



## wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 11:23 PM EDT

PDB ID : 9PSM / pdb\_00009psm  
EMDB ID : EMD-71829  
Title : In situ structure of the human mitoribosome in the A/P-P/E state  
Authors : Shuhui, W.; Yong, X.  
Deposited on : 2025-07-25  
Resolution : 2.98 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:

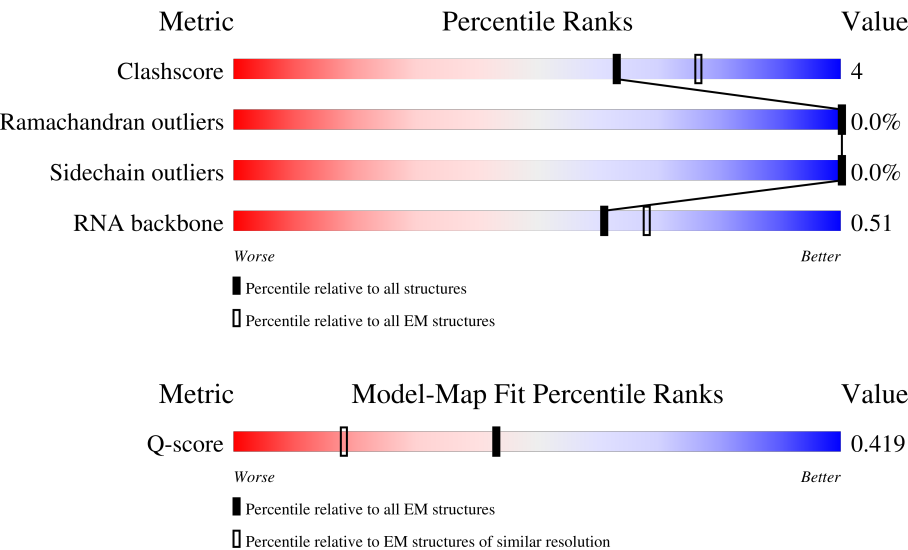
EMDB validation analysis : 0.0.1.dev133  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.50

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.98 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.



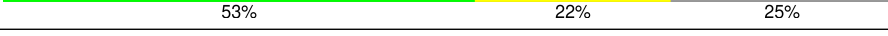
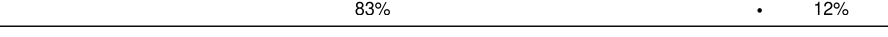
