



## wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 03:01 PM UTC

PDB ID : 7OG4 / pdb\_00007og4  
EMDB ID : EMD-12877  
Title : Human mitochondrial ribosome in complex with P/E-tRNA  
Authors : Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.  
Deposited on : 2021-05-06  
Resolution : 3.80 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](mailto: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>.

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

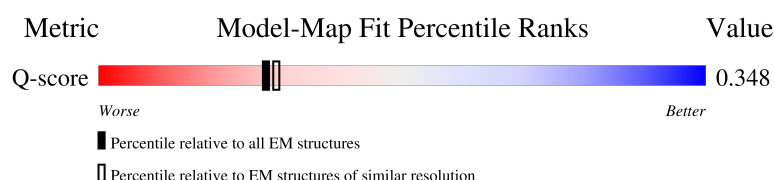
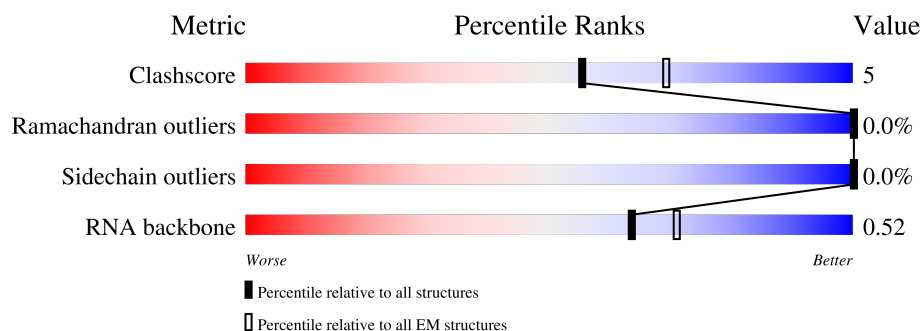
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 10198 ( 3.30 - 4.30 )                                    |

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 0     | 188    |                  |
| 2   | 1     | 65     |                  |
| 3   | 2     | 92     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | 3     | 188    |                  |
| 5   | 4     | 103    |                  |
| 6   | 5     | 423    |                  |
| 7   | 6     | 380    |                  |
| 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    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | AM    | 137    |                  |
| 30  | AN    | 130    |                  |
| 31  | AO    | 258    |                  |
| 32  | AP    | 142    |                  |
| 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    |                  |

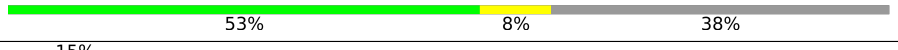
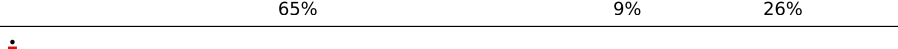
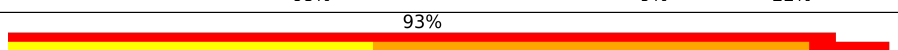
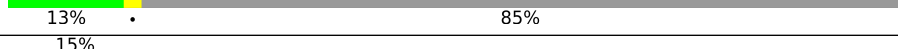
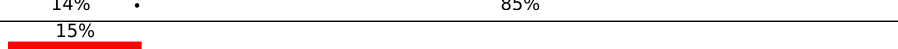
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | XO    | 175    |                  |
| 55  | XP    | 180    |                  |
| 56  | XQ    | 292    |                  |
| 57  | XR    | 149    |                  |
| 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    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 79  | o     | 102    |    |
| 80  | p     | 206    |    |
| 81  | q     | 222    |    |
| 82  | r     | 196    |    |
| 83  | r3    | 75     |    |
| 84  | s     | 439    |    |
| 85  | t1    | 198    |    |
| 85  | t2    | 198    |    |
| 85  | t3    | 198    |    |
| 85  | t4    | 198    |   |
| 85  | t5    | 198    |  |
| 85  | t6    | 198    |  |

## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 311905 atoms, of which 143004 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     |
|     |       |          | 702   | 217 | 361 | 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     | 134      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2301  | 724 | 1166 | 201 | 208 | 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    | 1498     | Total | C     | H     | N    | O     | P    | 0       | 0     |
|     |       |          | 47973 | 14274 | 16160 | 5751 | 10290 | 1498 |         |       |

- 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     |
|     |       |          | 3382  | 1069 | 1714 | 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     |
|     |       |          | 4997  | 1593 | 2492 | 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     |
|     |       |          | 2672  | 850 | 1342 | 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     |
|     |       |          | 5730  | 1841 | 2863 | 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     |
|     |       |          | 1867  | 621 | 911 | 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<sup>Val</sup>.

| 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     | 142      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2291  | 731 | 1152 | 185 | 219 | 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     |
|     |       |          | 2738  | 858 | 1359 | 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 P/E-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 83  | r3    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1468  | 714 | 228 | 451 | 75 |         |       |

- Molecule 84 is a protein called 39S ribosomal protein S30, mitochondrial.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 84  | s     | 370      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6059  | 1946 | 3023 | 542 | 534 | 14 |         |       |

- Molecule 85 is a protein called 39S ribosomal protein L12, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|-------|
| 85  | t1    | 46       | Total | C   | H   | N  | O  | 2       | 0     |
|     |       |          | 733   | 228 | 379 | 56 | 70 |         |       |
| 85  | t2    | 30       | Total | C   | H   | N  | O  | 0       | 0     |
|     |       |          | 506   | 154 | 268 | 38 | 46 |         |       |
| 85  | t3    | 30       | Total | C   | H   | N  | O  | 0       | 0     |
|     |       |          | 506   | 154 | 268 | 38 | 46 |         |       |
| 85  | t4    | 29       | Total | C   | H   | N  | O  | 0       | 0     |
|     |       |          | 484   | 148 | 255 | 36 | 45 |         |       |
| 85  | t5    | 29       | Total | C   | H   | N  | O  | 0       | 0     |
|     |       |          | 484   | 148 | 255 | 36 | 45 |         |       |
| 85  | t6    | 27       | Total | C   | H   | N  | O  | 0       | 0     |
|     |       |          | 450   | 137 | 236 | 34 | 43 |         |       |

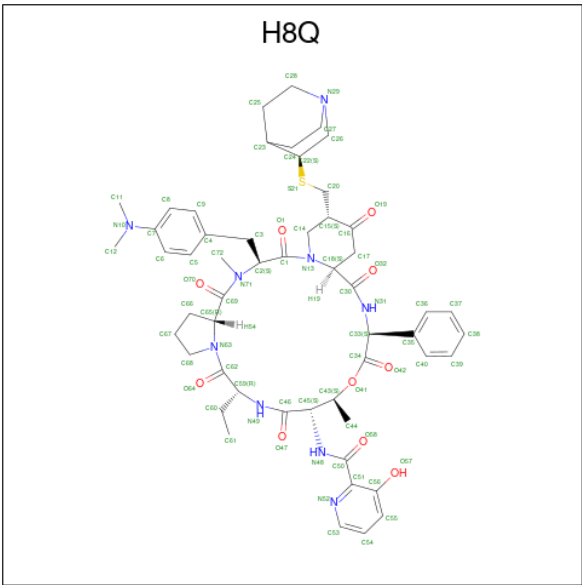
- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 86  | 0     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | AB    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | AO    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | AP    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | AT    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | r     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

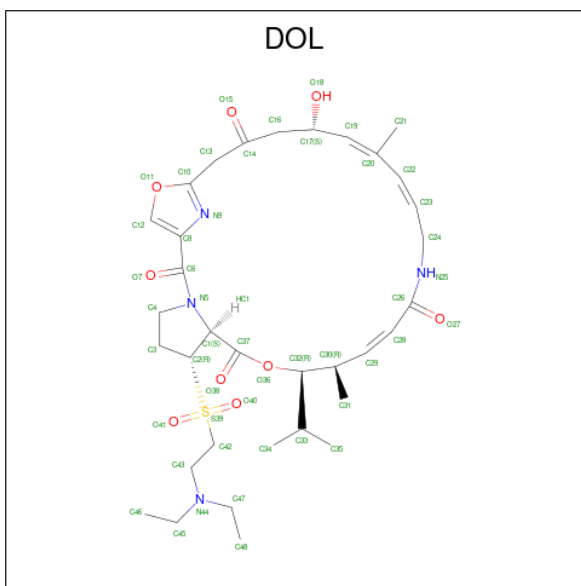
- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 87  | 9     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | XA    | 143      | Total | Mg  | 0       |
|     |       |          | 143   | 143 |         |
| 87  | AA    | 46       | Total | Mg  | 0       |
|     |       |          | 46    | 46  |         |
| 87  | XD    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | XI    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | XM    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | XW    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | g     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 88 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 (CCD ID: H8Q) (formula: C<sub>53</sub>H<sub>67</sub>N<sub>9</sub>O<sub>10</sub>S).

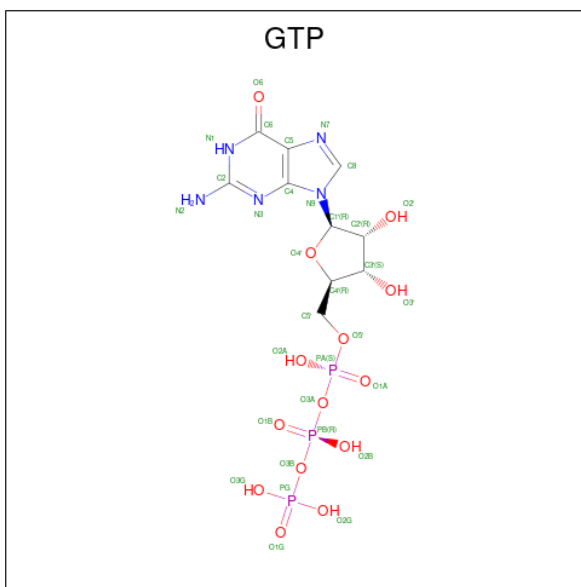


- Molecule 89 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (CCD ID: DOL) (formula:  $C_{34}H_{50}N_4O_9S$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |   |
|-----|-------|----------|-------|----|----|---|---|---------|---|
| 89  | XA    | 1        | Total | C  | H  | N | O | S       | 0 |
|     |       |          | 98    | 34 | 50 | 4 | 9 | 1       |   |

- Molecule 90 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

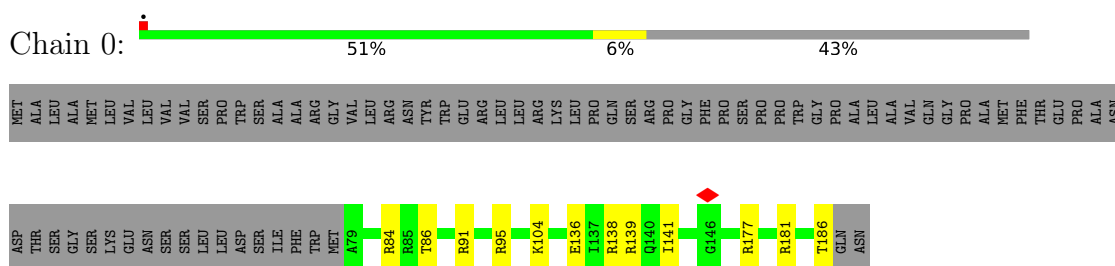


| Mol | Chain | Residues | Atoms |    |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
|     |       |          | Total | C  | H  | N | O  | P |         |
| 90  | AX    | 1        | 42    | 10 | 10 | 5 | 14 | 3 | 0       |

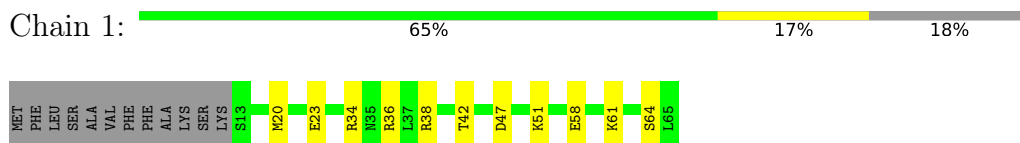
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

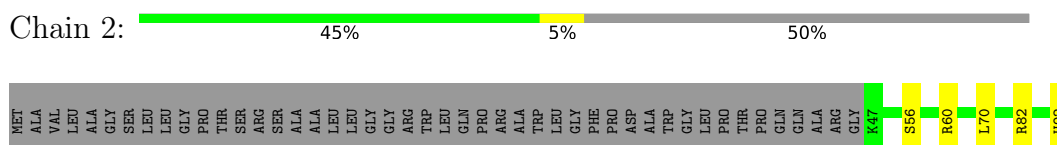
- Molecule 1: 39S ribosomal protein L32, mitochondrial



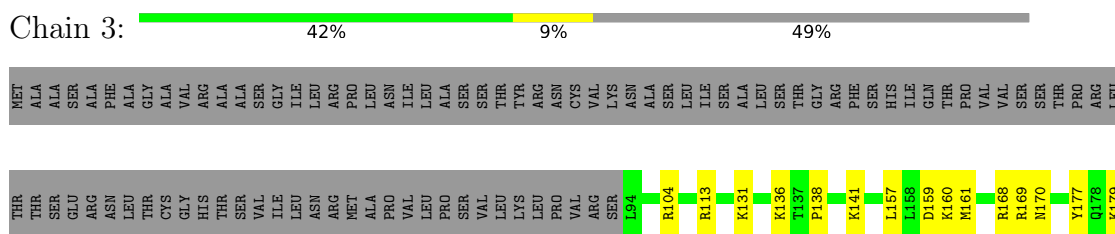
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial



- Molecule 4: 39S ribosomal protein L35, mitochondrial



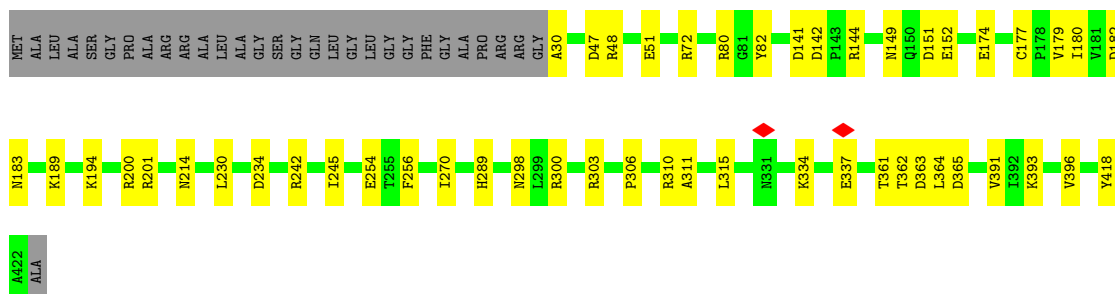
- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4:  29% 8% 63%



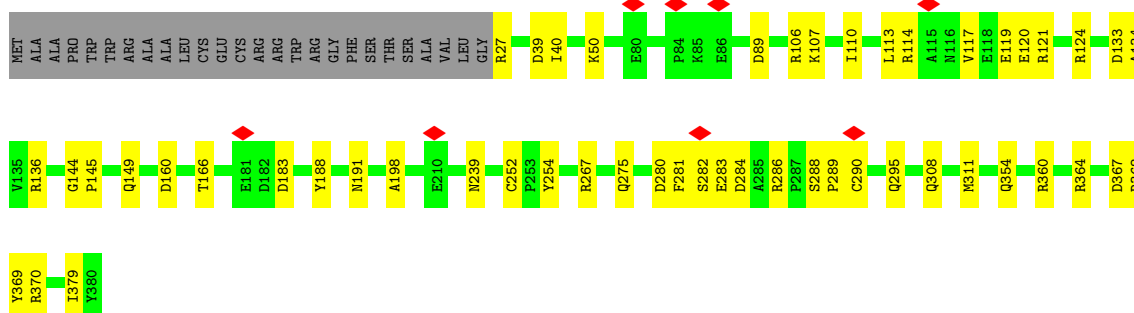
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:  81% 12% 7%



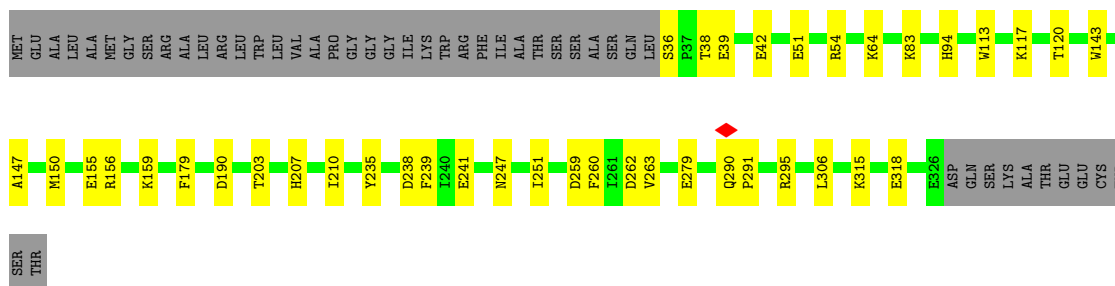
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:  79% 14% 7%



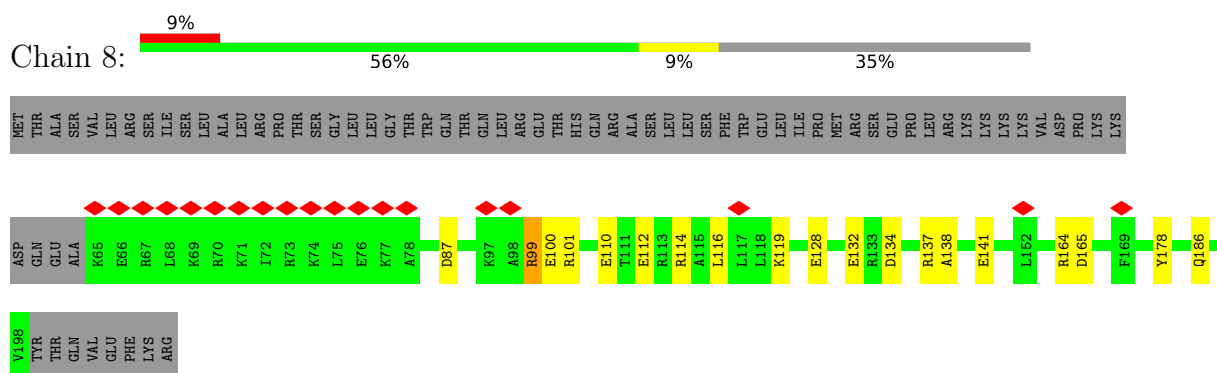
- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:  74% 12% 14%

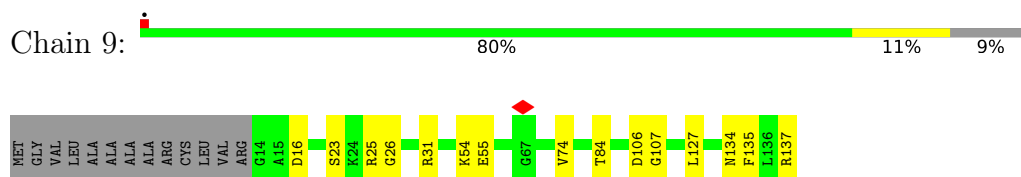


- Molecule 9: 39S ribosomal protein L40, mitochondrial

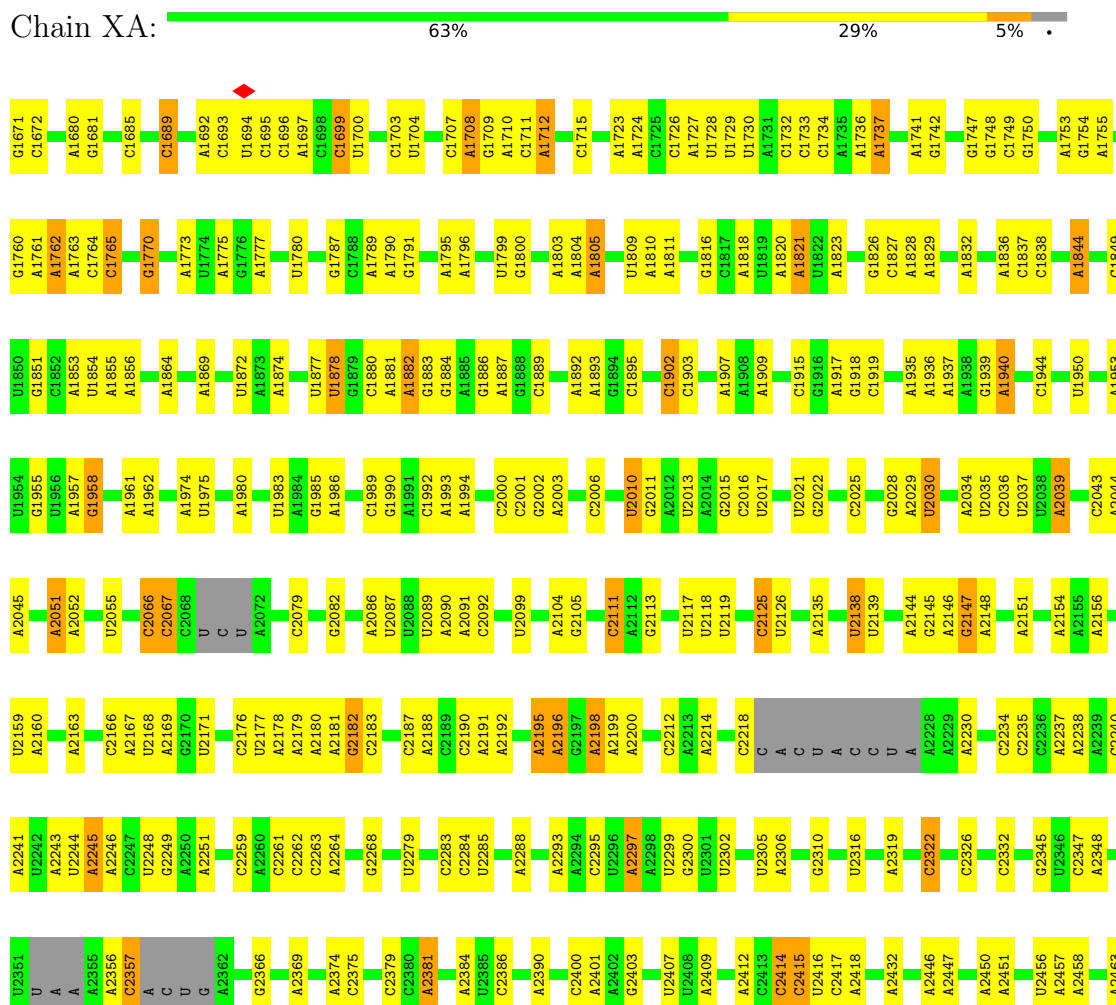


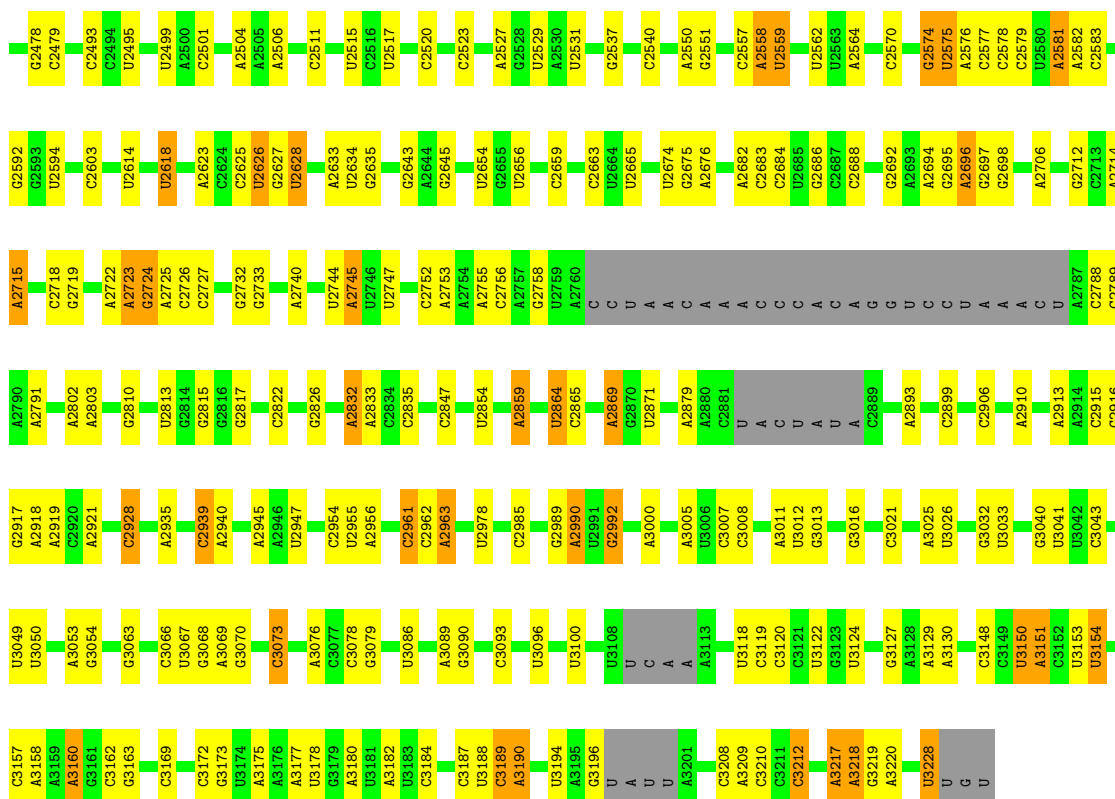


- Molecule 10: 39S ribosomal protein L41, mitochondrial

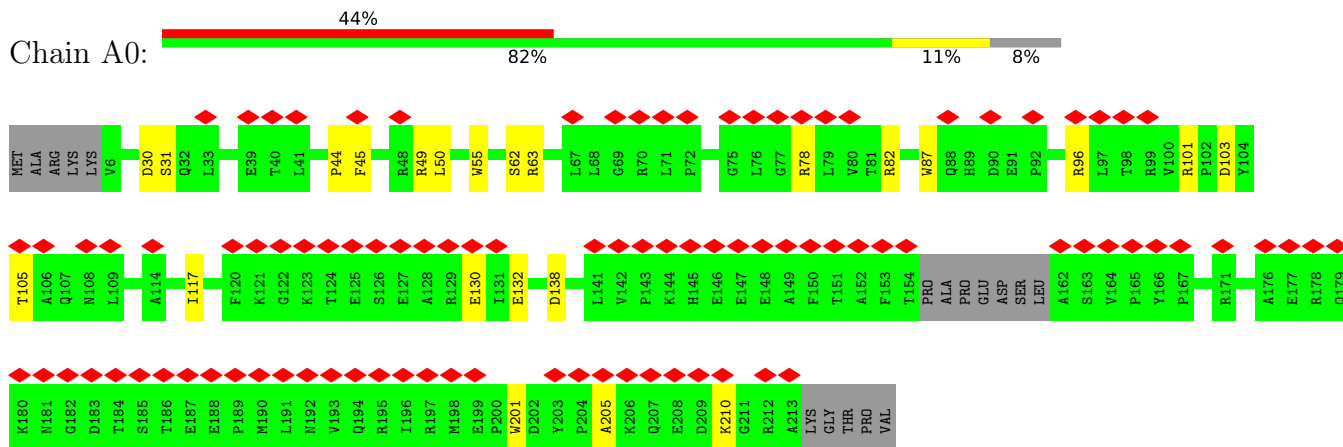


- Molecule 11: 16S mitochondrial rRNA

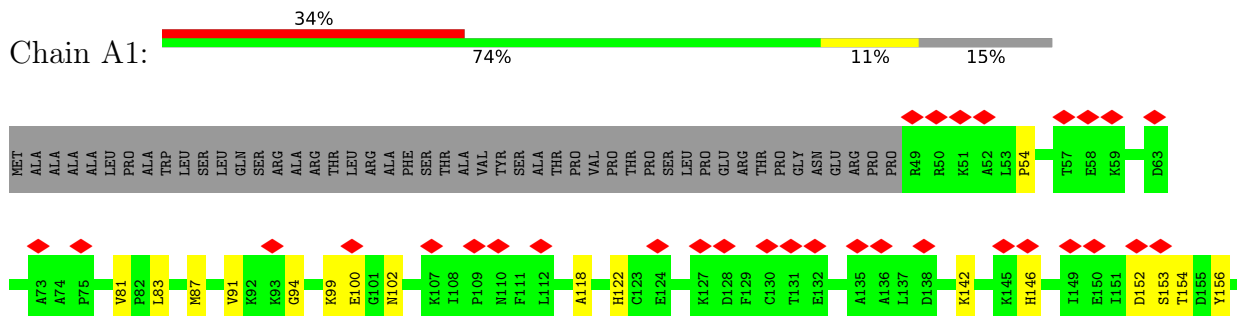


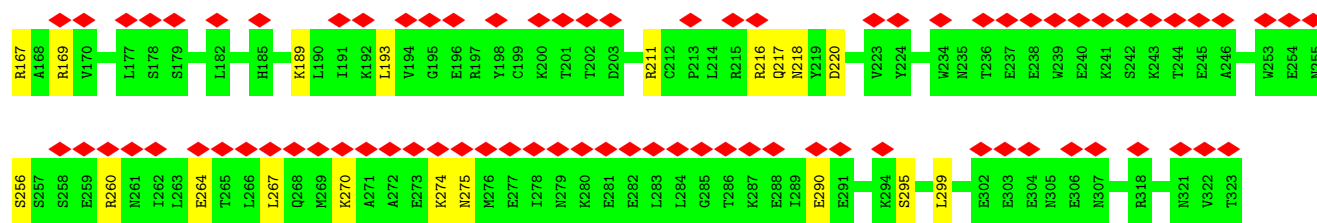


- Molecule 12: 28S ribosomal protein S34, mitochondrial

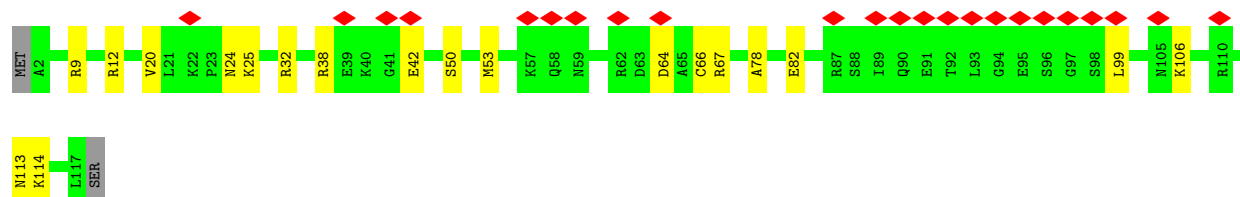
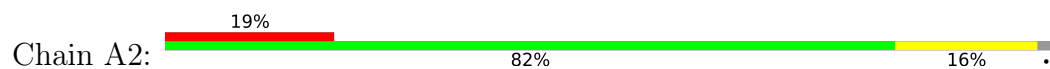


- Molecule 13: 28S ribosomal protein S35, mitochondrial

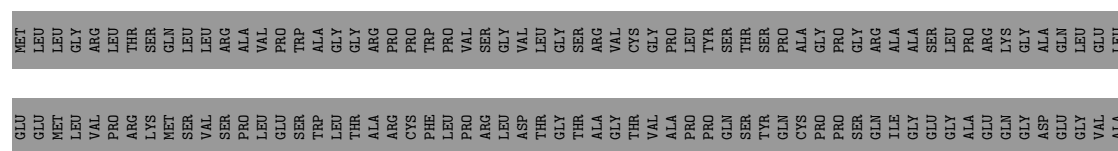




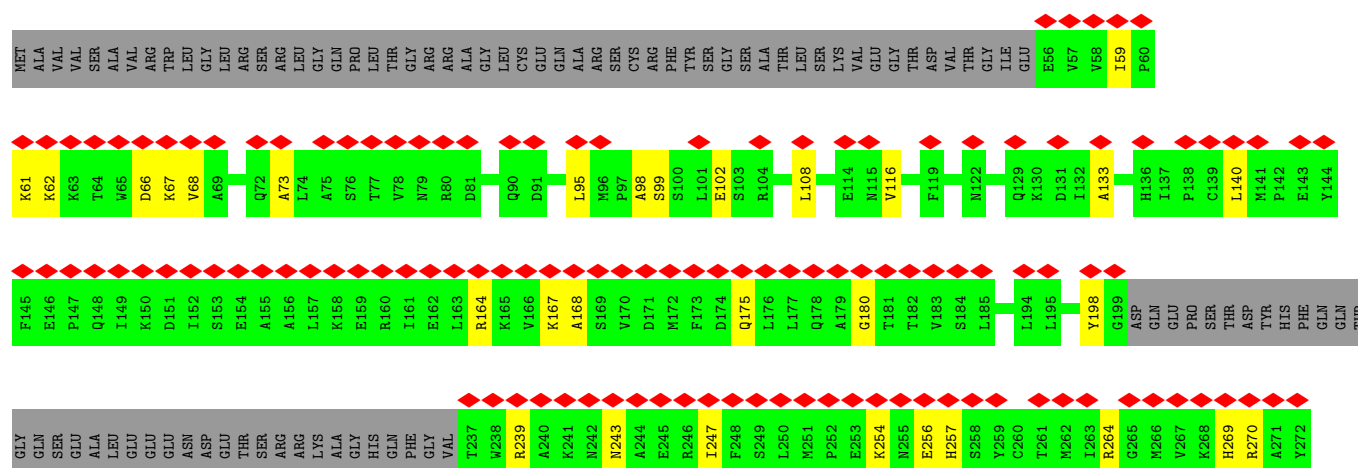
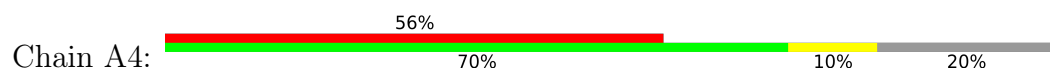
• Molecule 14: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

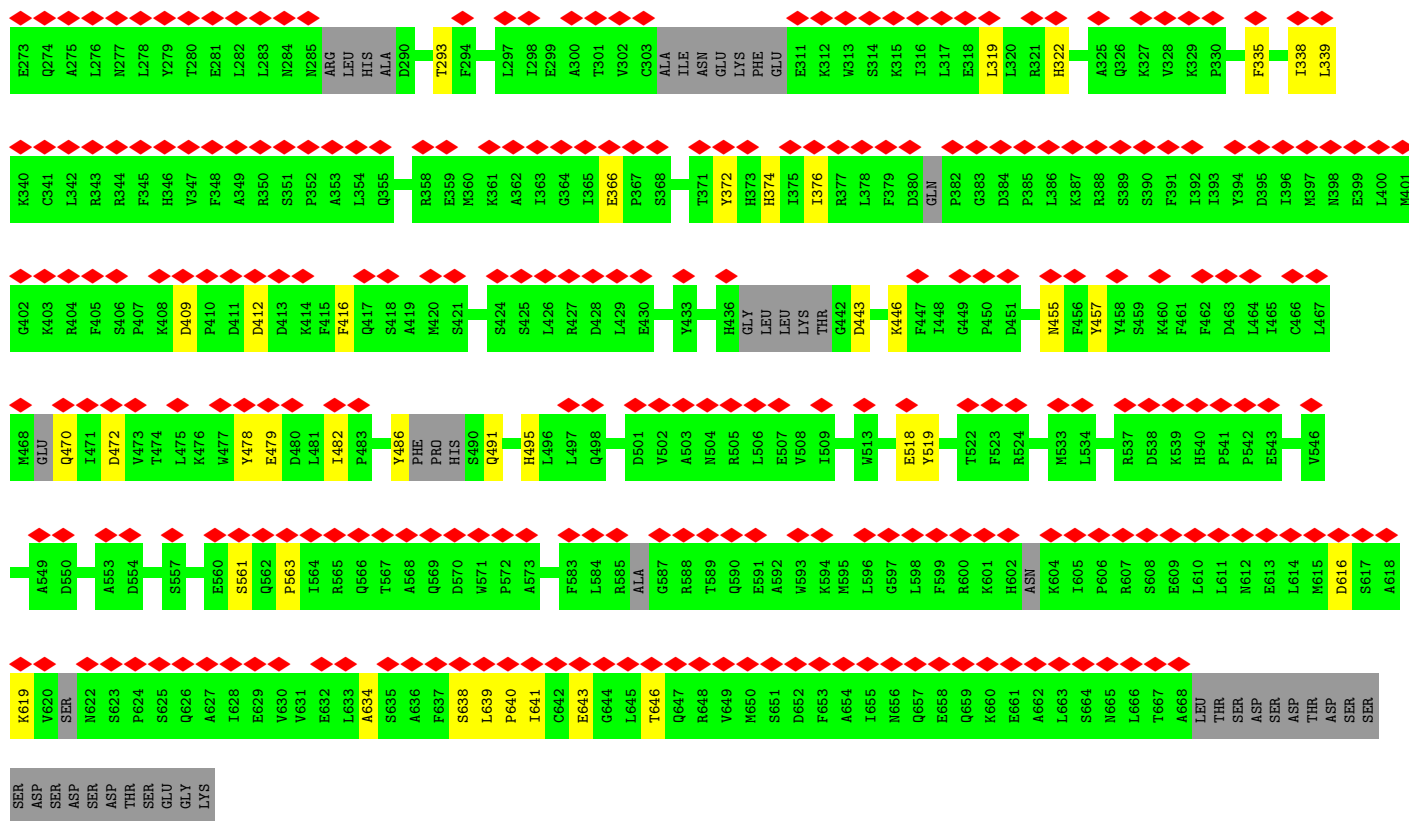


• Molecule 15: Aurora kinase A-interacting protein



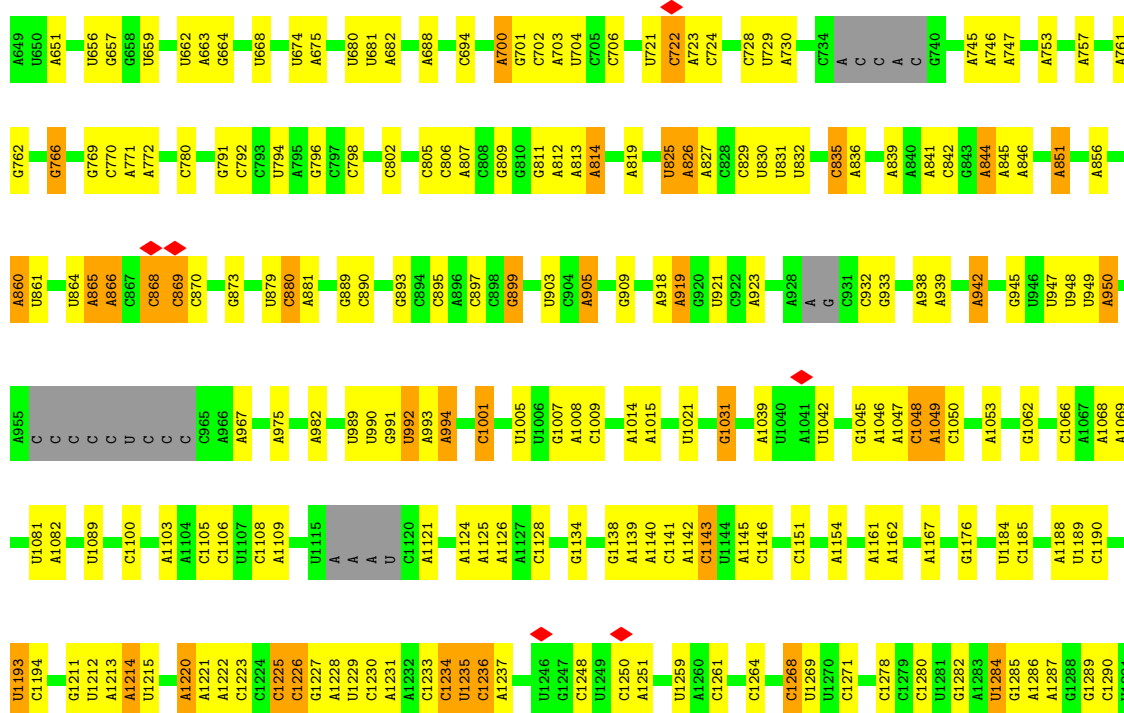
• Molecule 16: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

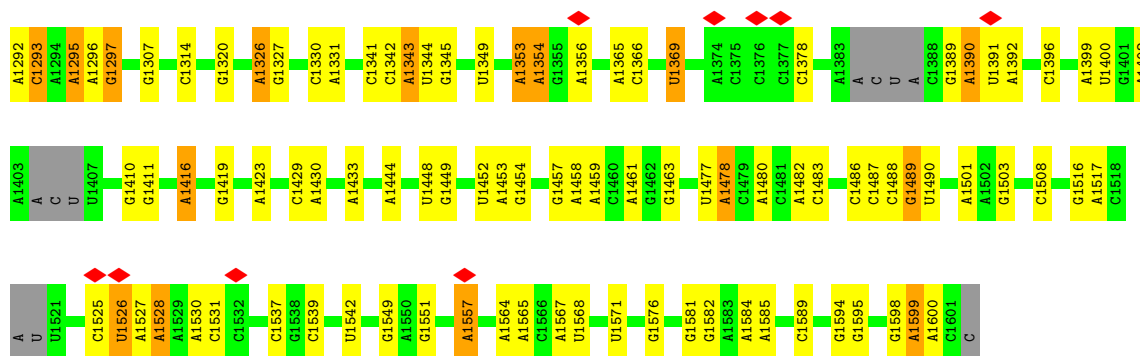




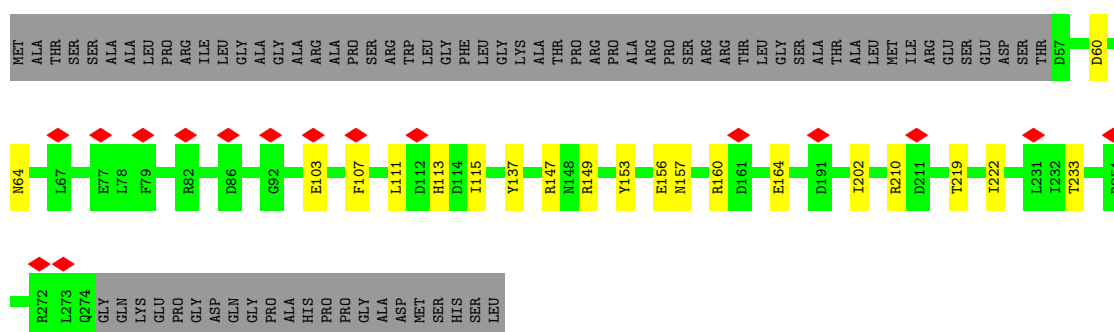
• Molecule 17: 12S mitochondrial rRNA

Chain AA: 64% 27% 6% •

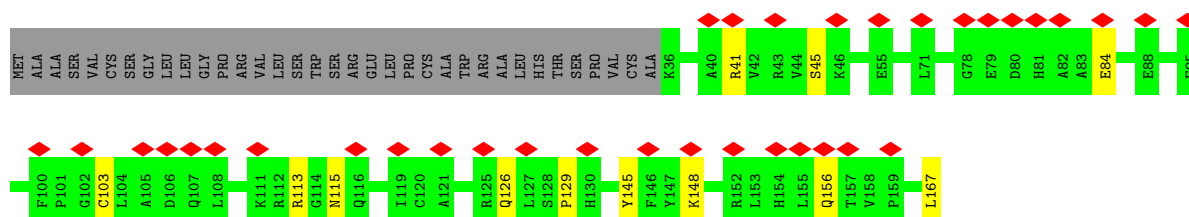
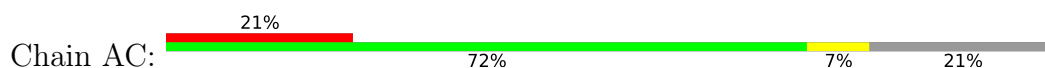




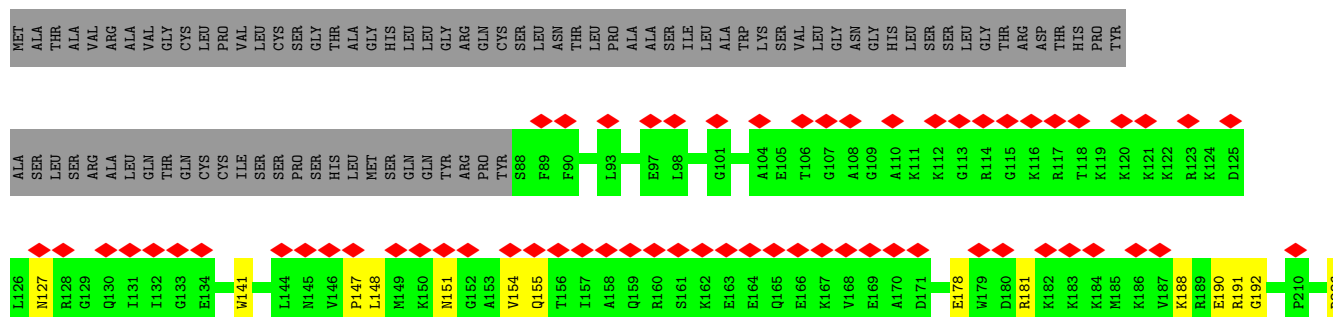
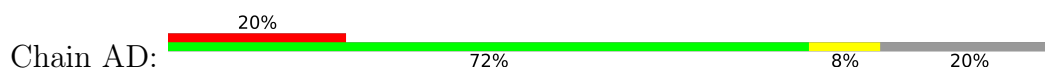
- Molecule 18: 28S ribosomal protein S2, mitochondrial

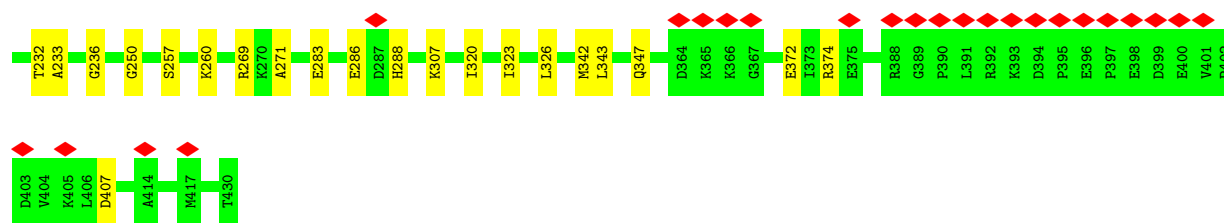


- Molecule 19: 28S ribosomal protein S24, mitochondrial



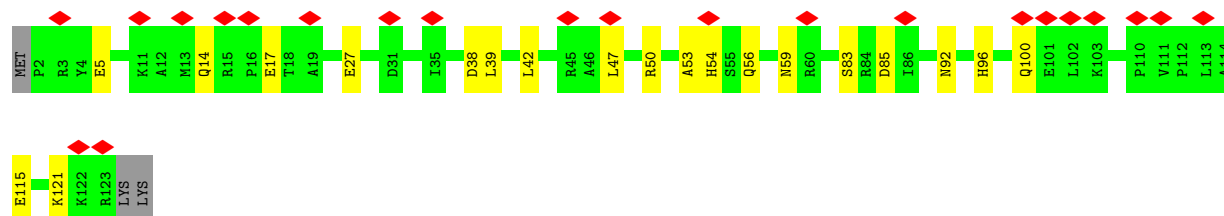
- Molecule 20: 28S ribosomal protein S5, mitochondrial





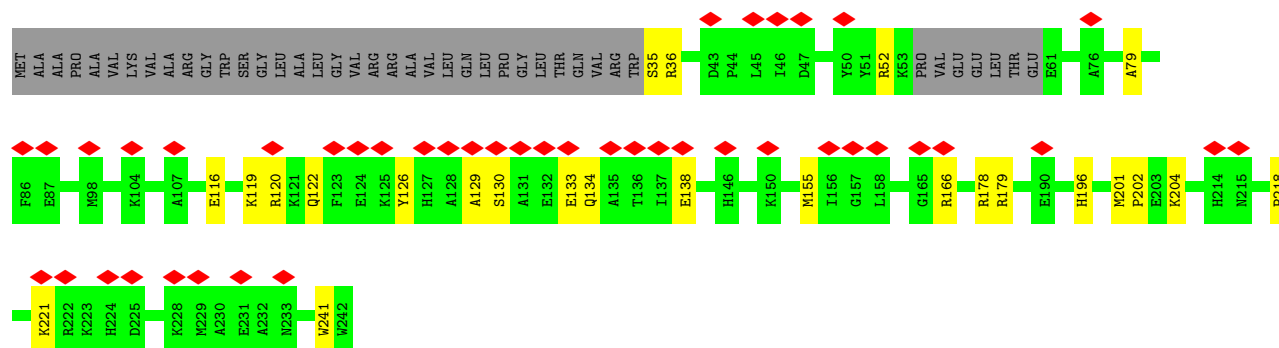
- Molecule 21: 28S ribosomal protein S6, mitochondrial

Chain AE:



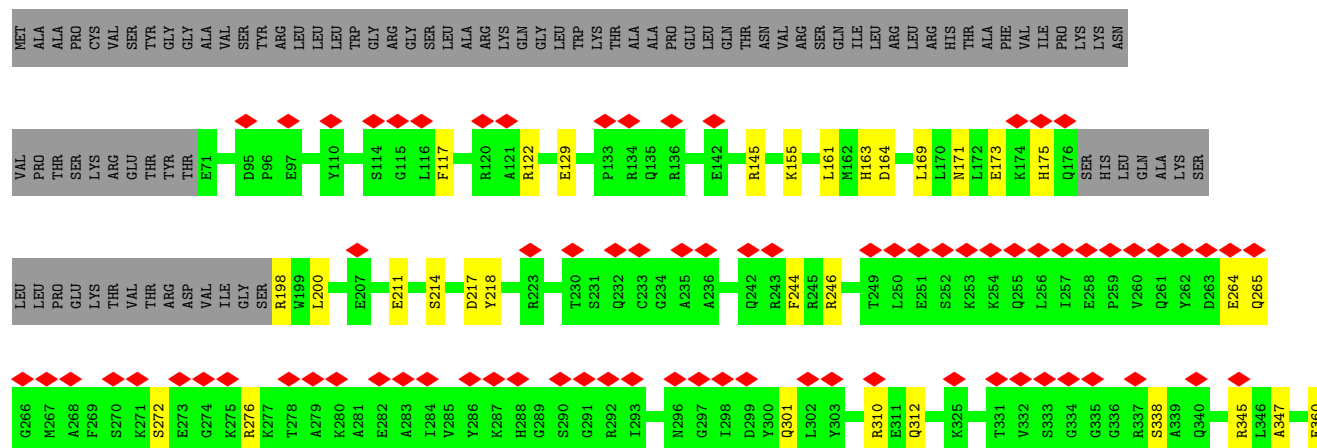
- Molecule 22: 28S ribosomal protein S7, mitochondrial

Chain AF:



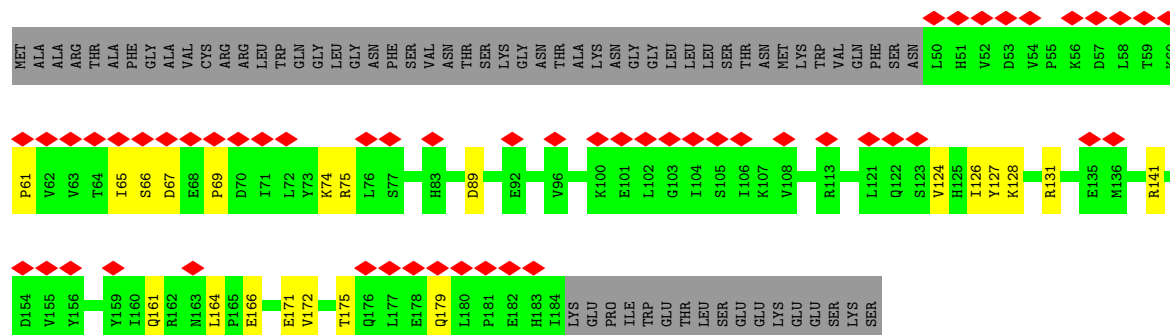
- Molecule 23: 28S ribosomal protein S9, mitochondrial

Chain AG:

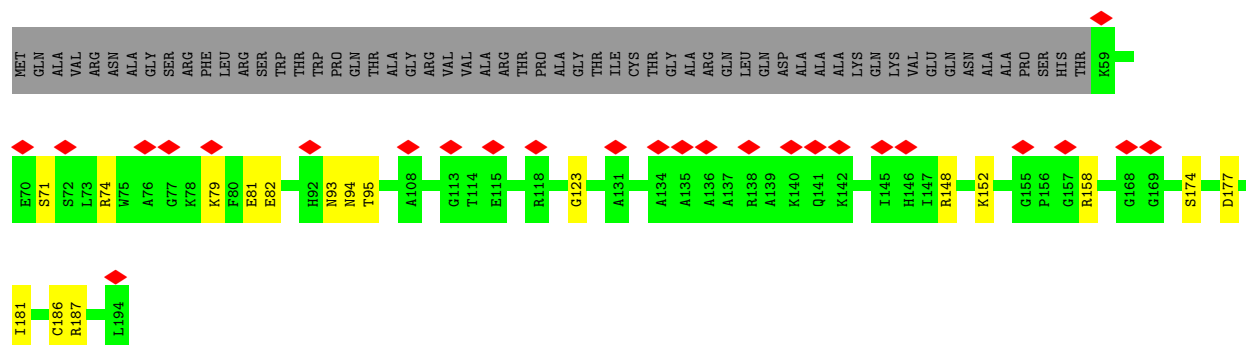




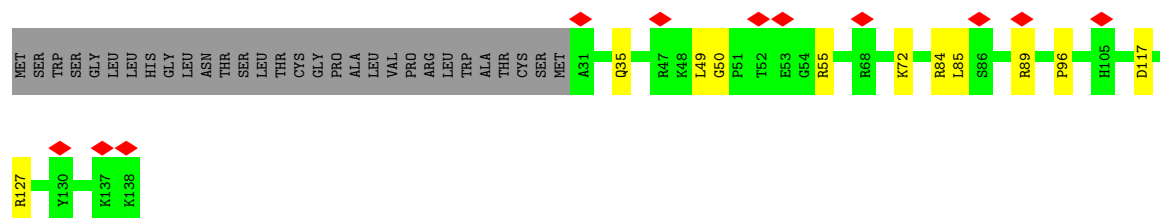
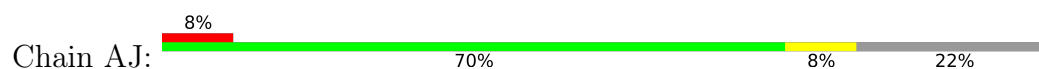
- Molecule 24: 28S ribosomal protein S10, mitochondrial



- Molecule 25: 28S ribosomal protein S11, mitochondrial

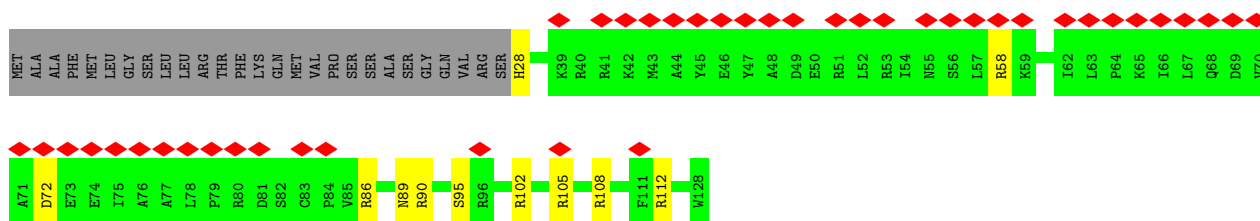


- Molecule 26: 28S ribosomal protein S12, mitochondrial

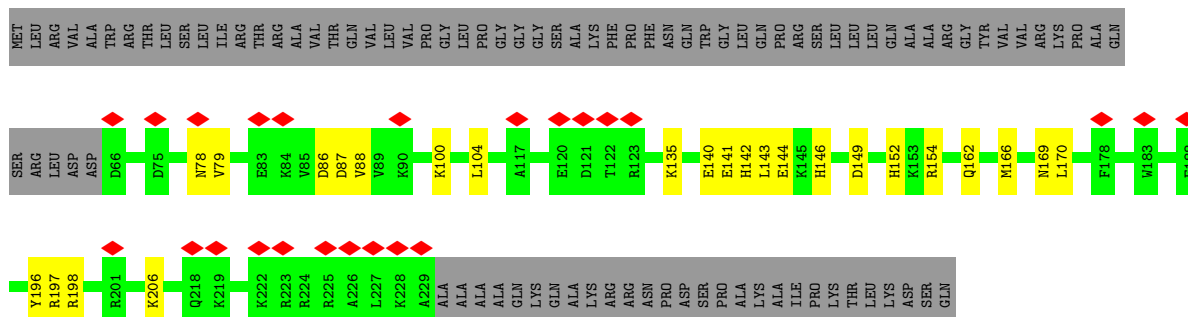


- Molecule 27: 28S ribosomal protein S14, mitochondrial

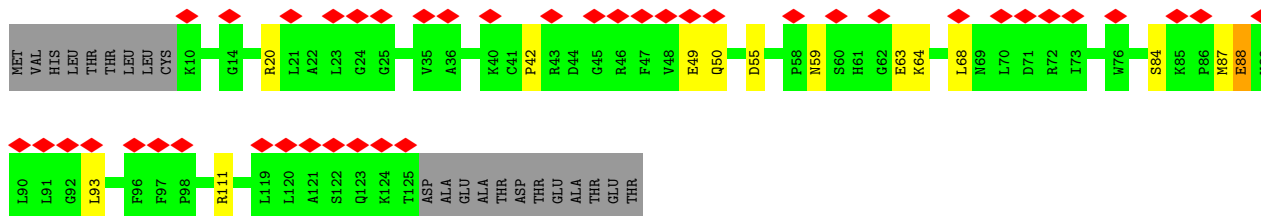
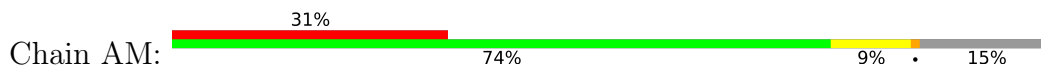




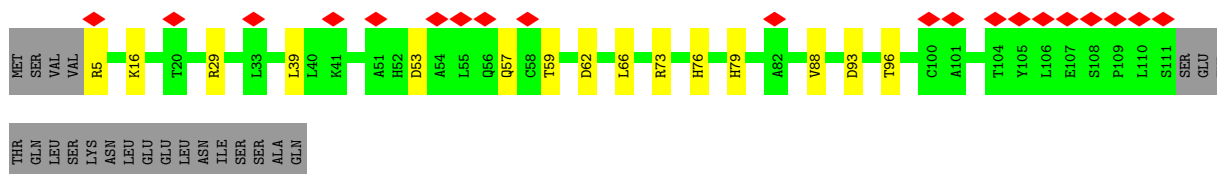
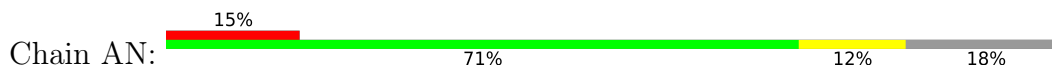
- Molecule 28: 28S ribosomal protein S15, mitochondrial



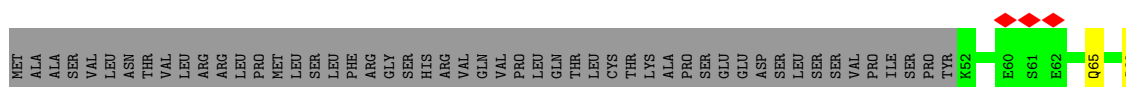
- Molecule 29: 28S ribosomal protein S16, mitochondrial



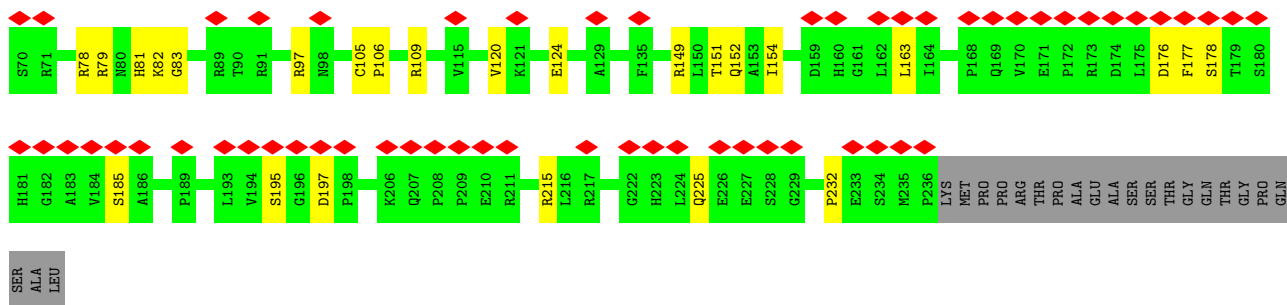
- Molecule 30: 28S ribosomal protein S17, mitochondrial



- Molecule 31: 28S ribosomal protein S18b, mitochondrial

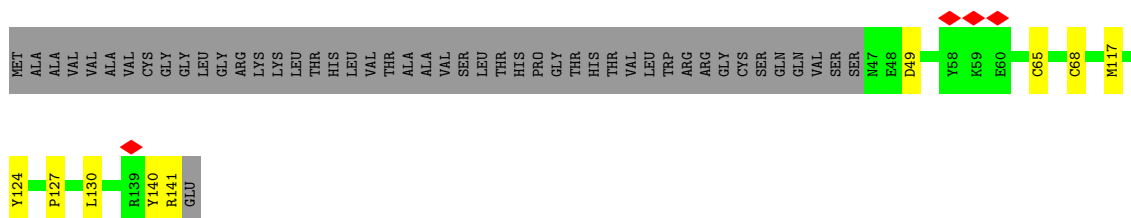






- Molecule 32: 28S ribosomal protein S18c, mitochondrial

Chain AP: 61% 6% 33%



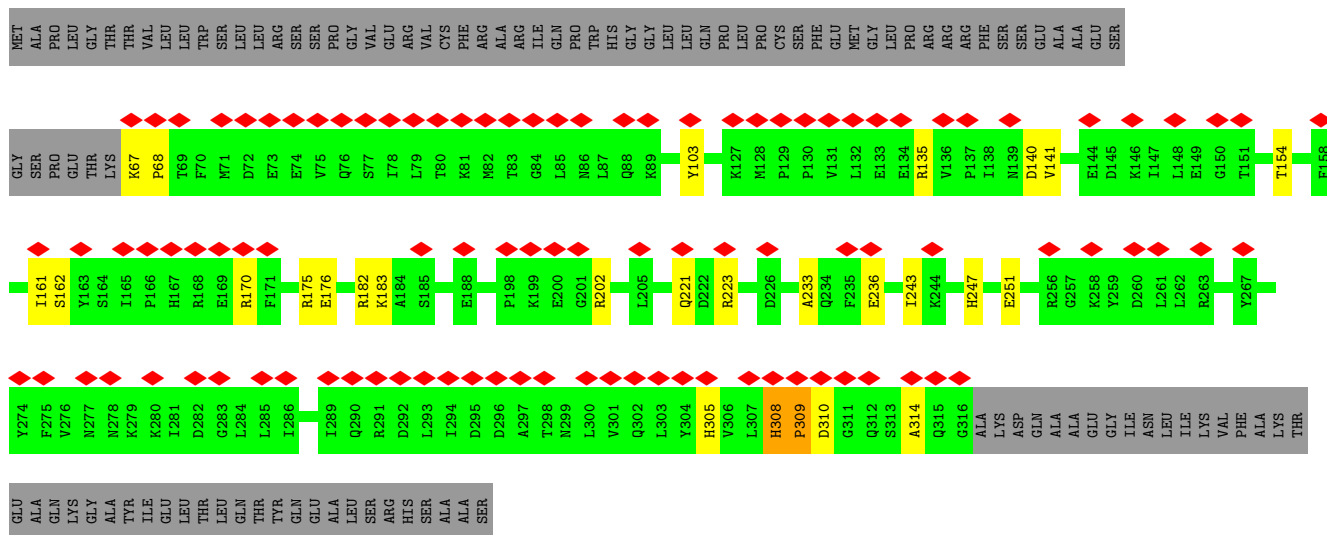
- Molecule 33: 28S ribosomal protein S21, mitochondrial

Chain AQ: 13% 86% 11%

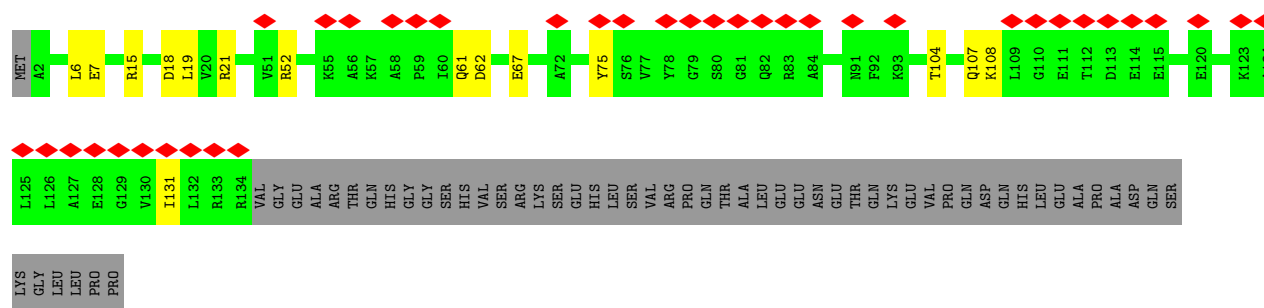


- Molecule 34: 28S ribosomal protein S22, mitochondrial

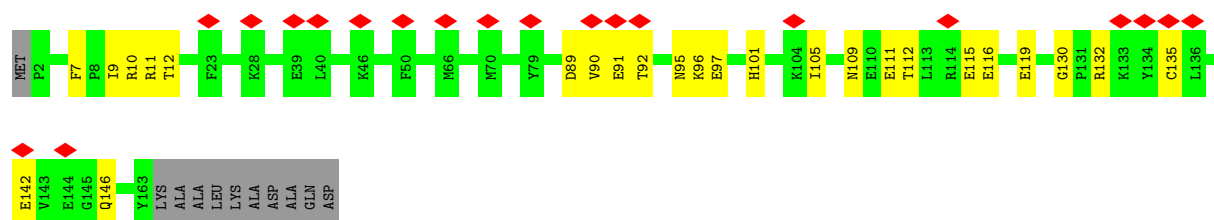
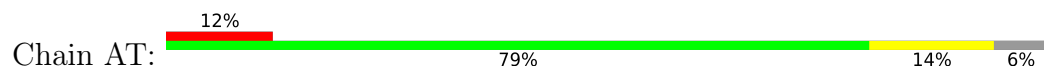
Chain AR: 28% 62% 7% 31%



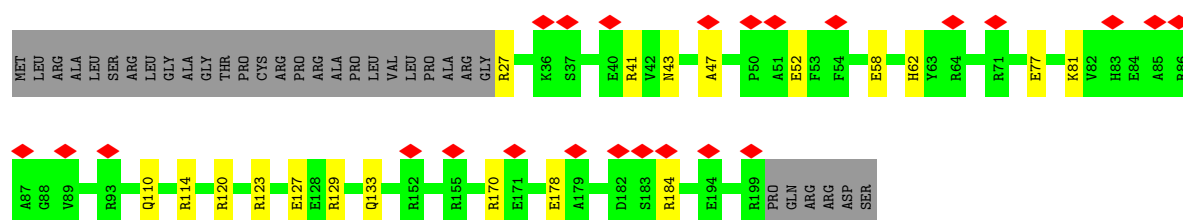
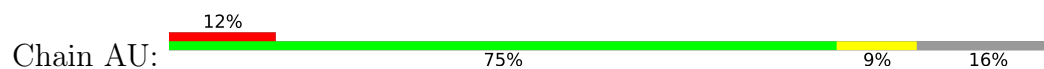
- Molecule 35: 28S ribosomal protein S23, mitochondrial



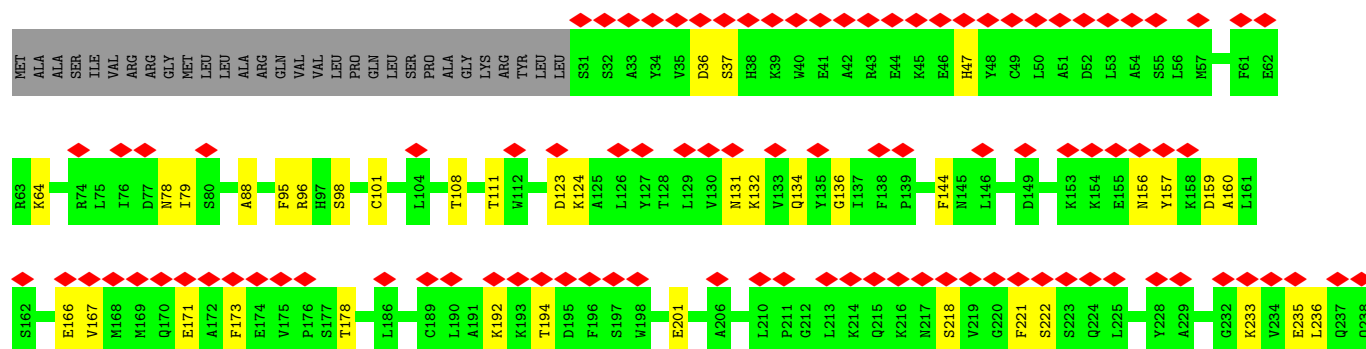
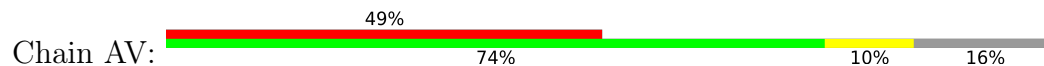
- Molecule 36: 28S ribosomal protein S25, mitochondrial

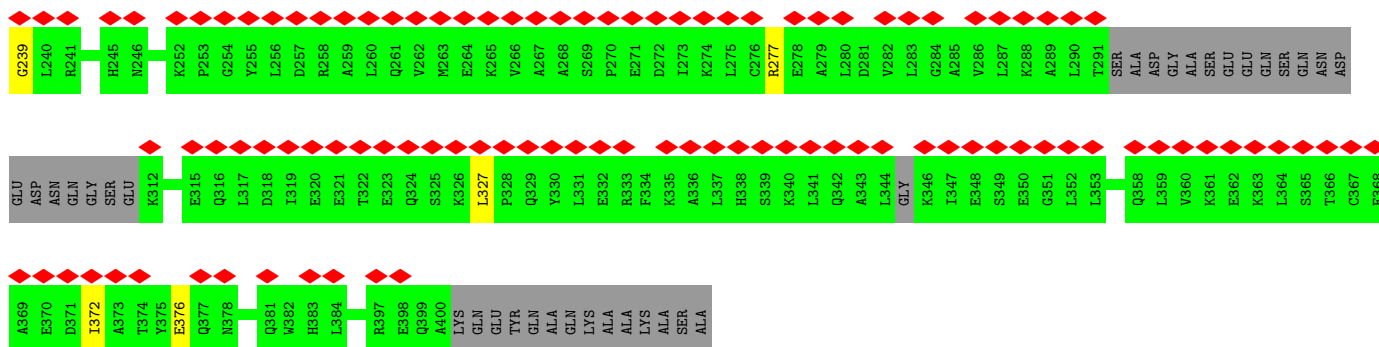


- Molecule 37: 28S ribosomal protein S26, mitochondrial

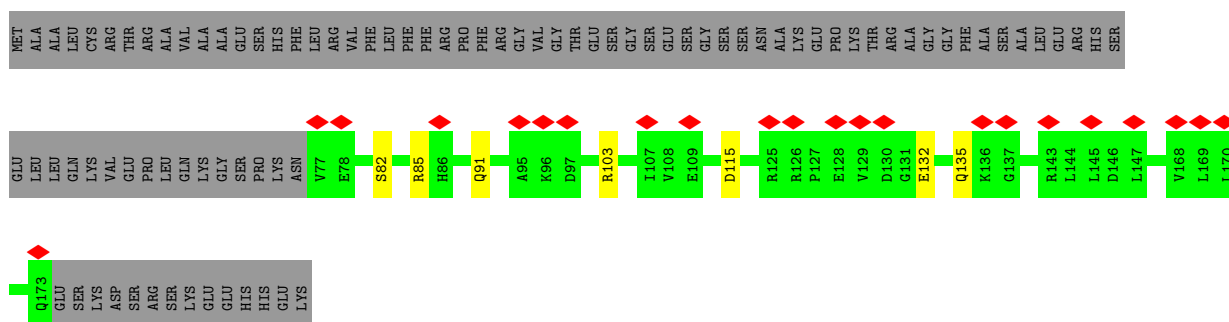


- Molecule 38: 28S ribosomal protein S27, mitochondrial

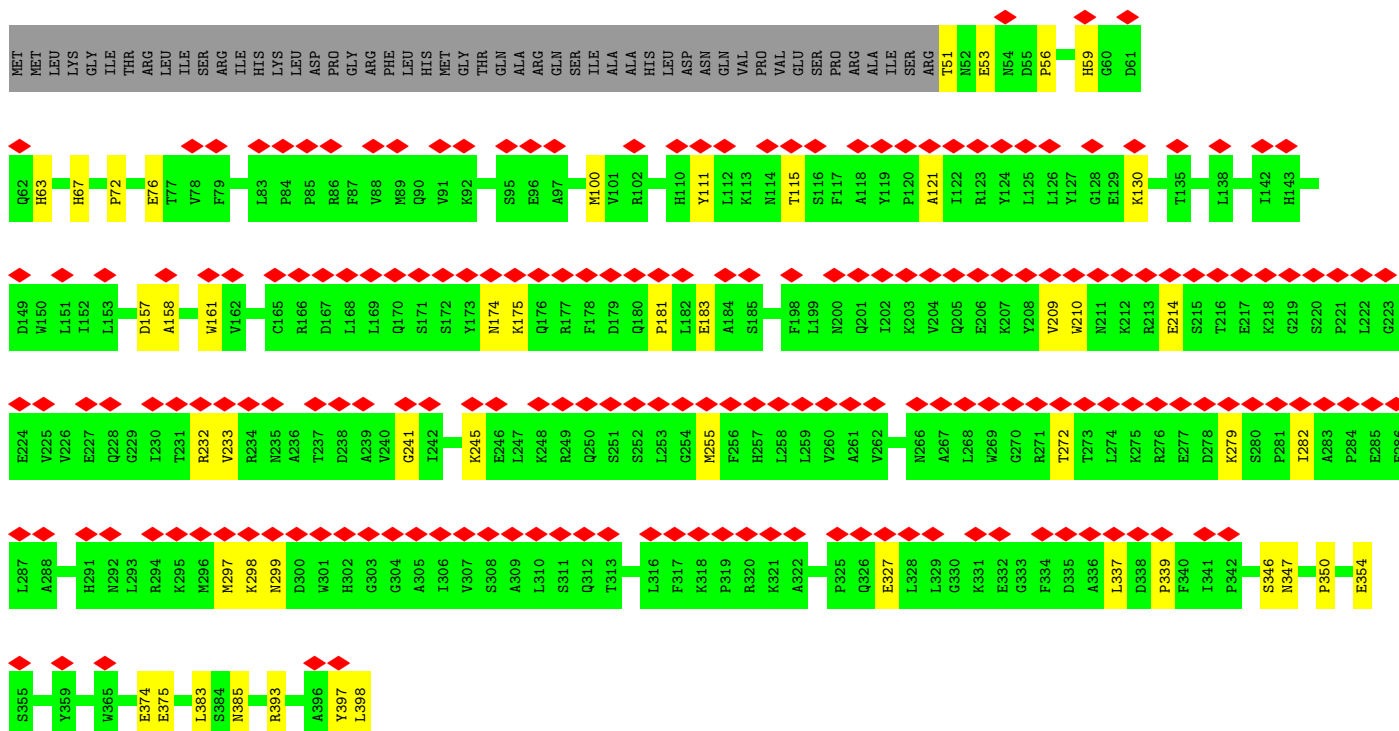
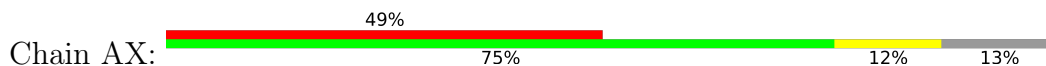


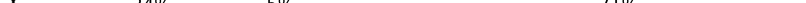


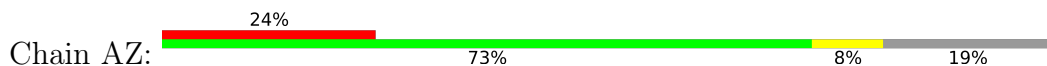
- Molecule 39: 28S ribosomal protein S28, mitochondrial



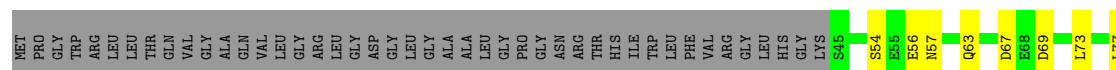
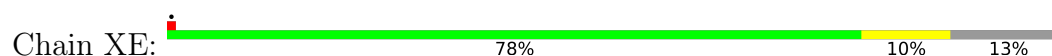
- Molecule 40: 28S ribosomal protein S29, mitochondrial



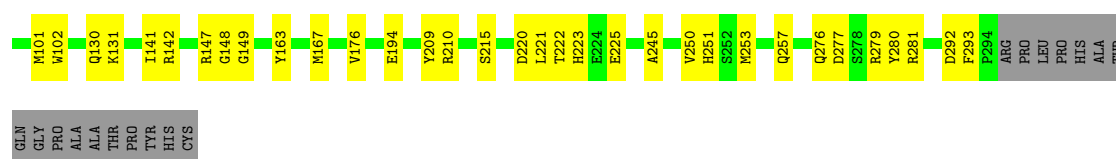
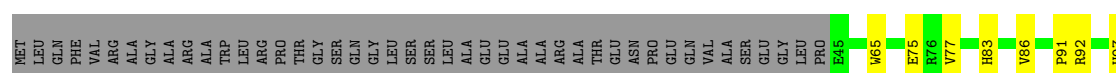
- Chain AY: 



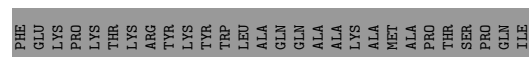
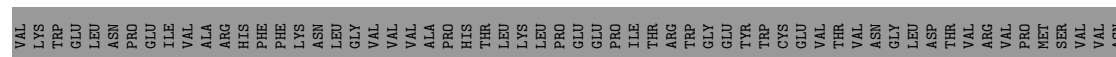
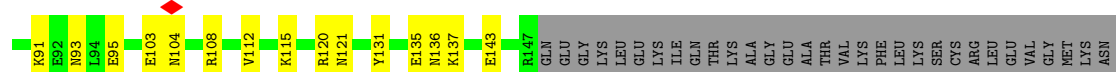
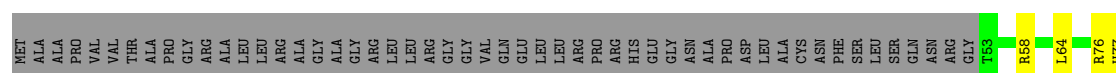
- Molecule 45: 39S ribosomal protein L3, mitochondrial



- Molecule 46: 39S ribosomal protein L4, mitochondrial

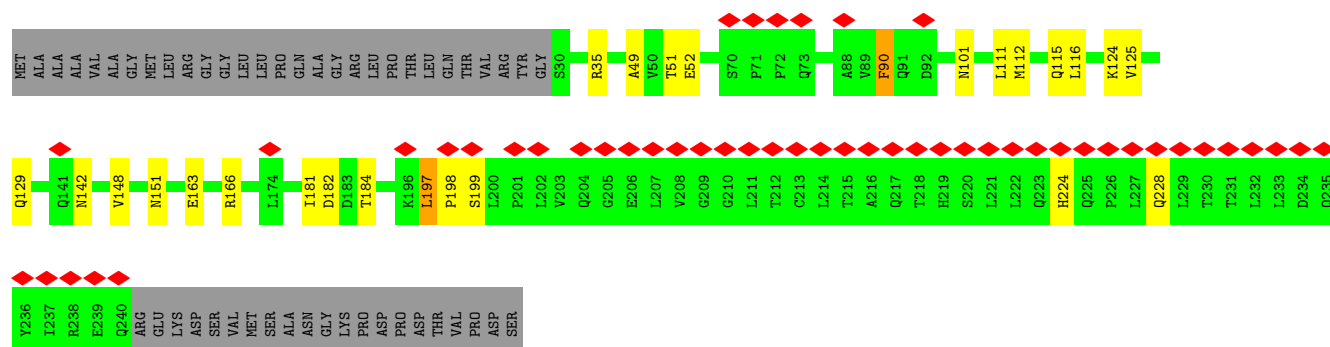


- Molecule 47: 39S ribosomal protein L9, mitochondrial

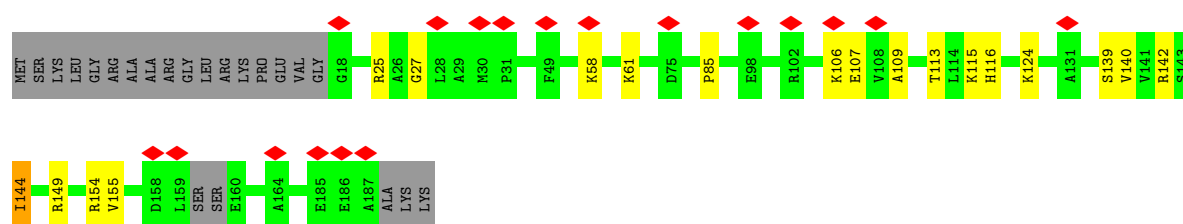
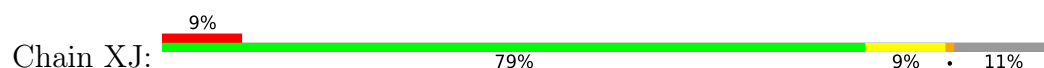


- Molecule 48: 39S ribosomal protein L10, mitochondrial

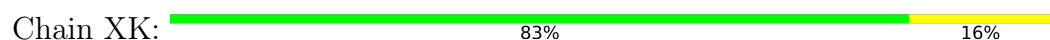




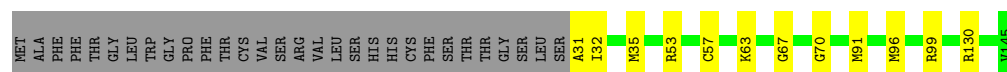
- Molecule 49: 39S ribosomal protein L11, mitochondrial



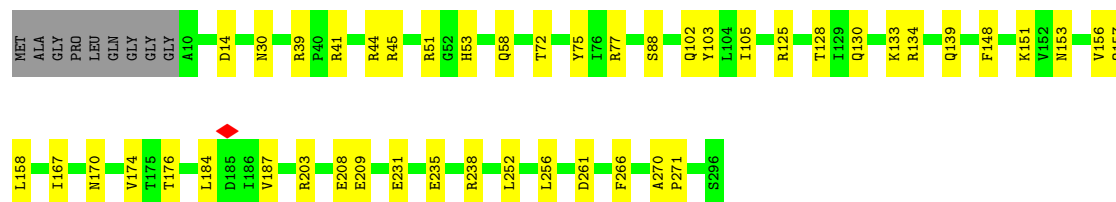
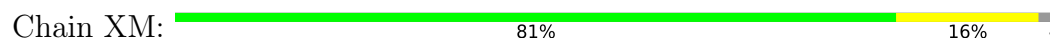
- Molecule 50: 39S ribosomal protein L13, mitochondrial



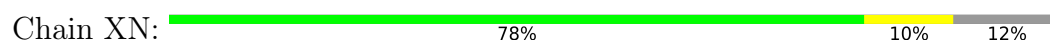
- Molecule 51: 39S ribosomal protein L14, mitochondrial

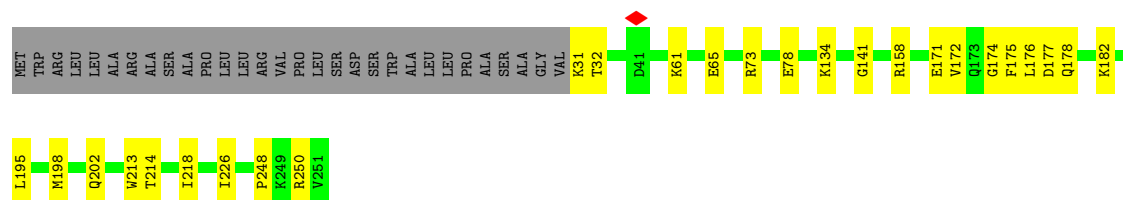


- Molecule 52: 39S ribosomal protein L15, mitochondrial



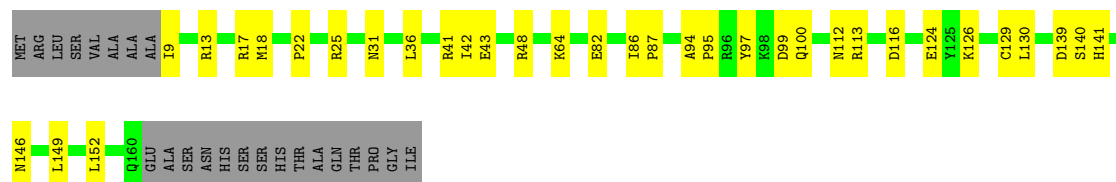
- Molecule 53: 39S ribosomal protein L16, mitochondrial





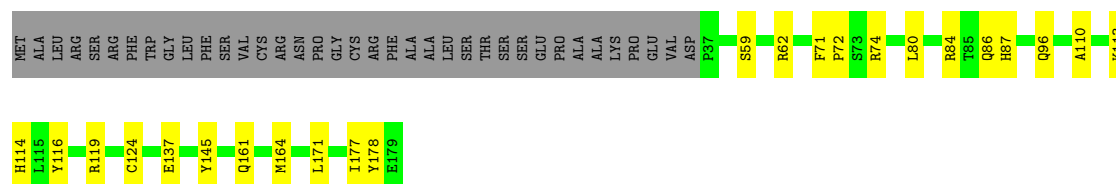
- Molecule 54: 39S ribosomal protein L17, mitochondrial

Chain XO: 67% 19% 13%



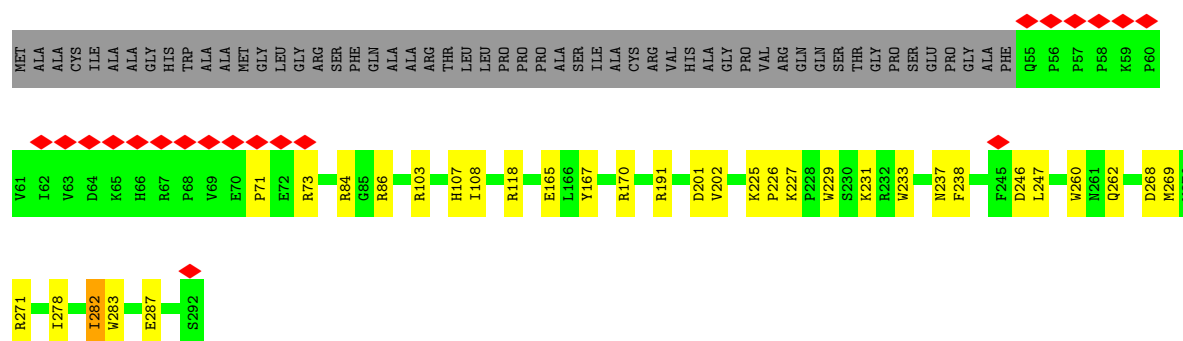
- Molecule 55: 39S ribosomal protein L18, mitochondrial

Chain XP: 67% 13% 21%



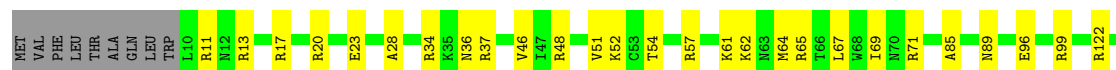
- Molecule 56: 39S ribosomal protein L19, mitochondrial

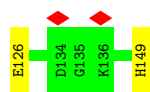
Chain XQ: 7% 70% 11% 18%



- Molecule 57: 39S ribosomal protein L20, mitochondrial

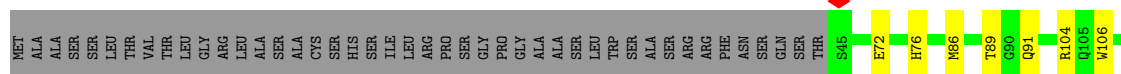
Chain XR: 74% 19% 6%





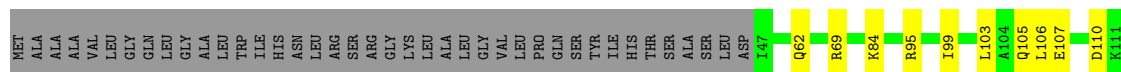
- Molecule 58: 39S ribosomal protein L21, mitochondrial

Chain XS: 67% 11% 22%



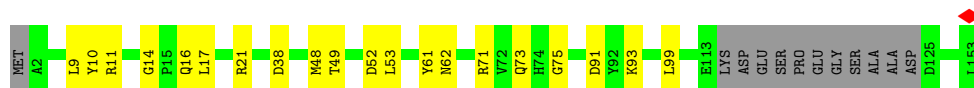
- Molecule 59: 39S ribosomal protein L22, mitochondrial

Chain XT: 66% 15% 19%



- Molecule 60: 39S ribosomal protein L23, mitochondrial

Chain XU: 79% 13% 8%



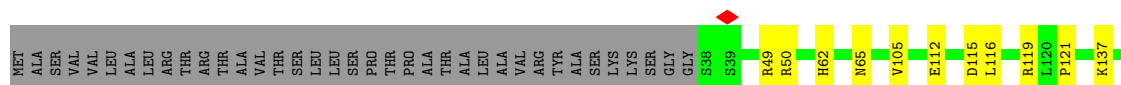
- Molecule 61: 39S ribosomal protein L24, mitochondrial

Chain XV: 83% 10% 6%



- Molecule 62: 39S ribosomal protein L27, mitochondrial

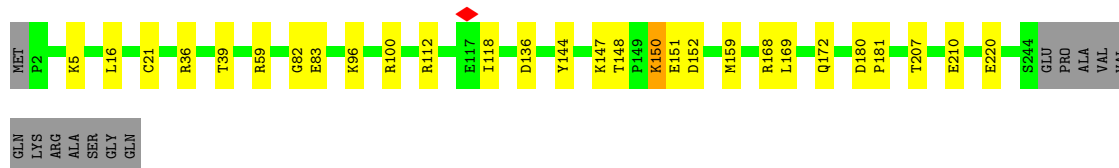
Chain XW: 68% 7% 25%



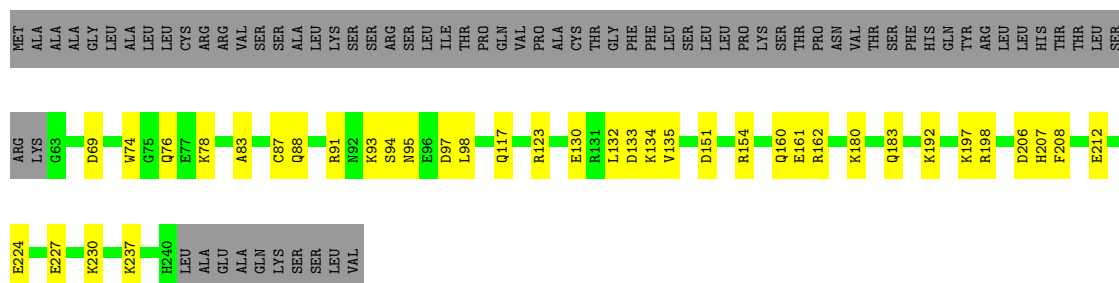


L148

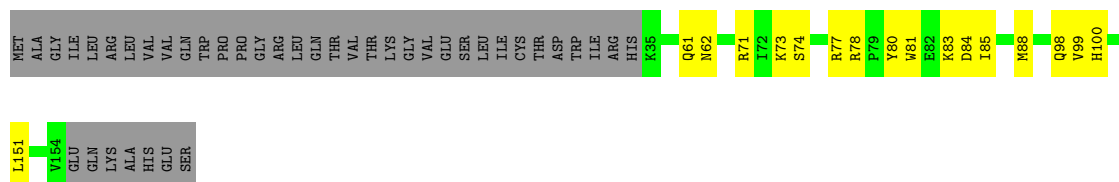
- Molecule 63: 39S ribosomal protein L28, mitochondrial

Chain XX:  84% 11% 5%

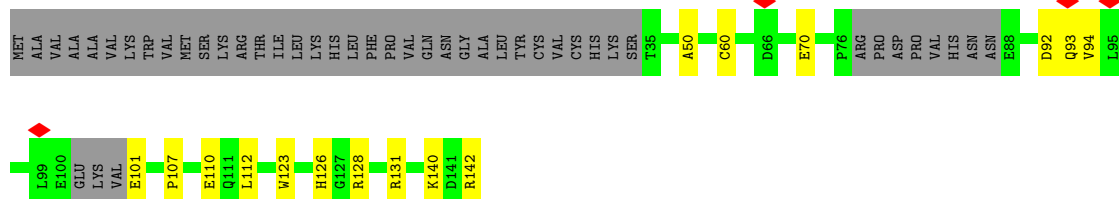
- Molecule 64: 39S ribosomal protein L47, mitochondrial

Chain XY:  56% 15% 29%

- Molecule 65: 39S ribosomal protein L30, mitochondrial

Chain XZ:  64% 11% 25%

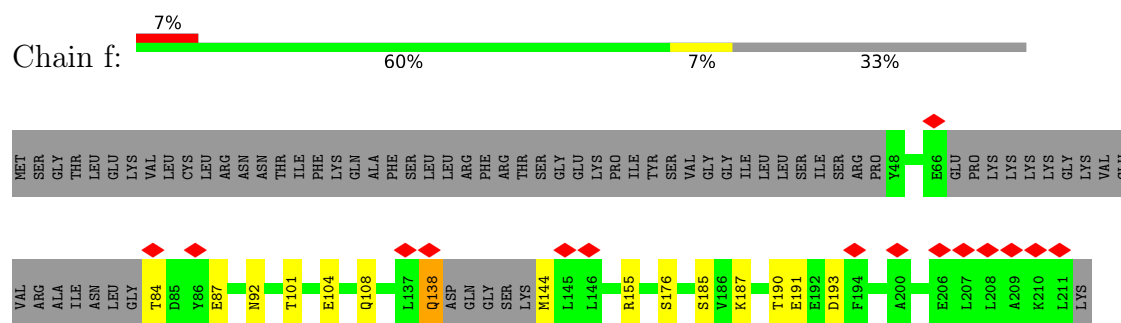
- Molecule 66: 39S ribosomal protein L42, mitochondrial

Chain a:  56% 12% 32%

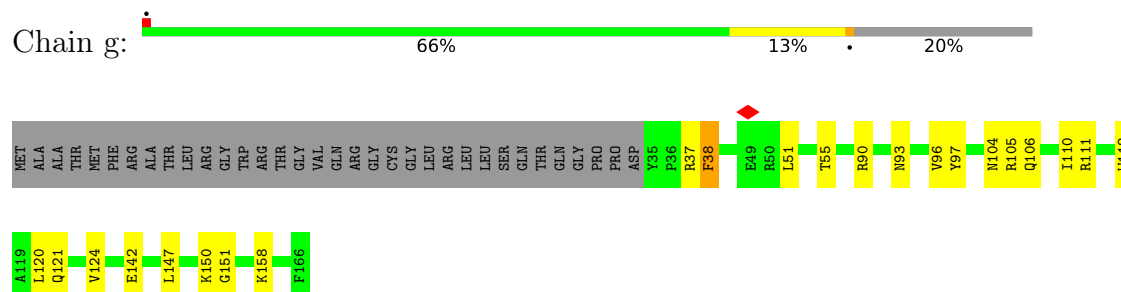
- Molecule 67: 39S ribosomal protein L43, mitochondrial

Chain b:  63% 6% 31%

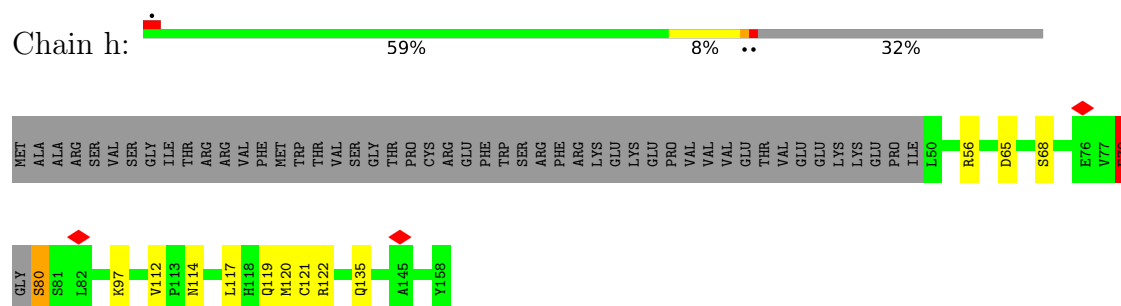




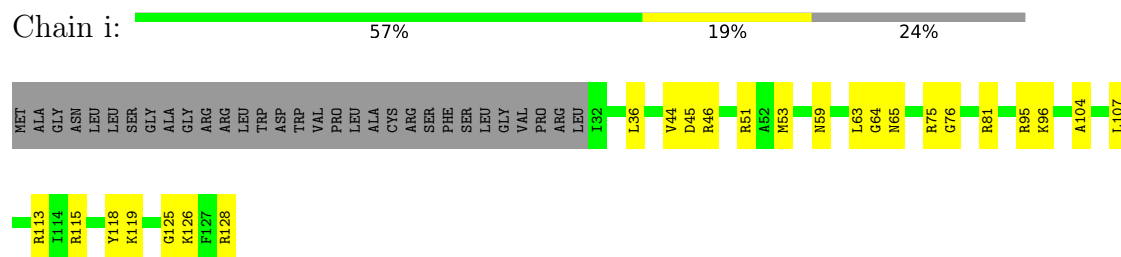
- Molecule 72: 39S ribosomal protein L49, mitochondrial



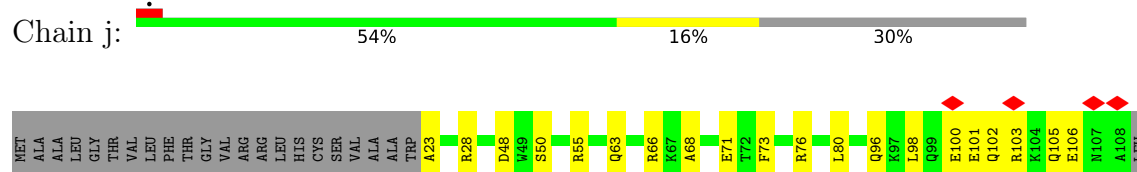
- Molecule 73: 39S ribosomal protein L50, mitochondrial



- Molecule 74: 39S ribosomal protein L51, mitochondrial



- Molecule 75: 39S ribosomal protein L52, mitochondrial



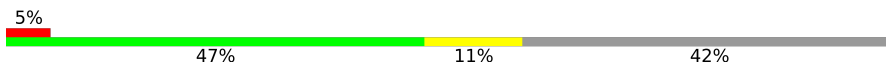
LYS  
PRO  
LYS  
GLY  
ALA  
SER  
LEU  
LYS  
SER  
PRO  
LEU  
PRO  
SER  
GLN

- Molecule 76: 39S ribosomal protein L53, mitochondrial

Chain k:  79% 6% 15%

MET  
A2  
G9  
L10  
Q19  
R31  
Q35  
R56  
H80  
A96  
ARG  
ASP  
ALA  
ALA  
GLY  
SER  
SER  
GLY  
ASP  
LYS  
PRO  
GLY  
ALA  
ASP  
THR  
GLY  
ARG

- Molecule 77: 39S ribosomal protein L54, mitochondrial

Chain l:  5% 47% 11% 42%

MET  
ALA  
THR  
LYS  
ARG  
LEU  
PHE  
GLY  
THR  
ARG  
THR  
TRP  
ALA  
GLY  
GLY  
ALA  
TRP  
GLU  
LEU  
LEU  
ASN  
PRO  
ALA  
THR  
SER  
GLY  
ARG  
LEU  
ALA  
ARG  
ASP  
TYR  
LYS  
LYS  
PRO  
VAL  
MET  
LYS  
GLY  
ALA  
LYS  
SER  
GLY  
GLY  
VAL  
THR  
SER  
GLU  
ALA  
LEU  
K57  
D58  
P59  
D60

V61  
I77  
K79  
E80  
D89  
Y92  
E98  
L101  
K105  
T106  
L107  
E108  
L110  
R119  
R120  
M135  
K136  
ARG  
LEU

- Molecule 78: 39S ribosomal protein L55, mitochondrial

Chain m:  5% 38% 9% 53%

MET  
ALA  
VAL  
GLY  
SER  
LEU  
LEU  
GLY  
ARG  
LEU  
ARG  
GLN  
SER  
THR  
VAL  
LYS  
ALA  
THR  
GLY  
PRO  
ALA  
LEU  
LEU  
ARG  
ARG  
LEU  
HIS  
THR  
SER  
SER  
TRP  
ARG  
ALA  
ASP  
S35  
S36  
R37  
R43  
V43  
H44  
R45  
Y52  
T63  
R67  
Y68  
D82  
T83  
LEU  
S84  
P85  
E86  
E87  
R88  
R89  
A90

R91  
K94  
ARG  
GLU  
ALA  
GLN  
LEU  
GLN  
SER  
ARG  
LYS  
GLU  
GLU  
GLN  
GLY  
LEU  
ASP  
ASP  
LEU  
HIS  
VAL  
GLU  
ARG  
GLY  
TYR  
GLN  
PHE  
THR  
THR  
LYS  
LYS

- Molecule 79: Ribosomal protein 63, mitochondrial

Chain o:  78% 14% 8%

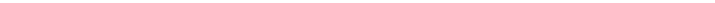
MET  
PHE  
LEU  
THR  
ALA  
LYS  
LEU  
LEU  
TRP  
R9  
R30  
Q33  
I36  
R37  
R38  
L39  
E40  
T55  
R56  
R66  
R67  
R68  
F71  
E72  
K75  
I88  
S102

- Molecule 80: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:  53% 8% 38%

MET  
ALA  
ALA  
THR  
CYS  
CYS  
ARG  
TRP  
GLY  
LEU  
SER  
ARG  
ALA  
VAL  
TRP  
LEU  
LEU  
PRO  
PRO  
PRO  
ALA  
CYS  
CYS  
PRO  
ARG  
ARG  
ALA  
LEU  
HIS  
LYS  
GLN  
LYS  
ASP  
GLY  
THR  
E38  
V61  
PRO  
ASN  
GLY  
ALA  
LYS  
GLN  
GLN  
ASP  
SER  
D70  
I71  
C81  
R82  
S83  
SER  
GLY  
PRO  
GLY  
GLY

GLN  
ASN  
VAL  
ASN  
ASN  
V95  
E113  
R116  
Q117  
N128  
R129  
N146  
D149  
C150  
R155  
Q163  
THR  
PRO  
LYS  
GLU  
PRO  
THR  
LYS  
GLU  
ASP  
VAL  
K174  
R177  
I178  
E181  
R189  
Q190  
I193  
HIS  
SER  
ALA  
VAL  
LYS  
THR  
ARG  
ARG  
VAL  
ASP  
MET  
ASP

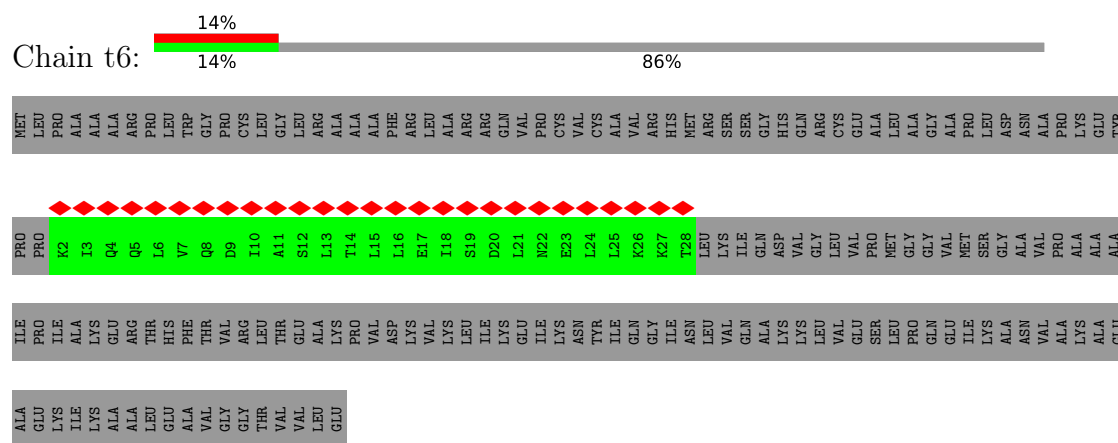
- Chain q: 





- Molecule 85: 39S ribosomal protein L12, mitochondrial

- Molecule 85: 39S ribosomal protein L12, mitochondrial



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 19968                                   | 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 |
| Maximum map value                    | 0.244                                   | Depositor |
| Minimum map value                    | -0.124                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.005                                   | Depositor |
| Recommended contour level            | 0.02                                    | Depositor |
| Map size (Å)                         | 546.0, 546.0, 546.0                     | wwPDB     |
| Map dimensions                       | 520, 520, 520                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.05, 1.05, 1.05                        | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$   |
| 1   | 0     | 0.21         | 0/895         | 0.33        | 0/1201        |
| 2   | 1     | 0.17         | 0/444         | 0.36        | 0/591         |
| 3   | 2     | 0.28         | 0/382         | 0.40        | 0/507         |
| 4   | 3     | 0.27         | 0/852         | 0.35        | 0/1136        |
| 5   | 4     | 0.22         | 0/349         | 0.38        | 0/461         |
| 6   | 5     | 0.16         | 0/3298        | 0.31        | 0/4492        |
| 7   | 6     | 0.15         | 0/3040        | 0.32        | 0/4134        |
| 8   | 7     | 0.16         | 0/2420        | 0.32        | 0/3270        |
| 9   | 8     | 1.52         | 1/1159 (0.1%) | 0.38        | 2/1559 (0.1%) |
| 10  | 9     | 0.17         | 0/1024        | 0.30        | 0/1379        |
| 11  | XA    | 0.18         | 0/35592       | 0.27        | 0/55390       |
| 12  | A0    | 0.11         | 0/1727        | 0.31        | 0/2338        |
| 13  | A1    | 0.10         | 0/2276        | 0.27        | 0/3079        |
| 14  | A2    | 0.13         | 0/939         | 0.33        | 0/1256        |
| 15  | A3    | 0.17         | 0/621         | 0.39        | 0/820         |
| 16  | A4    | 0.12         | 0/4559        | 0.32        | 0/6149        |
| 17  | AA    | 0.10         | 0/21952       | 0.22        | 0/34164       |
| 18  | AB    | 0.11         | 0/1819        | 0.28        | 0/2462        |
| 19  | AC    | 0.10         | 0/1112        | 0.26        | 0/1505        |
| 20  | AD    | 0.11         | 0/2768        | 0.31        | 0/3707        |
| 21  | AE    | 0.12         | 0/989         | 0.32        | 0/1335        |
| 22  | AF    | 0.10         | 0/1708        | 0.28        | 0/2291        |
| 23  | AG    | 0.11         | 0/2559        | 0.29        | 0/3429        |
| 24  | AH    | 0.11         | 0/1128        | 0.30        | 0/1529        |
| 25  | AI    | 0.11         | 0/1031        | 0.28        | 0/1390        |
| 26  | AJ    | 0.12         | 0/854         | 0.29        | 0/1148        |
| 27  | AK    | 0.12         | 0/879         | 0.32        | 0/1182        |
| 28  | AL    | 0.12         | 0/1406        | 0.30        | 0/1878        |
| 29  | AM    | 0.11         | 0/941         | 0.31        | 0/1265        |
| 30  | AN    | 0.10         | 0/864         | 0.30        | 0/1169        |
| 31  | AO    | 0.10         | 0/1580        | 0.27        | 0/2150        |
| 32  | AP    | 0.09         | 0/782         | 0.24        | 0/1050        |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 33  | AQ    | 0.13         | 0/746         | 0.28        | 0/993         |
| 34  | AR    | 1.12         | 1/2103 (0.0%) | 0.54        | 3/2842 (0.1%) |
| 35  | AS    | 0.11         | 0/1127        | 0.28        | 0/1518        |
| 36  | AT    | 0.12         | 0/1361        | 0.32        | 0/1829        |
| 37  | AU    | 0.13         | 0/1482        | 0.32        | 0/1987        |
| 38  | AV    | 0.10         | 0/2925        | 0.29        | 0/3948        |
| 39  | AW    | 0.10         | 0/778         | 0.26        | 0/1048        |
| 40  | AX    | 0.12         | 0/2886        | 0.32        | 0/3909        |
| 41  | AY    | 0.12         | 0/985         | 0.32        | 0/1329        |
| 42  | AZ    | 0.11         | 0/748         | 0.28        | 0/1000        |
| 43  | XB    | 0.09         | 0/1400        | 0.20        | 0/2168        |
| 44  | XD    | 0.21         | 0/1879        | 0.36        | 0/2527        |
| 45  | XE    | 0.20         | 0/2465        | 0.31        | 0/3344        |
| 46  | XF    | 0.25         | 0/2071        | 0.37        | 0/2817        |
| 47  | XH    | 0.16         | 0/798         | 0.34        | 0/1073        |
| 48  | XI    | 0.15         | 0/1727        | 0.34        | 0/2340        |
| 49  | XJ    | 0.11         | 0/1309        | 0.28        | 0/1764        |
| 50  | XK    | 0.24         | 0/1495        | 0.34        | 0/2029        |
| 51  | XL    | 0.19         | 0/904         | 0.30        | 0/1218        |
| 52  | XM    | 0.23         | 0/2359        | 0.36        | 0/3185        |
| 53  | XN    | 0.21         | 0/1825        | 0.33        | 0/2458        |
| 54  | XO    | 0.21         | 0/1269        | 0.37        | 0/1708        |
| 55  | XP    | 0.17         | 0/1190        | 0.36        | 0/1611        |
| 56  | XQ    | 0.17         | 0/2026        | 0.34        | 0/2734        |
| 57  | XR    | 0.28         | 0/1174        | 0.39        | 0/1572        |
| 58  | XS    | 0.25         | 0/1311        | 0.34        | 0/1778        |
| 59  | XT    | 0.25         | 0/1402        | 0.36        | 0/1886        |
| 60  | XU    | 0.20         | 0/1200        | 0.35        | 0/1623        |
| 61  | XV    | 0.16         | 0/1693        | 0.34        | 0/2297        |
| 62  | XW    | 0.23         | 0/893         | 0.33        | 0/1204        |
| 63  | XX    | 0.42         | 2/2090 (0.1%) | 0.54        | 6/2825 (0.2%) |
| 64  | XY    | 0.19         | 0/1571        | 0.33        | 0/2106        |
| 65  | XZ    | 0.24         | 0/1003        | 0.38        | 0/1354        |
| 66  | a     | 0.20         | 0/838         | 0.38        | 0/1138        |
| 67  | b     | 0.24         | 0/1202        | 0.36        | 0/1626        |
| 68  | c     | 0.18         | 0/2264        | 0.32        | 0/3059        |
| 69  | d     | 0.14         | 0/1807        | 0.29        | 0/2450        |
| 70  | e     | 0.77         | 6/1797 (0.3%) | 0.31        | 0/2422        |
| 71  | f     | 0.16         | 0/1159        | 0.31        | 0/1565        |
| 72  | g     | 0.29         | 0/1134        | 0.46        | 0/1547        |
| 73  | h     | 0.16         | 0/905         | 0.38        | 1/1233 (0.1%) |
| 74  | i     | 0.27         | 0/849         | 0.41        | 0/1135        |
| 75  | j     | 0.19         | 0/703         | 0.40        | 0/947         |

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 76  | k     | 0.13         | 0/743            | 0.33        | 0/1003           |
| 77  | l     | 0.11         | 0/692            | 0.29        | 0/939            |
| 78  | m     | 0.13         | 0/508            | 0.34        | 0/682            |
| 79  | o     | 0.24         | 0/818            | 0.40        | 0/1097           |
| 80  | p     | 0.14         | 0/1071           | 0.29        | 0/1433           |
| 81  | q     | 0.15         | 0/1413           | 0.32        | 0/1906           |
| 82  | r     | 0.19         | 0/1282           | 0.33        | 0/1734           |
| 84  | s     | 0.18         | 0/3114           | 0.33        | 0/4225           |
| 85  | t1    | 0.13         | 0/366            | 0.26        | 0/497            |
| 85  | t2    | 0.08         | 0/238            | 0.22        | 0/319            |
| 85  | t3    | 0.09         | 0/238            | 0.23        | 0/319            |
| 85  | t4    | 0.07         | 0/229            | 0.20        | 0/308            |
| 85  | t5    | 0.10         | 0/229            | 0.26        | 0/308            |
| 85  | t6    | 0.11         | 0/213            | 0.29        | 0/286            |
| All | All   | 0.25         | 10/175956 (0.0%) | 0.31        | 12/249618 (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                   | 2                   |
| 70  | e     | 0                   | 1                   |
| 71  | f     | 0                   | 1                   |
| 73  | h     | 0                   | 1                   |
| All | All   | 0                   | 6                   |

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

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | 8     | 99  | ARG  | CG-CD   | 51.30 | 3.06        | 1.52     |
| 34  | AR    | 308 | HIS  | C-N     | 50.85 | 1.89        | 1.34     |
| 70  | e     | 84  | TYR  | CD2-CE2 | 16.12 | 1.87        | 1.38     |
| 70  | e     | 84  | TYR  | CD1-CE1 | 15.79 | 1.86        | 1.38     |
| 63  | XX    | 150 | LYS  | C-N     | 12.58 | 1.51        | 1.33     |

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

| Mol | Chain | Res | Type | Atoms | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 63  | XX    | 147 | LYS  | O-C-N | 15.65 | 144.58      | 122.36   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 34  | AR    | 309 | PRO  | O-C-N  | 13.25  | 141.32      | 122.37   |
| 34  | AR    | 309 | PRO  | CA-C-N | -10.25 | 106.88      | 122.05   |
| 34  | AR    | 309 | PRO  | C-N-CA | -10.25 | 106.88      | 122.05   |
| 63  | XX    | 150 | LYS  | O-C-N  | -9.75  | 111.78      | 122.12   |

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 44  | XD    | 206 | TYR  | Peptide |
| 48  | XI    | 197 | LEU  | Peptide |
| 48  | XI    | 90  | PHE  | Peptide |
| 70  | e     | 265 | LYS  | Peptide |
| 71  | f     | 138 | GLN  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 880   | 903      | 903      | 10      | 0            |
| 2   | 1     | 439   | 480      | 480      | 8       | 0            |
| 3   | 2     | 376   | 406      | 406      | 4       | 0            |
| 4   | 3     | 831   | 883      | 883      | 12      | 0            |
| 5   | 4     | 341   | 361      | 361      | 6       | 0            |
| 6   | 5     | 3204  | 3200     | 3200     | 32      | 0            |
| 7   | 6     | 2947  | 2839     | 2839     | 38      | 0            |
| 8   | 7     | 2365  | 2373     | 2372     | 25      | 0            |
| 9   | 8     | 1135  | 1166     | 1166     | 41      | 0            |
| 10  | 9     | 996   | 987      | 987      | 11      | 0            |
| 11  | XA    | 31813 | 16160    | 16160    | 274     | 0            |
| 12  | A0    | 1684  | 1685     | 1685     | 16      | 0            |
| 13  | A1    | 2230  | 2261     | 2261     | 27      | 0            |
| 14  | A2    | 925   | 964      | 964      | 14      | 0            |
| 15  | A3    | 610   | 682      | 682      | 12      | 0            |
| 16  | A4    | 4470  | 4485     | 4486     | 65      | 0            |
| 17  | AA    | 19628 | 9970     | 9971     | 154     | 0            |
| 18  | AB    | 1776  | 1769     | 1769     | 15      | 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     | 36      | 0            |
| 21  | AE    | 972   | 1001     | 1001     | 14      | 0            |
| 22  | AF    | 1668  | 1714     | 1716     | 18      | 0            |
| 23  | AG    | 2505  | 2492     | 2490     | 27      | 0            |
| 24  | AH    | 1105  | 1136     | 1136     | 24      | 0            |
| 25  | AI    | 1011  | 1052     | 1052     | 13      | 0            |
| 26  | AJ    | 838   | 887      | 887      | 10      | 0            |
| 27  | AK    | 861   | 885      | 885      | 10      | 0            |
| 28  | AL    | 1382  | 1472     | 1472     | 18      | 0            |
| 29  | AM    | 920   | 951      | 951      | 11      | 0            |
| 30  | AN    | 846   | 908      | 908      | 12      | 0            |
| 31  | AO    | 1528  | 1490     | 1490     | 19      | 0            |
| 32  | AP    | 765   | 796      | 796      | 6       | 0            |
| 33  | AQ    | 734   | 749      | 749      | 7       | 0            |
| 34  | AR    | 2060  | 2074     | 2074     | 21      | 0            |
| 35  | AS    | 1100  | 1103     | 1103     | 12      | 0            |
| 36  | AT    | 1330  | 1342     | 1342     | 17      | 0            |
| 37  | AU    | 1461  | 1471     | 1471     | 14      | 0            |
| 38  | AV    | 2867  | 2863     | 2862     | 23      | 0            |
| 39  | AW    | 766   | 785      | 785      | 5       | 0            |
| 40  | AX    | 2814  | 2805     | 2804     | 33      | 0            |
| 41  | AY    | 956   | 911      | 911      | 12      | 0            |
| 42  | AZ    | 731   | 734      | 734      | 6       | 0            |
| 43  | XB    | 1255  | 640      | 640      | 11      | 0            |
| 44  | XD    | 1842  | 1896     | 1896     | 29      | 0            |
| 45  | XE    | 2396  | 2402     | 2402     | 25      | 0            |
| 46  | XF    | 2013  | 2045     | 2044     | 32      | 0            |
| 47  | XH    | 784   | 832      | 832      | 14      | 0            |
| 48  | XI    | 1691  | 1783     | 1783     | 21      | 0            |
| 49  | XJ    | 1291  | 1367     | 1364     | 15      | 0            |
| 50  | XK    | 1451  | 1448     | 1448     | 20      | 0            |
| 51  | XL    | 889   | 941      | 941      | 8       | 0            |
| 52  | XM    | 2305  | 2378     | 2378     | 36      | 0            |
| 53  | XN    | 1778  | 1808     | 1808     | 19      | 0            |
| 54  | XO    | 1245  | 1283     | 1283     | 25      | 0            |
| 55  | XP    | 1164  | 1162     | 1162     | 21      | 0            |
| 56  | XQ    | 1978  | 2022     | 2022     | 22      | 0            |
| 57  | XR    | 1153  | 1214     | 1214     | 26      | 0            |
| 58  | XS    | 1284  | 1354     | 1354     | 18      | 0            |
| 59  | XT    | 1368  | 1410     | 1410     | 24      | 0            |
| 60  | XU    | 1171  | 1164     | 1164     | 13      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 61  | XV    | 1648  | 1656     | 1654     | 16      | 0            |
| 62  | XW    | 871   | 898      | 898      | 11      | 0            |
| 63  | XX    | 2035  | 2054     | 2054     | 28      | 0            |
| 64  | XY    | 1534  | 1575     | 1575     | 28      | 0            |
| 65  | XZ    | 978   | 1030     | 1030     | 15      | 0            |
| 66  | a     | 813   | 777      | 777      | 13      | 0            |
| 67  | b     | 1178  | 1180     | 1180     | 10      | 0            |
| 68  | c     | 2217  | 2220     | 2220     | 28      | 0            |
| 69  | d     | 1758  | 1743     | 1742     | 17      | 0            |
| 70  | e     | 1762  | 1767     | 1767     | 41      | 0            |
| 71  | f     | 1139  | 1152     | 1152     | 12      | 0            |
| 72  | g     | 1097  | 1086     | 1085     | 19      | 0            |
| 73  | h     | 882   | 866      | 867      | 10      | 0            |
| 74  | i     | 827   | 857      | 857      | 21      | 0            |
| 75  | j     | 689   | 678      | 678      | 16      | 0            |
| 76  | k     | 732   | 745      | 745      | 5       | 0            |
| 77  | l     | 673   | 654      | 653      | 15      | 0            |
| 78  | m     | 500   | 525      | 525      | 10      | 0            |
| 79  | o     | 797   | 804      | 804      | 9       | 0            |
| 80  | p     | 1058  | 1083     | 1083     | 13      | 0            |
| 81  | q     | 1379  | 1359     | 1359     | 14      | 0            |
| 82  | r     | 1247  | 1267     | 1267     | 13      | 0            |
| 83  | r3    | 1468  | 0        | 823      | 24      | 0            |
| 84  | s     | 3036  | 3023     | 3022     | 40      | 0            |
| 85  | t1    | 354   | 379      | 374      | 2       | 0            |
| 85  | t2    | 238   | 268      | 270      | 2       | 0            |
| 85  | t3    | 238   | 268      | 270      | 1       | 0            |
| 85  | t4    | 229   | 255      | 257      | 1       | 0            |
| 85  | t5    | 229   | 255      | 257      | 0       | 0            |
| 85  | t6    | 214   | 236      | 236      | 0       | 0            |
| 86  | 0     | 1     | 0        | 0        | 0       | 0            |
| 86  | 4     | 1     | 0        | 0        | 0       | 0            |
| 86  | AB    | 1     | 0        | 0        | 0       | 0            |
| 86  | AO    | 1     | 0        | 0        | 0       | 0            |
| 86  | AP    | 1     | 0        | 0        | 0       | 0            |
| 86  | AT    | 1     | 0        | 0        | 0       | 0            |
| 86  | r     | 1     | 0        | 0        | 0       | 0            |
| 87  | 9     | 1     | 0        | 0        | 0       | 0            |
| 87  | AA    | 46    | 0        | 0        | 0       | 0            |
| 87  | XA    | 143   | 0        | 0        | 0       | 0            |
| 87  | XD    | 1     | 0        | 0        | 0       | 0            |
| 87  | XI    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 87  | XM    | 1      | 0        | 0        | 0       | 0            |
| 87  | XW    | 1      | 0        | 0        | 0       | 0            |
| 87  | g     | 1      | 0        | 0        | 0       | 0            |
| 88  | XA    | 73     | 67       | 0        | 2       | 0            |
| 89  | XA    | 48     | 50       | 50       | 0       | 0            |
| 90  | AX    | 32     | 10       | 12       | 1       | 0            |
| All | All   | 168901 | 143004   | 143755   | 1524    | 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 1524 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 70:e:84:TYR:CE1 | 70:e:84:TYR:CD1 | 1.86                     | 1.61              |
| 70:e:84:TYR:CD2 | 70:e:84:TYR:CE2 | 1.87                     | 1.56              |
| 34:AR:308:HIS:C | 34:AR:309:PRO:N | 1.88                     | 1.31              |
| 9:8:99:ARG:CD   | 70:e:84:TYR:CD1 | 2.25                     | 1.19              |
| 9:8:99:ARG:CD   | 70:e:84:TYR:CD2 | 2.28                     | 1.16              |

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%)   | 44 (100%) | 0       | 0        | 100         | 100 |
| 4   | 3     | 93/188 (50%)  | 91 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 5   | 4     | 36/103 (35%)  | 35 (97%)  | 1 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 6   | 5     | 389/423 (92%) | 366 (94%) | 23 (6%) | 0        | 100         | 100 |
| 7   | 6     | 348/380 (92%) | 321 (92%) | 27 (8%) | 0        | 100         | 100 |
| 8   | 7     | 285/338 (84%) | 262 (92%) | 23 (8%) | 0        | 100         | 100 |
| 9   | 8     | 132/206 (64%) | 126 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 10  | 9     | 122/137 (89%) | 116 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 12  | A0    | 197/218 (90%) | 188 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 13  | A1    | 273/323 (84%) | 255 (93%) | 18 (7%) | 0        | 100         | 100 |
| 14  | A2    | 114/118 (97%) | 109 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 15  | A3    | 67/199 (34%)  | 67 (100%) | 0       | 0        | 100         | 100 |
| 16  | A4    | 526/689 (76%) | 493 (94%) | 33 (6%) | 0        | 100         | 100 |
| 18  | AB    | 216/296 (73%) | 214 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 19  | AC    | 130/167 (78%) | 127 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 20  | AD    | 341/430 (79%) | 324 (95%) | 17 (5%) | 0        | 100         | 100 |
| 21  | AE    | 120/125 (96%) | 115 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 22  | AF    | 197/242 (81%) | 192 (98%) | 5 (2%)  | 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%) | 130 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 26  | AJ    | 106/138 (77%) | 99 (93%)  | 7 (7%)  | 0        | 100         | 100 |
| 27  | AK    | 99/128 (77%)  | 98 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 28  | AL    | 162/257 (63%) | 157 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 29  | AM    | 114/137 (83%) | 113 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 30  | AN    | 105/130 (81%) | 101 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 31  | AO    | 183/258 (71%) | 179 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 32  | AP    | 93/142 (66%)  | 87 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 33  | AQ    | 83/87 (95%)   | 79 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 34  | AR    | 248/360 (69%) | 238 (96%) | 10 (4%) | 0        | 100         | 100 |
| 35  | AS    | 131/190 (69%) | 123 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 36  | AT    | 160/173 (92%) | 147 (92%) | 13 (8%) | 0        | 100         | 100 |
| 37  | AU    | 171/205 (83%) | 169 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 38  | AV    | 341/414 (82%) | 322 (94%) | 19 (6%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 39  | AW    | 95/187 (51%)  | 90 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 40  | AX    | 346/398 (87%) | 329 (95%) | 17 (5%) | 0        | 100         | 100 |
| 41  | AY    | 111/395 (28%) | 104 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 42  | AZ    | 84/106 (79%)  | 83 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 44  | XD    | 234/305 (77%) | 219 (94%) | 13 (6%) | 2 (1%)   | 14          | 45  |
| 45  | XE    | 302/348 (87%) | 288 (95%) | 14 (5%) | 0        | 100         | 100 |
| 46  | XF    | 248/311 (80%) | 239 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 47  | XH    | 93/267 (35%)  | 87 (94%)  | 6 (6%)  | 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%) | 169 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 51  | XL    | 113/145 (78%) | 106 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 52  | XM    | 285/296 (96%) | 277 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 53  | XN    | 219/251 (87%) | 208 (95%) | 11 (5%) | 0        | 100         | 100 |
| 54  | XO    | 150/175 (86%) | 145 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 55  | XP    | 141/180 (78%) | 130 (92%) | 11 (8%) | 0        | 100         | 100 |
| 56  | XQ    | 236/292 (81%) | 226 (96%) | 10 (4%) | 0        | 100         | 100 |
| 57  | XR    | 138/149 (93%) | 132 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 58  | XS    | 158/205 (77%) | 153 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 59  | XT    | 164/206 (80%) | 161 (98%) | 3 (2%)  | 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%) | 234 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 64  | XY    | 176/250 (70%) | 173 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 65  | XZ    | 118/161 (73%) | 114 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 66  | a     | 93/142 (66%)  | 87 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 67  | b     | 146/215 (68%) | 135 (92%) | 11 (8%) | 0        | 100         | 100 |
| 68  | c     | 271/332 (82%) | 260 (96%) | 11 (4%) | 0        | 100         | 100 |
| 69  | d     | 212/306 (69%) | 201 (95%) | 10 (5%) | 1 (0%)   | 24          | 57  |
| 70  | e     | 211/279 (76%) | 202 (96%) | 9 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 71  | f     | 138/212 (65%)     | 132 (96%)   | 6 (4%)   | 0        | 100         | 100 |
| 72  | g     | 130/166 (78%)     | 122 (94%)   | 7 (5%)   | 1 (1%)   | 16          | 48  |
| 73  | h     | 106/158 (67%)     | 103 (97%)   | 2 (2%)   | 1 (1%)   | 14          | 45  |
| 74  | i     | 95/128 (74%)      | 91 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| 75  | j     | 84/123 (68%)      | 83 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 76  | k     | 93/112 (83%)      | 90 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 77  | l     | 78/138 (56%)      | 73 (94%)    | 5 (6%)   | 0        | 100         | 100 |
| 78  | m     | 58/128 (45%)      | 53 (91%)    | 5 (9%)   | 0        | 100         | 100 |
| 79  | o     | 92/102 (90%)      | 88 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| 80  | p     | 119/206 (58%)     | 113 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| 81  | q     | 162/222 (73%)     | 157 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 82  | r     | 144/196 (74%)     | 137 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 84  | s     | 366/439 (83%)     | 351 (96%)   | 15 (4%)  | 0        | 100         | 100 |
| 85  | t1    | 45/198 (23%)      | 40 (89%)    | 5 (11%)  | 0        | 100         | 100 |
| 85  | t2    | 28/198 (14%)      | 28 (100%)   | 0        | 0        | 100         | 100 |
| 85  | t3    | 28/198 (14%)      | 28 (100%)   | 0        | 0        | 100         | 100 |
| 85  | t4    | 27/198 (14%)      | 26 (96%)    | 1 (4%)   | 0        | 100         | 100 |
| 85  | t5    | 27/198 (14%)      | 26 (96%)    | 1 (4%)   | 0        | 100         | 100 |
| 85  | t6    | 25/198 (13%)      | 25 (100%)   | 0        | 0        | 100         | 100 |
| All | All   | 13778/19160 (72%) | 13145 (95%) | 628 (5%) | 5 (0%)   | 100         | 100 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 72  | g     | 38  | PHE  |
| 44  | XD    | 207 | ILE  |
| 44  | XD    | 208 | ARG  |
| 73  | h     | 78  | PHE  |
| 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%) | 353 (100%) | 0        | 100         | 100 |
| 7   | 6     | 313/332 (94%) | 313 (100%) | 0        | 100         | 100 |
| 8   | 7     | 267/303 (88%) | 267 (100%) | 0        | 100         | 100 |
| 9   | 8     | 124/190 (65%) | 124 (100%) | 0        | 100         | 100 |
| 10  | 9     | 104/112 (93%) | 104 (100%) | 0        | 100         | 100 |
| 12  | A0    | 176/190 (93%) | 176 (100%) | 0        | 100         | 100 |
| 13  | A1    | 253/291 (87%) | 253 (100%) | 0        | 100         | 100 |
| 14  | A2    | 99/101 (98%)  | 99 (100%)  | 0        | 100         | 100 |
| 15  | A3    | 63/166 (38%)  | 63 (100%)  | 0        | 100         | 100 |
| 16  | A4    | 494/609 (81%) | 494 (100%) | 0        | 100         | 100 |
| 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%) | 283 (100%) | 0        | 100         | 100 |
| 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 |
| 29  | AM    | 95/113 (84%)  | 94 (99%)   | 1 (1%)   | 65          | 73  |
| 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 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 33  | AQ    | 77/79 (98%)   | 77 (100%)  | 0        | 100         | 100 |
| 34  | AR    | 229/318 (72%) | 229 (100%) | 0        | 100         | 100 |
| 35  | AS    | 115/164 (70%) | 115 (100%) | 0        | 100         | 100 |
| 36  | AT    | 150/157 (96%) | 150 (100%) | 0        | 100         | 100 |
| 37  | AU    | 149/174 (86%) | 149 (100%) | 0        | 100         | 100 |
| 38  | AV    | 315/364 (86%) | 315 (100%) | 0        | 100         | 100 |
| 39  | AW    | 84/158 (53%)  | 84 (100%)  | 0        | 100         | 100 |
| 40  | AX    | 307/351 (88%) | 307 (100%) | 0        | 100         | 100 |
| 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%) | 190 (100%) | 0        | 100         | 100 |
| 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%) | 132 (99%)  | 1 (1%)   | 73          | 76  |
| 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%) | 245 (100%) | 0        | 100         | 100 |
| 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%) | 219 (100%) | 1 (0%)   | 81          | 81  |
| 57  | XR    | 118/126 (94%) | 118 (100%) | 0        | 100         | 100 |
| 58  | XS    | 145/180 (81%) | 145 (100%) | 0        | 100         | 100 |
| 59  | XT    | 146/176 (83%) | 146 (100%) | 0        | 100         | 100 |
| 60  | XU    | 126/135 (93%) | 126 (100%) | 0        | 100         | 100 |
| 61  | XV    | 179/191 (94%) | 179 (100%) | 0        | 100         | 100 |
| 62  | XW    | 91/119 (76%)  | 91 (100%)  | 0        | 100         | 100 |
| 63  | XX    | 219/229 (96%) | 219 (100%) | 0        | 100         | 100 |
| 64  | XY    | 161/223 (72%) | 161 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 65  | XZ    | 111/147 (76%)     | 111 (100%)   | 0        | 100         | 100 |
| 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%)     | 241 (100%)   | 0        | 100         | 100 |
| 69  | d     | 196/274 (72%)     | 196 (100%)   | 0        | 100         | 100 |
| 70  | e     | 188/236 (80%)     | 188 (100%)   | 0        | 100         | 100 |
| 71  | f     | 127/188 (68%)     | 127 (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%)     | 141 (100%)   | 0        | 100         | 100 |
| 82  | r     | 138/169 (82%)     | 138 (100%)   | 0        | 100         | 100 |
| 84  | s     | 326/381 (86%)     | 326 (100%)   | 0        | 100         | 100 |
| 85  | t1    | 41/158 (26%)      | 40 (98%)     | 1 (2%)   | 43          | 62  |
| 85  | t2    | 29/158 (18%)      | 29 (100%)    | 0        | 100         | 100 |
| 85  | t3    | 29/158 (18%)      | 29 (100%)    | 0        | 100         | 100 |
| 85  | t4    | 28/158 (18%)      | 28 (100%)    | 0        | 100         | 100 |
| 85  | t5    | 28/158 (18%)      | 28 (100%)    | 0        | 100         | 100 |
| 85  | t6    | 26/158 (16%)      | 26 (100%)    | 0        | 100         | 100 |
| All | All   | 12392/16507 (75%) | 12388 (100%) | 4 (0%)   | 100         | 100 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | AM    | 88  | GLU  |
| 49  | XJ    | 144 | ILE  |
| 56  | XQ    | 282 | ILE  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 85  | t1    | 21[A] | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | XE    | 216 | GLN  |
| 59  | XT    | 202 | GLN  |
| 46  | XF    | 251 | HIS  |
| 55  | XP    | 54  | ASN  |
| 63  | XX    | 240 | GLN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 11  | XA    | 1489/1561 (95%) | 262 (17%)         | 7 (0%)          |
| 17  | AA    | 916/954 (96%)   | 161 (17%)         | 3 (0%)          |
| 43  | XB    | 55/72 (76%)     | 12 (21%)          | 0               |
| 83  | r3    | 74/75 (98%)     | 25 (33%)          | 0               |
| All | All   | 2534/2662 (95%) | 460 (18%)         | 10 (0%)         |

5 of 460 RNA backbone outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | XA    | 1681 | G    |
| 11  | XA    | 1685 | C    |
| 11  | XA    | 1689 | C    |
| 11  | XA    | 1692 | A    |
| 11  | XA    | 1693 | C    |

5 of 10 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 17  | AA    | 770  | C    |
| 17  | AA    | 1048 | C    |
| 17  | AA    | 1234 | C    |
| 11  | XA    | 2558 | A    |
| 11  | XA    | 2574 | G    |

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

75 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$ |
| 83  | Y5P  | r3    | 4   | 83   | 14,19,20     | 7.39 | 3 (21%)     | 18,26,29    | 0.57 | 0           |
| 83  | P5P  | r3    | 14  | 83   | 20,23,24     | 1.27 | 3 (15%)     | 27,33,36    | 2.48 | 11 (40%)    |
| 83  | P5P  | r3    | 24  | 83   | 20,23,24     | 1.28 | 3 (15%)     | 27,33,36    | 2.47 | 11 (40%)    |
| 83  | Y5P  | r3    | 49  | 83   | 14,19,20     | 7.37 | 3 (21%)     | 18,26,29    | 0.55 | 0           |
| 83  | P5P  | r3    | 10  | 83   | 20,23,24     | 1.27 | 3 (15%)     | 27,33,36    | 2.48 | 11 (40%)    |
| 83  | Y5P  | r3    | 54  | 83   | 14,19,20     | 7.40 | 3 (21%)     | 18,26,29    | 0.55 | 0           |
| 83  | P5P  | r3    | 22  | 83   | 20,23,24     | 1.27 | 3 (15%)     | 27,33,36    | 2.48 | 11 (40%)    |
| 83  | P5P  | r3    | 65  | 83   | 20,23,24     | 1.28 | 3 (15%)     | 27,33,36    | 2.49 | 11 (40%)    |
| 83  | Y5P  | r3    | 48  | 83   | 14,19,20     | 7.38 | 3 (21%)     | 18,26,29    | 0.52 | 0           |
| 83  | Y5P  | r3    | 55  | 83   | 14,19,20     | 7.42 | 3 (21%)     | 18,26,29    | 0.55 | 0           |
| 83  | P5P  | r3    | 6   | 83   | 20,23,24     | 1.27 | 3 (15%)     | 27,33,36    | 2.48 | 11 (40%)    |
| 83  | Y5P  | r3    | 72  | 83   | 14,19,20     | 7.37 | 3 (21%)     | 18,26,29    | 0.56 | 0           |
| 83  | Y5P  | r3    | 68  | 83   | 14,19,20     | 7.37 | 3 (21%)     | 18,26,29    | 0.57 | 0           |
| 83  | Y5P  | r3    | 67  | 83   | 14,19,20     | 7.40 | 3 (21%)     | 18,26,29    | 0.55 | 0           |
| 83  | P5P  | r3    | 57  | 83   | 20,23,24     | 1.27 | 3 (15%)     | 27,33,36    | 2.49 | 11 (40%)    |
| 83  | P5P  | r3    | 28  | 83   | 20,23,24     | 1.26 | 3 (15%)     | 27,33,36    | 2.48 | 11 (40%)    |
| 83  | P5P  | r3    | 27  | 83   | 20,23,24     | 1.27 | 3 (15%)     | 27,33,36    | 2.48 | 11 (40%)    |
| 83  | Y5P  | r3    | 43  | 83   | 14,19,20     | 7.41 | 3 (21%)     | 18,26,29    | 0.55 | 0           |
| 83  | P5P  | r3    | 70  | 83   | 20,23,24     | 1.27 | 3 (15%)     | 27,33,36    | 2.48 | 11 (40%)    |
| 83  | P5P  | r3    | 37  | 83   | 24,24,24     | 1.19 | 3 (12%)     | 34,36,36    | 4.14 | 17 (50%)    |
| 83  | P5P  | r3    | 1   | 83   | 20,23,24     | 1.28 | 3 (15%)     | 27,33,36    | 2.47 | 11 (40%)    |
| 83  | P5P  | r3    | 34  | 83   | 20,23,24     | 1.28 | 3 (15%)     | 27,33,36    | 2.50 | 11 (40%)    |
| 83  | Y5P  | r3    | 41  | 83   | 14,19,20     | 7.39 | 3 (21%)     | 18,26,29    | 0.56 | 0           |
| 83  | Y5P  | r3    | 2   | 83   | 14,19,20     | 7.37 | 3 (21%)     | 18,26,29    | 0.55 | 0           |
| 83  | P5P  | r3    | 21  | 83   | 20,23,24     | 1.27 | 3 (15%)     | 27,33,36    | 2.47 | 11 (40%)    |
| 83  | P5P  | r3    | 53  | 83   | 20,23,24     | 1.28 | 3 (15%)     | 27,33,36    | 2.49 | 11 (40%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 83  | P5P  | r3    | 58  | 83   | 20,23,24     | 1.27 | 3 (15%)  | 27,33,36    | 2.47 | 11 (40%) |
| 83  | Y5P  | r3    | 66  | 83   | 14,19,20     | 7.39 | 3 (21%)  | 18,26,29    | 0.54 | 0        |
| 83  | Y5P  | r3    | 51  | 83   | 14,19,20     | 7.39 | 3 (21%)  | 18,26,29    | 0.56 | 0        |
| 83  | P5P  | r3    | 73  | 83   | 20,23,24     | 1.29 | 3 (15%)  | 27,33,36    | 2.51 | 11 (40%) |
| 83  | P5P  | r3    | 18  | 83   | 20,23,24     | 1.26 | 3 (15%)  | 27,33,36    | 2.48 | 11 (40%) |
| 83  | P5P  | r3    | 9   | 83   | 20,23,24     | 1.28 | 3 (15%)  | 27,33,36    | 2.47 | 11 (40%) |
| 83  | Y5P  | r3    | 13  | 83   | 14,19,20     | 7.39 | 3 (21%)  | 18,26,29    | 0.54 | 0        |
| 83  | P5P  | r3    | 44  | 83   | 20,23,24     | 1.27 | 3 (15%)  | 27,33,36    | 2.50 | 11 (40%) |
| 83  | P5P  | r3    | 15  | 83   | 20,23,24     | 1.27 | 3 (15%)  | 27,33,36    | 2.48 | 11 (40%) |
| 83  | P5P  | r3    | 36  | 83   | 20,23,24     | 1.29 | 3 (15%)  | 27,33,36    | 2.53 | 11 (40%) |
| 83  | Y5P  | r3    | 45  | 83   | 14,19,20     | 7.40 | 3 (21%)  | 18,26,29    | 0.54 | 0        |
| 83  | P5P  | r3    | 69  | 83   | 20,23,24     | 1.27 | 3 (15%)  | 27,33,36    | 2.48 | 11 (40%) |
| 83  | P5P  | r3    | 5   | 83   | 20,23,24     | 1.27 | 3 (15%)  | 27,33,36    | 2.48 | 11 (40%) |
| 83  | Y5P  | r3    | 20  | 83   | 14,19,20     | 7.41 | 3 (21%)  | 18,26,29    | 0.56 | 0        |
| 83  | Y5P  | r3    | 11  | 83   | 14,19,20     | 7.38 | 3 (21%)  | 18,26,29    | 0.55 | 0        |
| 83  | Y5P  | r3    | 75  | 83   | 14,19,20     | 7.36 | 3 (21%)  | 18,26,29    | 0.56 | 0        |
| 83  | Y5P  | r3    | 61  | 83   | 14,19,20     | 7.37 | 3 (21%)  | 18,26,29    | 0.54 | 0        |
| 83  | Y5P  | r3    | 3   | 83   | 14,19,20     | 7.36 | 3 (21%)  | 18,26,29    | 0.55 | 0        |
| 83  | P5P  | r3    | 64  | 83   | 20,23,24     | 1.28 | 3 (15%)  | 27,33,36    | 2.48 | 11 (40%) |
| 83  | Y5P  | r3    | 25  | 83   | 14,19,20     | 7.38 | 3 (21%)  | 18,26,29    | 0.54 | 0        |
| 83  | P5P  | r3    | 38  | 83   | 20,23,24     | 1.27 | 3 (15%)  | 27,33,36    | 2.48 | 11 (40%) |
| 83  | Y5P  | r3    | 39  | 83   | 14,19,20     | 7.36 | 3 (21%)  | 18,26,29    | 0.55 | 0        |
| 83  | P5P  | r3    | 46  | 83   | 20,23,24     | 1.28 | 3 (15%)  | 27,33,36    | 2.45 | 10 (37%) |
| 83  | P5P  | r3    | 7   | 83   | 20,23,24     | 1.28 | 3 (15%)  | 27,33,36    | 2.48 | 11 (40%) |
| 83  | P5P  | r3    | 29  | 83   | 20,23,24     | 1.26 | 3 (15%)  | 27,33,36    | 2.51 | 11 (40%) |
| 83  | Y5P  | r3    | 17  | 83   | 14,19,20     | 7.43 | 3 (21%)  | 18,26,29    | 0.55 | 0        |
| 83  | Y5P  | r3    | 16  | 83   | 14,19,20     | 7.43 | 3 (21%)  | 18,26,29    | 0.57 | 0        |
| 83  | P5P  | r3    | 23  | 83   | 20,23,24     | 1.28 | 3 (15%)  | 27,33,36    | 2.50 | 11 (40%) |
| 83  | Y5P  | r3    | 32  | 83   | 14,19,20     | 7.39 | 3 (21%)  | 18,26,29    | 0.58 | 0        |
| 83  | P5P  | r3    | 26  | 83   | 20,23,24     | 1.28 | 3 (15%)  | 27,33,36    | 2.48 | 11 (40%) |
| 83  | Y5P  | r3    | 50  | 83   | 14,19,20     | 7.38 | 3 (21%)  | 18,26,29    | 0.55 | 0        |
| 83  | Y5P  | r3    | 42  | 83   | 14,19,20     | 7.38 | 3 (21%)  | 18,26,29    | 0.54 | 0        |
| 83  | Y5P  | r3    | 8   | 83   | 14,19,20     | 7.39 | 3 (21%)  | 18,26,29    | 0.54 | 0        |
| 83  | P5P  | r3    | 35  | 83   | 20,23,24     | 1.28 | 3 (15%)  | 27,33,36    | 2.47 | 11 (40%) |
| 83  | P5P  | r3    | 31  | 83   | 20,23,24     | 1.28 | 3 (15%)  | 27,33,36    | 2.48 | 10 (37%) |



| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 83  | Y5P  | r3    | 47  | 83    | 14,19,20     | 7.41 | 3 (21%)  | 18,26,29    | 0.59 | 0        |
| 83  | Y5P  | r3    | 33  | 83    | 14,19,20     | 7.41 | 3 (21%)  | 18,26,29    | 0.52 | 0        |
| 83  | Y5P  | r3    | 56  | 83    | 14,19,20     | 7.40 | 3 (21%)  | 18,26,29    | 0.55 | 0        |
| 83  | P5P  | r3    | 52  | 83    | 20,23,24     | 1.28 | 3 (15%)  | 27,33,36    | 2.48 | 11 (40%) |
| 83  | Y5P  | r3    | 62  | 83    | 14,19,20     | 7.43 | 3 (21%)  | 18,26,29    | 0.57 | 0        |
| 83  | Y5P  | r3    | 40  | 83    | 14,19,20     | 7.41 | 3 (21%)  | 18,26,29    | 0.55 | 0        |
| 83  | P5P  | r3    | 63  | 83    | 20,23,24     | 1.27 | 3 (15%)  | 27,33,36    | 2.49 | 11 (40%) |
| 83  | P5P  | r3    | 71  | 83    | 20,23,24     | 1.27 | 3 (15%)  | 27,33,36    | 2.47 | 11 (40%) |
| 83  | Y5P  | r3    | 12  | 83    | 14,19,20     | 7.41 | 3 (21%)  | 18,26,29    | 0.54 | 0        |
| 83  | P5P  | r3    | 19  | 83    | 20,23,24     | 1.28 | 3 (15%)  | 27,33,36    | 2.47 | 11 (40%) |
| 83  | Y5P  | r3    | 60  | 83    | 14,19,20     | 7.38 | 3 (21%)  | 18,26,29    | 0.57 | 0        |
| 83  | P5P  | r3    | 74  | 11,83 | 20,23,24     | 1.31 | 3 (15%)  | 27,33,36    | 2.52 | 11 (40%) |
| 83  | Y5P  | r3    | 59  | 83    | 14,19,20     | 7.41 | 3 (21%)  | 18,26,29    | 0.56 | 0        |
| 83  | P5P  | r3    | 30  | 83    | 20,23,24     | 1.27 | 3 (15%)  | 27,33,36    | 2.47 | 11 (40%) |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 83  | Y5P  | r3    | 4   | 83   | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 14  | 83   | -       | 0/7/25/26 | 0/3/3/3 |
| 83  | P5P  | r3    | 24  | 83   | -       | 0/7/25/26 | 0/3/3/3 |
| 83  | Y5P  | r3    | 49  | 83   | -       | 3/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 10  | 83   | -       | 2/7/25/26 | 0/3/3/3 |
| 83  | Y5P  | r3    | 54  | 83   | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 22  | 83   | -       | 3/7/25/26 | 0/3/3/3 |
| 83  | P5P  | r3    | 65  | 83   | -       | 0/7/25/26 | 0/3/3/3 |
| 83  | Y5P  | r3    | 48  | 83   | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | Y5P  | r3    | 55  | 83   | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 6   | 83   | -       | 2/7/25/26 | 0/3/3/3 |
| 83  | Y5P  | r3    | 72  | 83   | -       | 3/7/33/34 | 0/2/2/2 |
| 83  | Y5P  | r3    | 68  | 83   | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | Y5P  | r3    | 67  | 83   | -       | 2/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 57  | 83   | -       | 0/7/25/26 | 0/3/3/3 |
| 83  | P5P  | r3    | 28  | 83   | -       | 2/7/25/26 | 0/3/3/3 |
| 83  | P5P  | r3    | 27  | 83   | -       | 3/7/25/26 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 83  | Y5P  | r3    | 43  | 83   | -       | 1/7/33/34  | 0/2/2/2 |
| 83  | P5P  | r3    | 70  | 83   | -       | 0/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 37  | 83   | -       | 2/10/26/26 | 0/3/3/3 |
| 83  | P5P  | r3    | 1   | 83   | -       | 0/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 34  | 83   | -       | 0/7/25/26  | 0/3/3/3 |
| 83  | Y5P  | r3    | 41  | 83   | -       | 3/7/33/34  | 0/2/2/2 |
| 83  | Y5P  | r3    | 2   | 83   | -       | 1/7/33/34  | 0/2/2/2 |
| 83  | P5P  | r3    | 21  | 83   | -       | 1/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 53  | 83   | -       | 0/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 58  | 83   | -       | 0/7/25/26  | 0/3/3/3 |
| 83  | Y5P  | r3    | 66  | 83   | -       | 3/7/33/34  | 0/2/2/2 |
| 83  | Y5P  | r3    | 51  | 83   | -       | 1/7/33/34  | 0/2/2/2 |
| 83  | P5P  | r3    | 73  | 83   | -       | 4/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 18  | 83   | -       | 1/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 9   | 83   | -       | 2/7/25/26  | 0/3/3/3 |
| 83  | Y5P  | r3    | 13  | 83   | -       | 3/7/33/34  | 0/2/2/2 |
| 83  | P5P  | r3    | 44  | 83   | -       | 0/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 15  | 83   | -       | 0/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 36  | 83   | -       | 0/7/25/26  | 0/3/3/3 |
| 83  | Y5P  | r3    | 45  | 83   | -       | 4/7/33/34  | 0/2/2/2 |
| 83  | P5P  | r3    | 69  | 83   | -       | 0/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 5   | 83   | -       | 0/7/25/26  | 0/3/3/3 |
| 83  | Y5P  | r3    | 20  | 83   | -       | 2/7/33/34  | 0/2/2/2 |
| 83  | Y5P  | r3    | 11  | 83   | -       | 1/7/33/34  | 0/2/2/2 |
| 83  | Y5P  | r3    | 75  | 83   | -       | 6/7/33/34  | 0/2/2/2 |
| 83  | Y5P  | r3    | 61  | 83   | -       | 1/7/33/34  | 0/2/2/2 |
| 83  | Y5P  | r3    | 3   | 83   | -       | 1/7/33/34  | 0/2/2/2 |
| 83  | P5P  | r3    | 64  | 83   | -       | 2/7/25/26  | 0/3/3/3 |
| 83  | Y5P  | r3    | 25  | 83   | -       | 3/7/33/34  | 0/2/2/2 |
| 83  | P5P  | r3    | 38  | 83   | -       | 1/7/25/26  | 0/3/3/3 |
| 83  | Y5P  | r3    | 39  | 83   | -       | 1/7/33/34  | 0/2/2/2 |
| 83  | P5P  | r3    | 46  | 83   | -       | 3/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 7   | 83   | -       | 1/7/25/26  | 0/3/3/3 |
| 83  | P5P  | r3    | 29  | 83   | -       | 4/7/25/26  | 0/3/3/3 |
| 83  | Y5P  | r3    | 17  | 83   | -       | 3/7/33/34  | 0/2/2/2 |
| 83  | Y5P  | r3    | 16  | 83   | -       | 1/7/33/34  | 0/2/2/2 |
| 83  | P5P  | r3    | 23  | 83   | -       | 5/7/25/26  | 0/3/3/3 |
| 83  | Y5P  | r3    | 32  | 83   | -       | 1/7/33/34  | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 83  | P5P  | r3    | 26  | 83    | -       | 2/7/25/26 | 0/3/3/3 |
| 83  | Y5P  | r3    | 50  | 83    | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | Y5P  | r3    | 42  | 83    | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | Y5P  | r3    | 8   | 83    | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 35  | 83    | -       | 0/7/25/26 | 0/3/3/3 |
| 83  | P5P  | r3    | 31  | 83    | -       | 2/7/25/26 | 0/3/3/3 |
| 83  | Y5P  | r3    | 47  | 83    | -       | 4/7/33/34 | 0/2/2/2 |
| 83  | Y5P  | r3    | 33  | 83    | -       | 2/7/33/34 | 0/2/2/2 |
| 83  | Y5P  | r3    | 56  | 83    | -       | 3/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 52  | 83    | -       | 3/7/25/26 | 0/3/3/3 |
| 83  | Y5P  | r3    | 62  | 83    | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | Y5P  | r3    | 40  | 83    | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 63  | 83    | -       | 0/7/25/26 | 0/3/3/3 |
| 83  | P5P  | r3    | 71  | 83    | -       | 0/7/25/26 | 0/3/3/3 |
| 83  | Y5P  | r3    | 12  | 83    | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 19  | 83    | -       | 0/7/25/26 | 0/3/3/3 |
| 83  | Y5P  | r3    | 60  | 83    | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 74  | 11,83 | -       | 3/7/25/26 | 0/3/3/3 |
| 83  | Y5P  | r3    | 59  | 83    | -       | 1/7/33/34 | 0/2/2/2 |
| 83  | P5P  | r3    | 30  | 83    | -       | 1/7/25/26 | 0/3/3/3 |

The worst 5 of 225 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 83  | r3    | 62  | Y5P  | C2-N3 | 26.89 | 1.48        | 1.27     |
| 83  | r3    | 16  | Y5P  | C2-N3 | 26.88 | 1.48        | 1.27     |
| 83  | r3    | 17  | Y5P  | C2-N3 | 26.87 | 1.48        | 1.27     |
| 83  | r3    | 55  | Y5P  | C2-N3 | 26.86 | 1.48        | 1.27     |
| 83  | r3    | 59  | Y5P  | C2-N3 | 26.83 | 1.48        | 1.27     |

The worst 5 of 433 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 83  | r3    | 37  | P5P  | OP2-P-O5' | -10.44 | 79.46       | 106.67   |
| 83  | r3    | 37  | P5P  | O5'-P-OP1 | -9.71  | 80.20       | 106.44   |
| 83  | r3    | 37  | P5P  | OP2-P-OP1 | 8.11   | 142.42      | 110.83   |
| 83  | r3    | 37  | P5P  | OP3-P-O5' | 7.22   | 125.48      | 106.67   |
| 83  | r3    | 37  | P5P  | OP3-P-OP1 | -6.97  | 83.67       | 110.83   |

There are no chirality outliers.

5 of 115 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 83  | r3    | 9   | P5P  | O4'-C4'-C5'-O5' |
| 83  | r3    | 13  | Y5P  | C3'-C4'-C5'-O5' |
| 83  | r3    | 13  | Y5P  | O4'-C1'-N1-C2   |
| 83  | r3    | 16  | Y5P  | O4'-C1'-N1-C2   |
| 83  | r3    | 20  | Y5P  | O4'-C1'-N1-C2   |

There are no ring outliers.

26 monomers are involved in 24 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 83  | r3    | 49  | Y5P  | 1       | 0            |
| 83  | r3    | 55  | Y5P  | 1       | 0            |
| 83  | r3    | 68  | Y5P  | 1       | 0            |
| 83  | r3    | 67  | Y5P  | 2       | 0            |
| 83  | r3    | 37  | P5P  | 1       | 0            |
| 83  | r3    | 1   | P5P  | 1       | 0            |
| 83  | r3    | 41  | Y5P  | 2       | 0            |
| 83  | r3    | 66  | Y5P  | 2       | 0            |
| 83  | r3    | 51  | Y5P  | 1       | 0            |
| 83  | r3    | 75  | Y5P  | 2       | 0            |
| 83  | r3    | 3   | Y5P  | 1       | 0            |
| 83  | r3    | 38  | P5P  | 1       | 0            |
| 83  | r3    | 16  | Y5P  | 1       | 0            |
| 83  | r3    | 23  | P5P  | 1       | 0            |
| 83  | r3    | 8   | Y5P  | 1       | 0            |
| 83  | r3    | 31  | P5P  | 2       | 0            |
| 83  | r3    | 47  | Y5P  | 1       | 0            |
| 83  | r3    | 33  | Y5P  | 1       | 0            |
| 83  | r3    | 52  | P5P  | 1       | 0            |
| 83  | r3    | 62  | Y5P  | 1       | 0            |
| 83  | r3    | 40  | Y5P  | 2       | 0            |
| 83  | r3    | 71  | P5P  | 1       | 0            |
| 83  | r3    | 12  | Y5P  | 1       | 0            |
| 83  | r3    | 74  | P5P  | 2       | 0            |
| 83  | r3    | 59  | Y5P  | 1       | 0            |
| 83  | r3    | 30  | P5P  | 2       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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  | DOL  | XA    | 5145 | -    | 47,50,50     | 3.90 | 19 (40%) | 57,70,70    | 3.04 | 13 (22%) |
| 90  | GTP  | AX    | 500  | -    | 33,34,34     | 0.94 | 1 (3%)   | 50,54,54    | 1.56 | 8 (16%)  |
| 88  | H8Q  | XA    | 5144 | -    | 78,80,80     | 1.12 | 5 (6%)   | 102,115,115 | 1.40 | 15 (14%) |

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  | DOL  | XA    | 5145 | -    | -       | 19/64/77/77   | 0/2/3/3 |
| 90  | GTP  | AX    | 500  | -    | -       | 7/22/38/38    | 0/3/3/3 |
| 88  | H8Q  | XA    | 5144 | -    | -       | 31/83/127/127 | 0/8/8/8 |

The worst 5 of 25 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 89  | XA    | 5145 | DOL  | C28-C29 | 10.58 | 1.56        | 1.32     |
| 89  | XA    | 5145 | DOL  | C6-N5   | 10.34 | 1.49        | 1.34     |
| 89  | XA    | 5145 | DOL  | C22-C23 | 9.01  | 1.57        | 1.32     |
| 89  | XA    | 5145 | DOL  | C10-N9  | 8.73  | 1.38        | 1.29     |
| 89  | XA    | 5145 | DOL  | C19-C20 | 8.50  | 1.57        | 1.34     |

The worst 5 of 36 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 89  | XA    | 5145 | DOL  | O40-S39-O41 | -15.17 | 100.93      | 118.13   |
| 89  | XA    | 5145 | DOL  | O11-C10-C13 | 9.90   | 126.84      | 117.70   |
| 89  | XA    | 5145 | DOL  | C24-N25-C26 | -5.53  | 113.21      | 122.17   |
| 89  | XA    | 5145 | DOL  | O11-C10-N9  | -5.22  | 108.44      | 114.09   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 90  | AX    | 500 | GTP  | C5-C4-N3 | -5.11 | 120.26      | 128.39   |

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 88  | XA    | 5144 | H8Q  | C2-C1-N13-C14   |
| 88  | XA    | 5144 | H8Q  | C2-C1-N13-C18   |
| 88  | XA    | 5144 | H8Q  | O1-C1-N13-C14   |
| 88  | XA    | 5144 | H8Q  | O1-C1-N13-C18   |
| 88  | XA    | 5144 | H8Q  | C33-C34-O41-C43 |

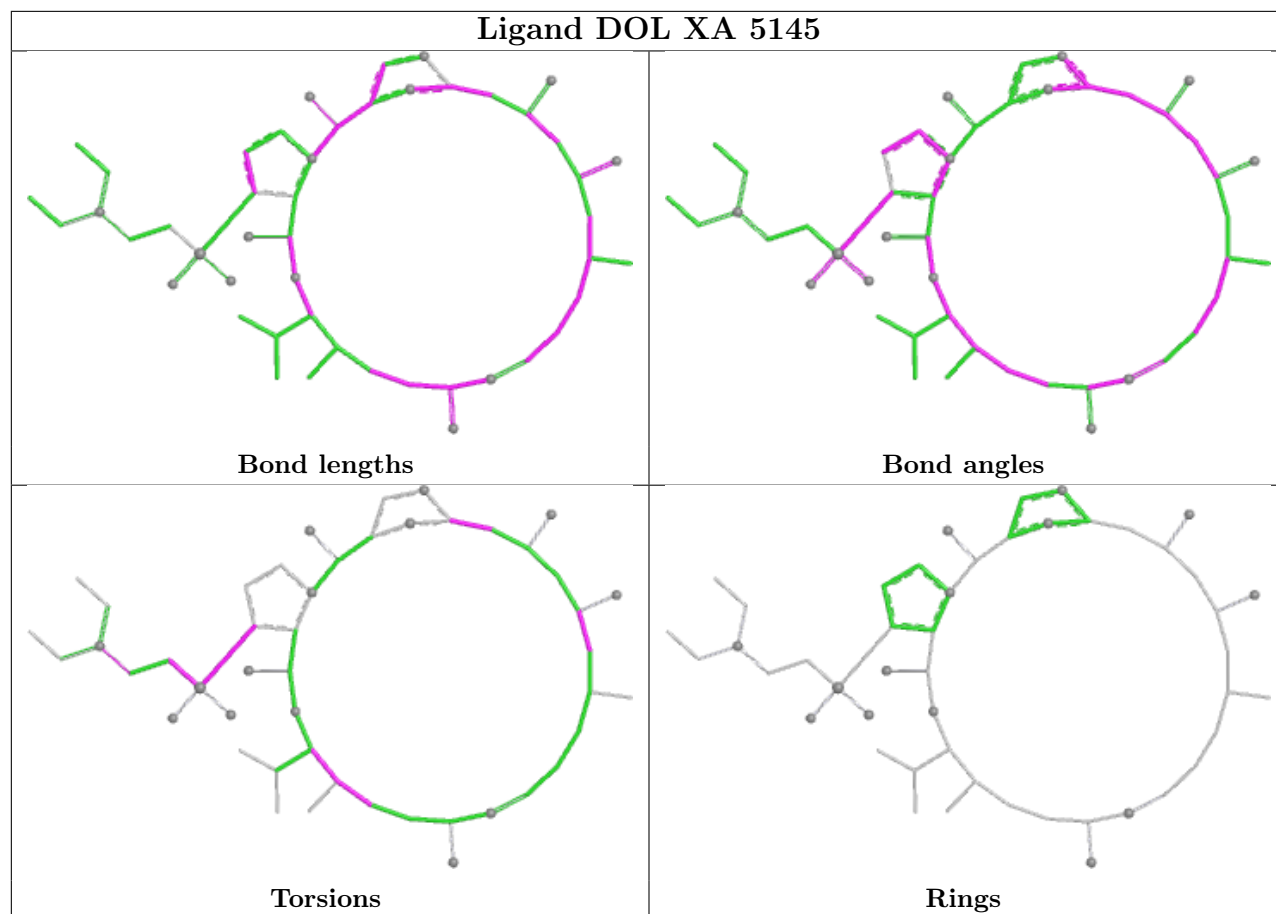
There are no ring outliers.

2 monomers are involved in 3 short contacts:

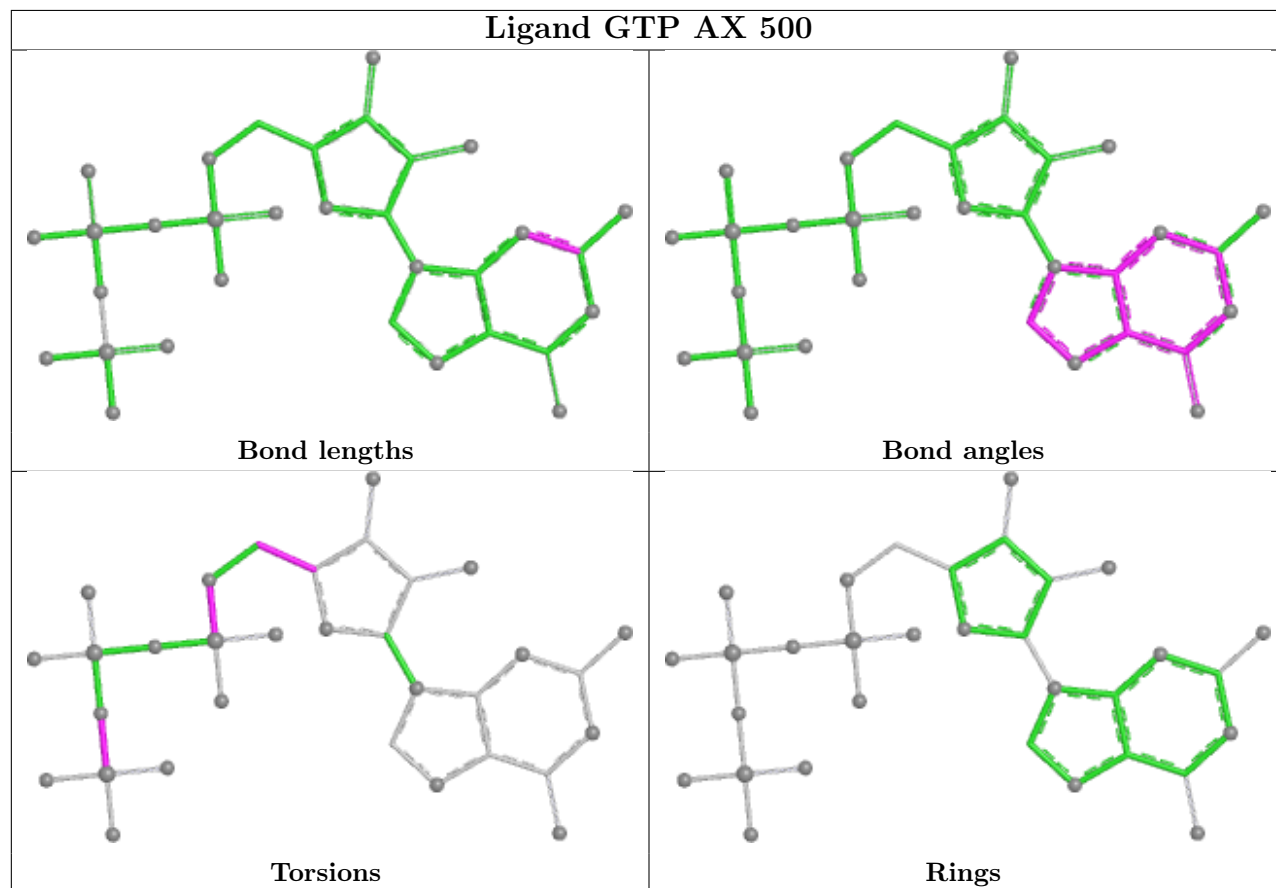
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 90  | AX    | 500  | GTP  | 1       | 0            |
| 88  | XA    | 5144 | H8Q  | 2       | 0            |

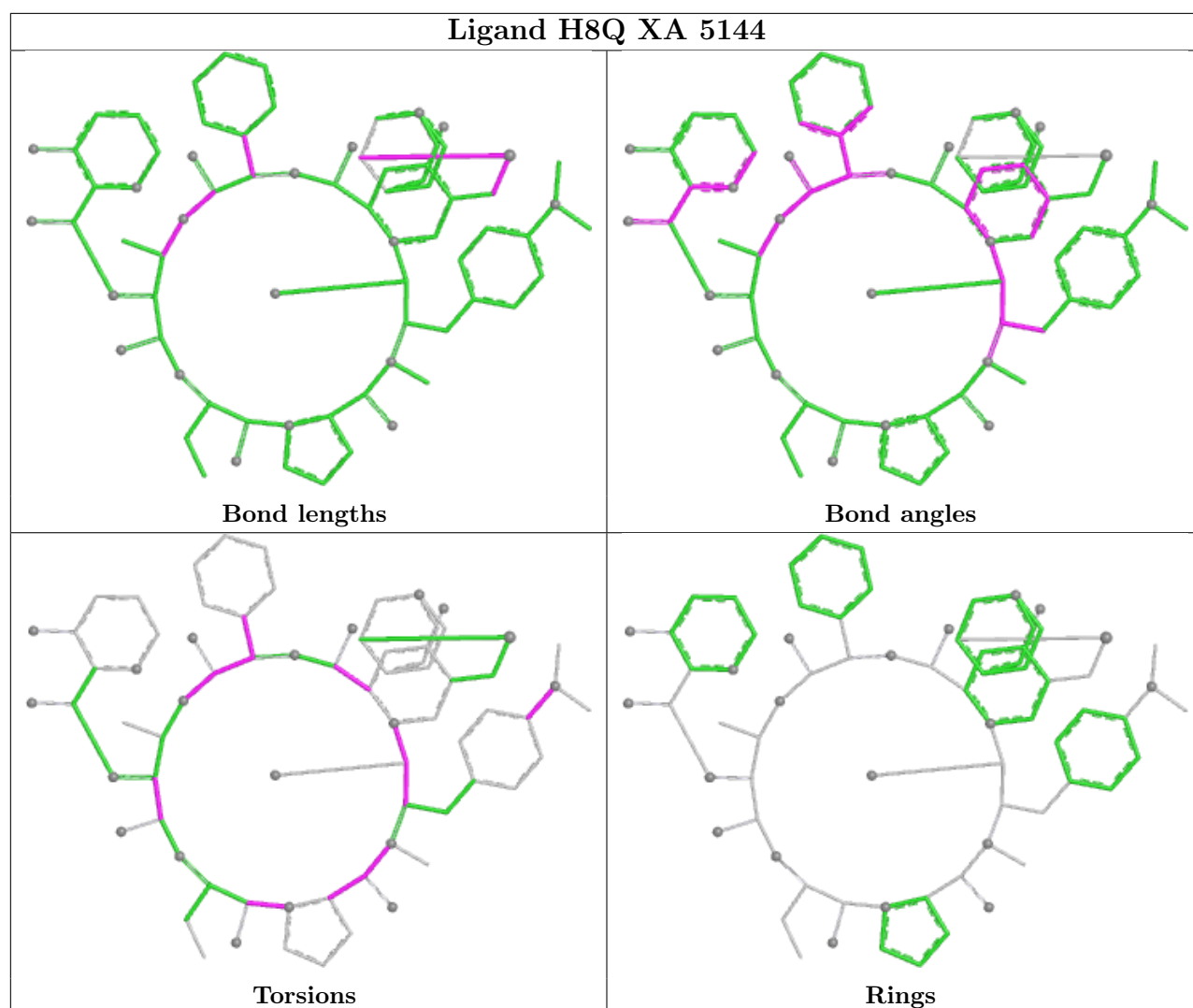
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 DOL XA 5145



## Ligand GTP AX 500





## 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                |
| 7   | 6     | 2                |
| 82  | r     | 1                |
| 38  | AV    | 1                |
| 6   | 5     | 1                |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 34  | AR    | 1                |

The worst 5 of 10 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      | 5.98         |
| 1     | r     | 134:ARG   | C      | 135:LEU   | N      | 5.26         |
| 1     | AV    | 269:SER   | C      | 270:PRO   | N      | 4.49         |
| 1     | 7     | 185:LEU   | C      | 186:ASP   | N      | 3.31         |

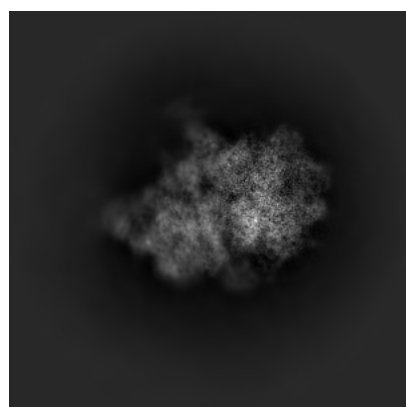
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12877. These allow visual inspection of the internal detail of the map and identification of artifacts.

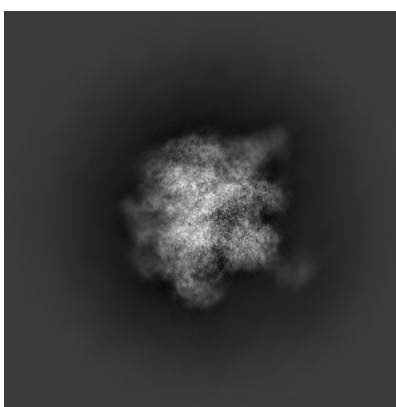
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

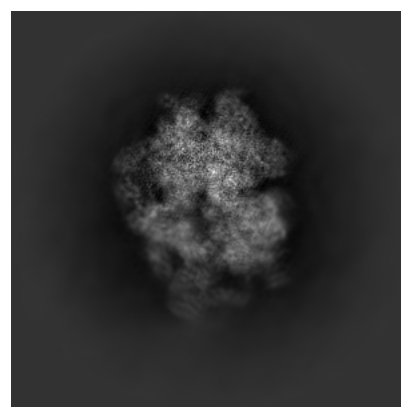
#### 6.1.1 Primary map



X



Y

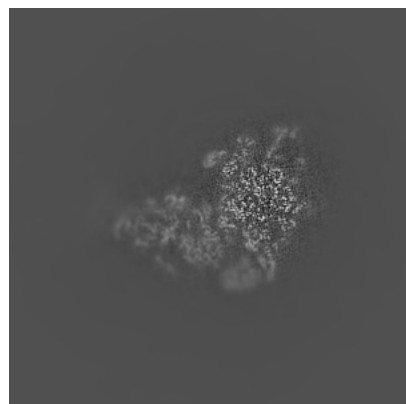


Z

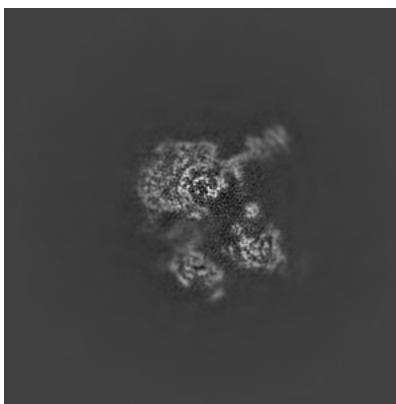
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

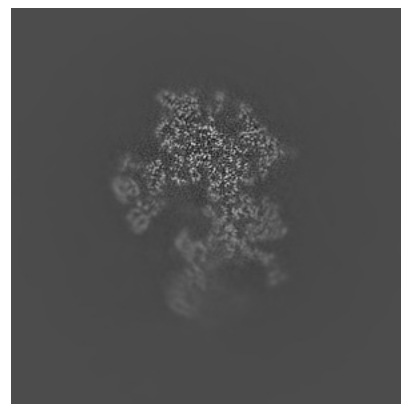
#### 6.2.1 Primary map



X Index: 260



Y Index: 260

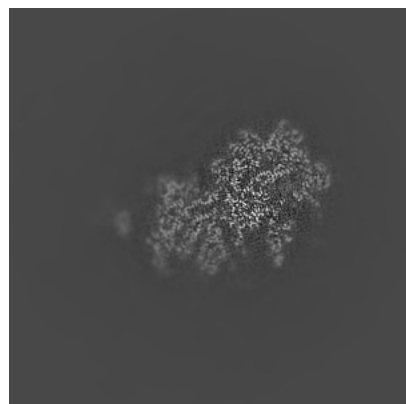


Z Index: 260

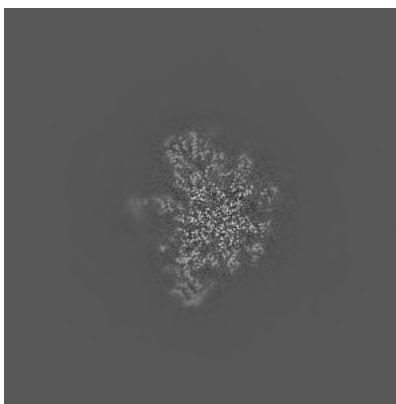
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

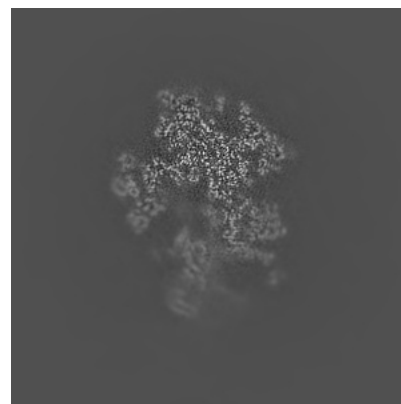
### 6.3.1 Primary map



X Index: 282



Y Index: 321

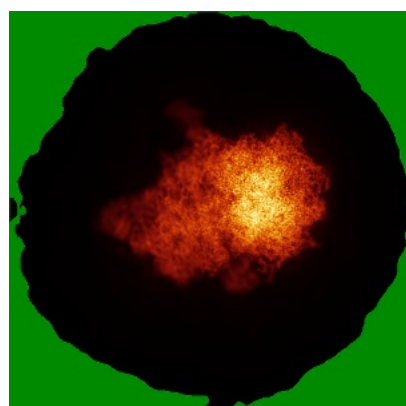


Z Index: 257

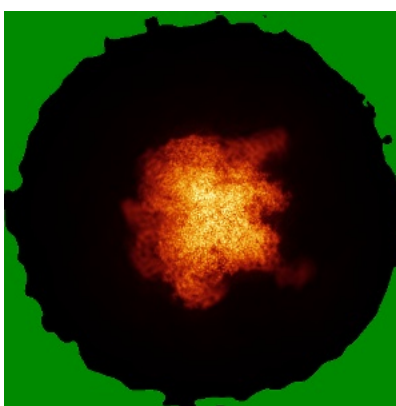
The images above show the largest variance slices of the map in three orthogonal directions.

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

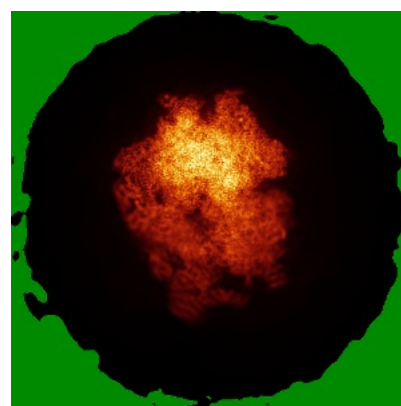
### 6.4.1 Primary map



X



Y

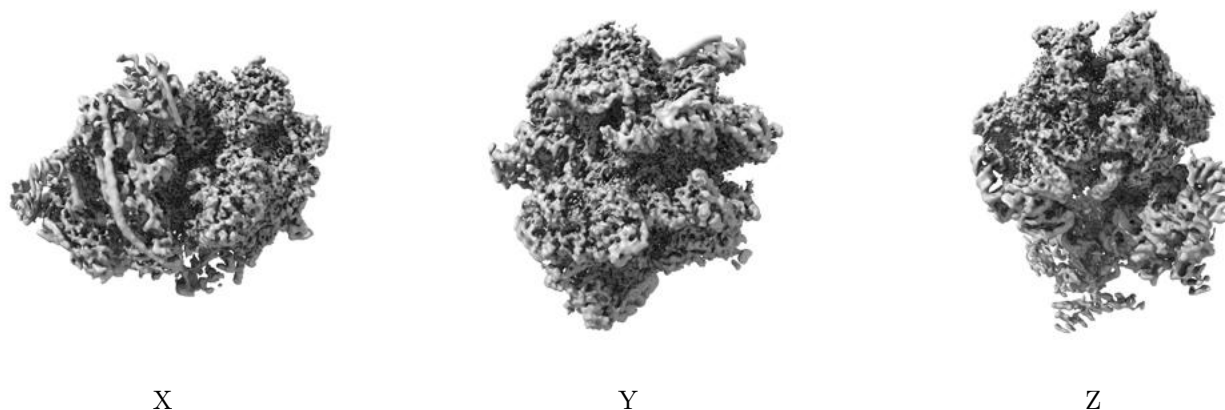


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

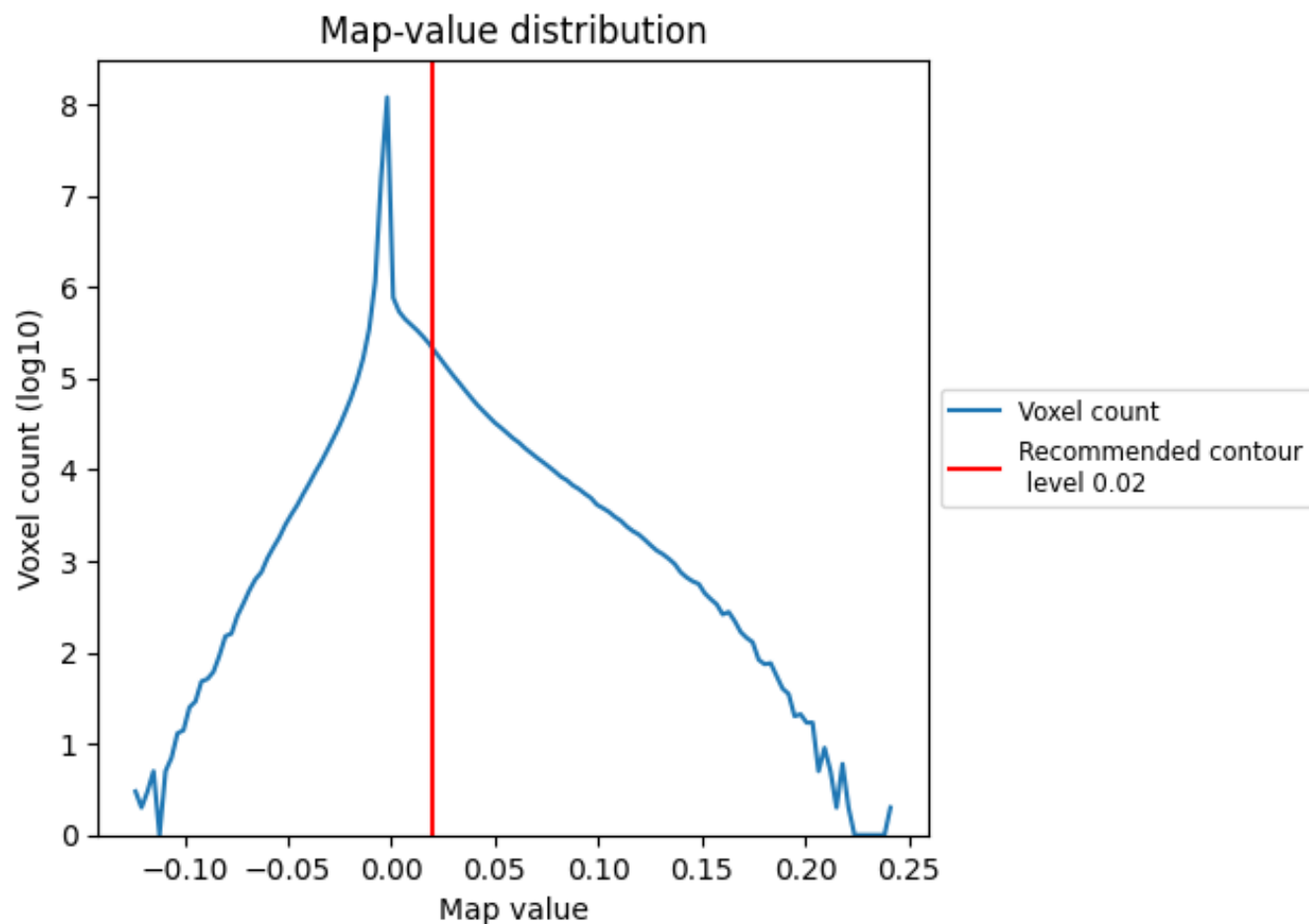
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

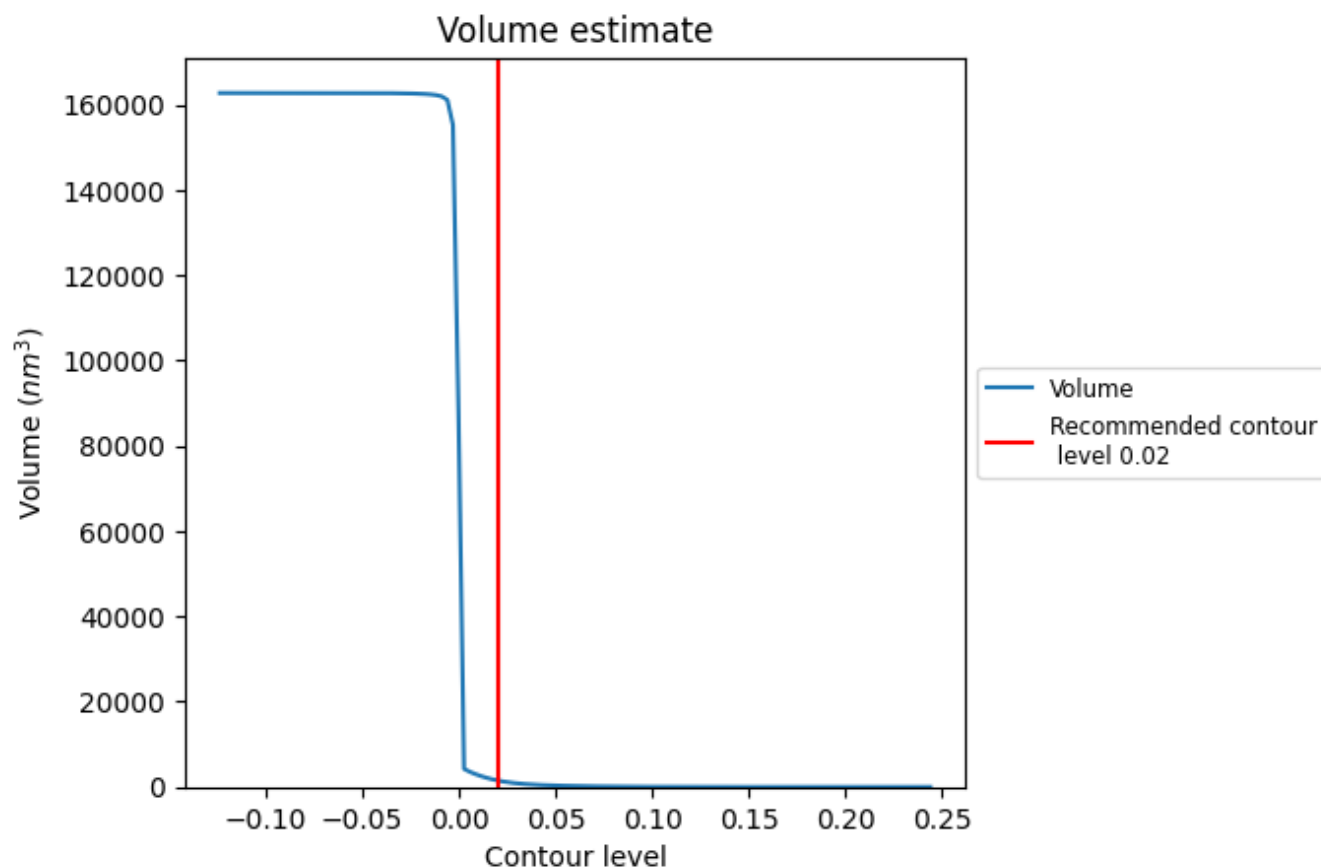
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

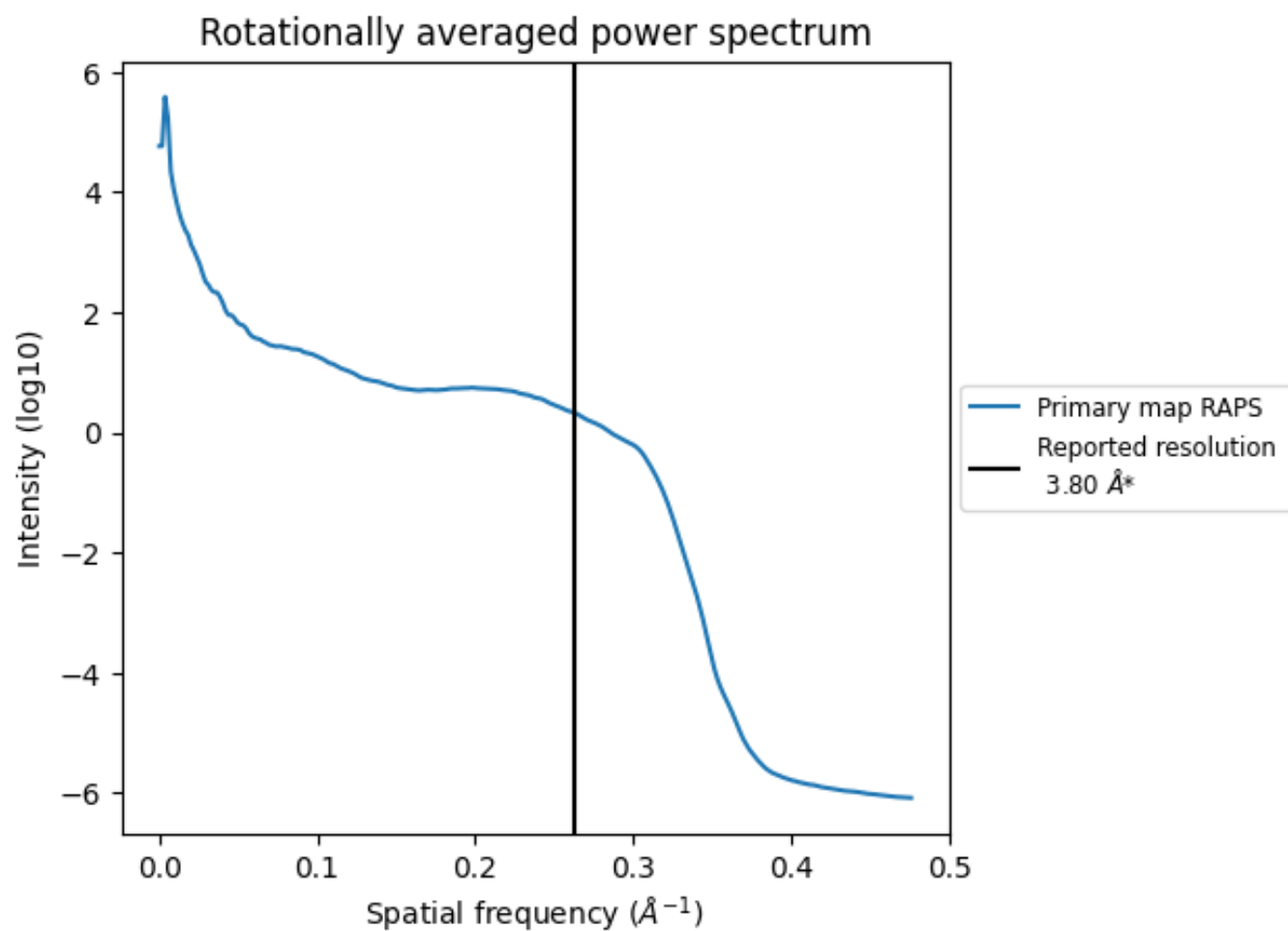
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1527  $\text{nm}^3$ ; this corresponds to an approximate mass of 1379 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

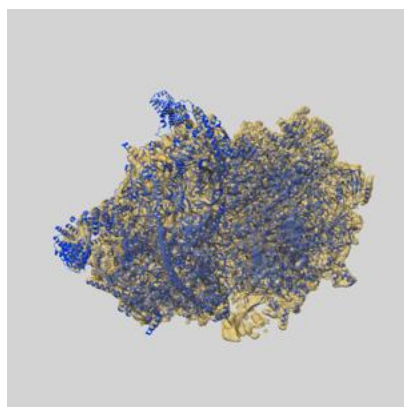
This section was not generated. No FSC curve or half-maps provided.



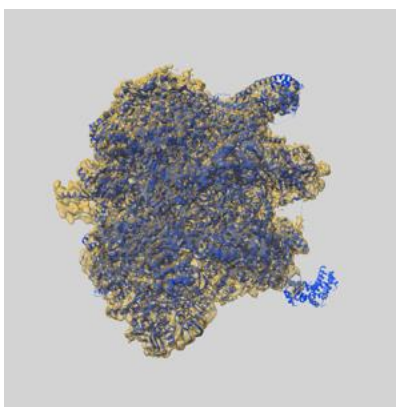
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12877 and PDB model 7OG4. Per-residue inclusion information can be found in section 3 on page 23.

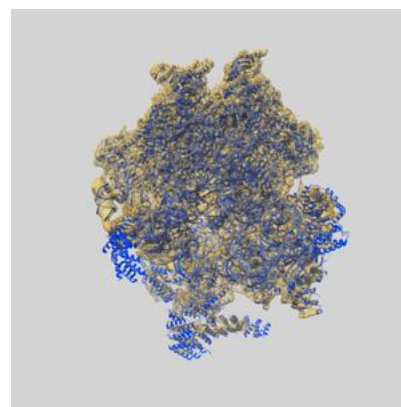
### 9.1 Map-model overlay [i](#)



X



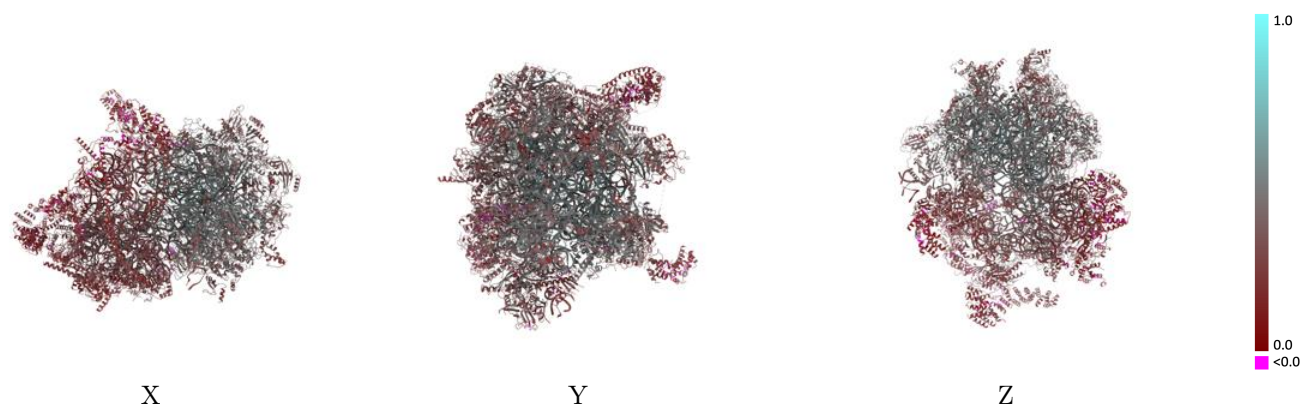
Y



Z

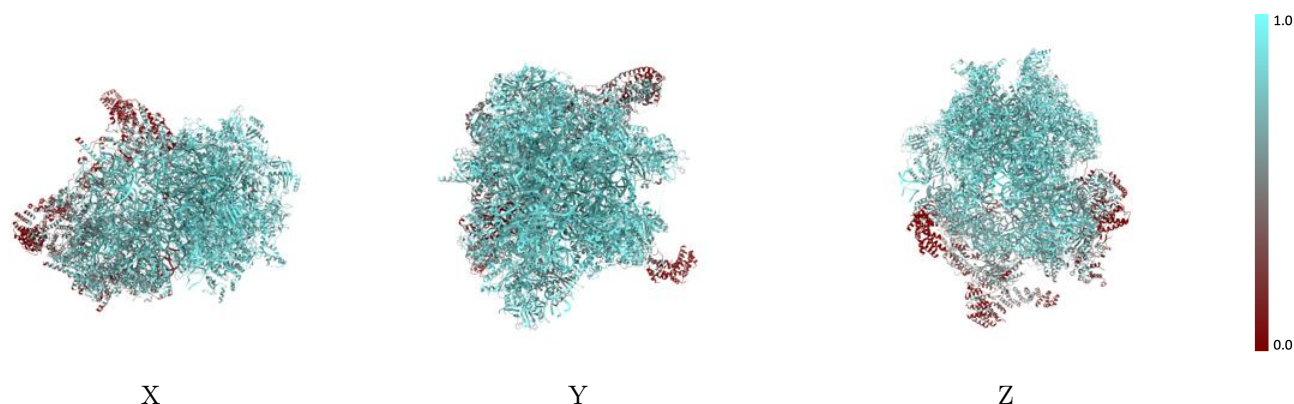
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



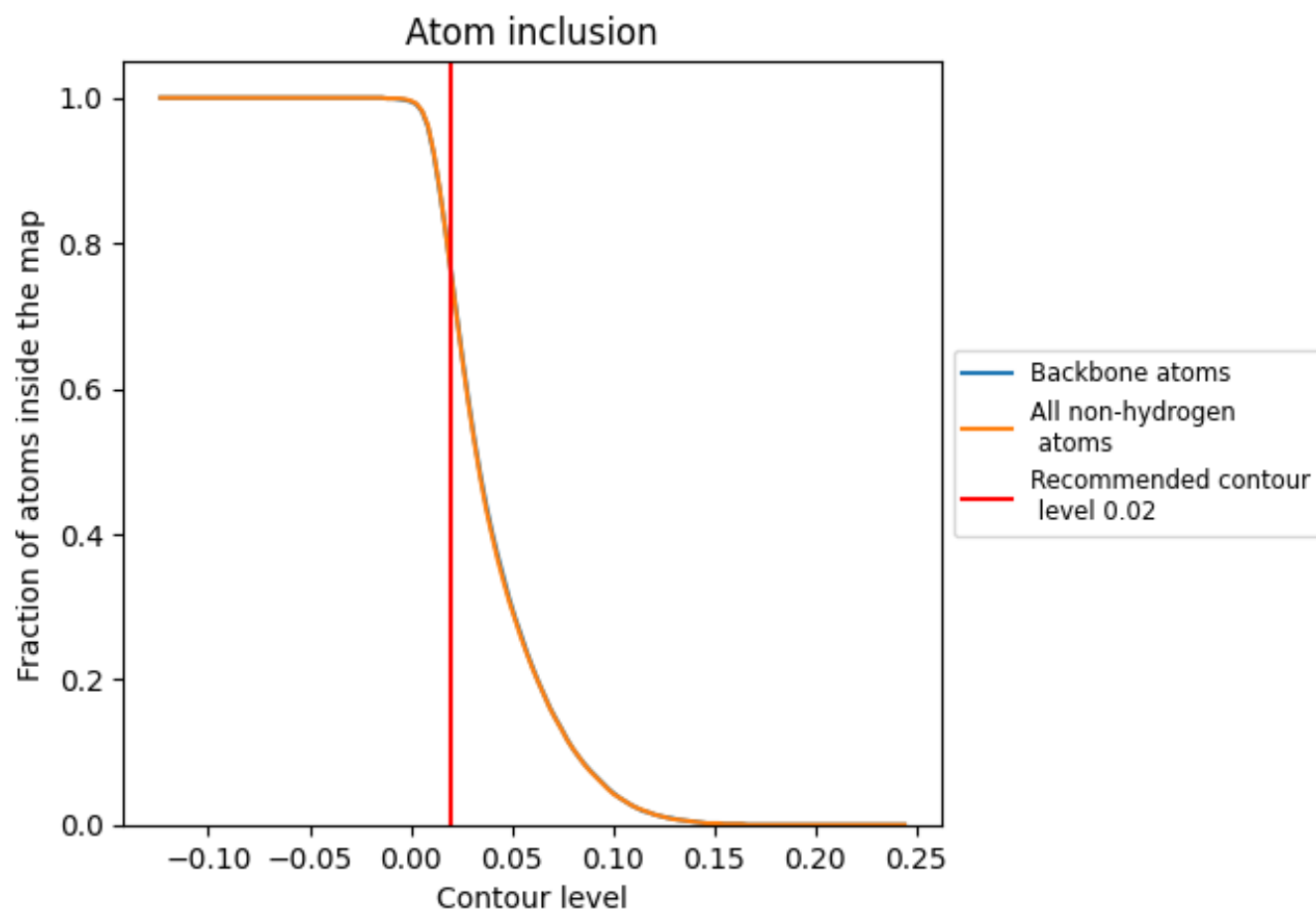
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

## 9.4 Atom inclusion [i](#)



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

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7570   |  0.3480   |
| 0     |  0.8310   |  0.4140   |
| 1     |  0.8520   |  0.4090   |
| 2     |  0.9110   |  0.5090   |
| 3     |  0.9000   |  0.5010   |
| 4     |  0.9230   |  0.4730   |
| 5     |  0.8510   |  0.4010   |
| 6     |  0.8100   |  0.3530   |
| 7     |  0.8160   |  0.3660   |
| 8     |  0.6130   |  0.2280   |
| 9     |  0.8210   |  0.3930   |
| A0    |  0.4230   |  0.1660   |
| A1    |  0.4360   |  0.1900   |
| A2    |  0.6190   |  0.2530   |
| A3    |  0.7610  |  0.3660  |
| A4    |  0.2550 |  0.1590 |
| AA    |  0.9010 |  0.3120 |
| AB    |  0.7040 |  0.2630 |
| AC    |  0.5440 |  0.2180 |
| AD    |  0.5760 |  0.2700 |
| AE    |  0.6670 |  0.3280 |
| AF    |  0.5720 |  0.2160 |
| AG    |  0.5560 |  0.2180 |
| AH    |  0.4310 |  0.1890 |
| AI    |  0.6470 |  0.2900 |
| AJ    |  0.7070 |  0.2690 |
| AK    |  0.4610 |  0.1940 |
| AL    |  0.6610 |  0.2720 |
| AM    |  0.5650 |  0.1930 |
| AN    |  0.6070 |  0.2600 |
| AO    |  0.5460 |  0.2210 |
| AP    |  0.6940 |  0.3120 |
| AQ    |  0.6960 |  0.3220 |
| AR    |  0.4620 |  0.1700 |
| AS    |  0.5840 |  0.2390 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| AT    |  0.6490   |  0.2540   |
| AU    |  0.6340   |  0.2070   |
| AV    |  0.3560   |  0.1550   |
| AW    |  0.5900   |  0.2570   |
| AX    |  0.3540   |  0.1600   |
| AY    |  0.2540   |  0.1750   |
| AZ    |  0.5460   |  0.1760   |
| XA    |  0.9600   |  0.4830   |
| XB    |  0.9550   |  0.3170   |
| XD    |  0.8790   |  0.4480   |
| XE    |  0.8620   |  0.4440   |
| XF    |  0.8870   |  0.4530   |
| XH    |  0.8090   |  0.3640   |
| XI    |  0.6040   |  0.2720   |
| XJ    |  0.6600   |  0.2230   |
| XK    |  0.8740   |  0.4570   |
| XL    |  0.8820   |  0.4540   |
| XM    |  0.8590   |  0.4430   |
| XN    |  0.8530   |  0.4370   |
| XO    |  0.8670  |  0.4240  |
| XP    |  0.8360 |  0.3850 |
| XQ    |  0.7730 |  0.3860 |
| XR    |  0.8740 |  0.4730 |
| XS    |  0.8680 |  0.4600 |
| XT    |  0.8890 |  0.4680 |
| XU    |  0.8780 |  0.4400 |
| XV    |  0.8090 |  0.3720 |
| XW    |  0.9010 |  0.4750 |
| XX    |  0.8210 |  0.3930 |
| XY    |  0.8680 |  0.4270 |
| XZ    |  0.8880 |  0.4660 |
| a     |  0.8280 |  0.4140 |
| b     |  0.8870 |  0.4540 |
| c     |  0.8410 |  0.3890 |
| d     |  0.7830 |  0.3510 |
| e     |  0.6590 |  0.1920 |
| f     |  0.6870 |  0.2630 |
| g     |  0.8650 |  0.4310 |
| h     |  0.7990 |  0.3490 |
| i     |  0.8890 |  0.4810 |
| j     |  0.8380 |  0.4150 |
| k     |  0.7840 |  0.3040 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| l     |  0.7130 |  0.2600 |
| m     |  0.6960 |  0.2260 |
| o     |  0.9020 |  0.4730 |
| p     |  0.8170 |  0.3490 |
| q     |  0.6530 |  0.3050 |
| r     |  0.8810 |  0.4210 |
| r3    |  0.0760 |  0.0780 |
| s     |  0.8620 |  0.4190 |
| t1    |  0.2180 |  0.1990 |
| t2    |  0.1810 |  0.1860 |
| t3    |  0.0000 |  0.1740 |
| t4    |  0.0000 |  0.1200 |
| t5    |  0.0000 |  0.1370 |
| t6    |  0.0000 |  0.1020 |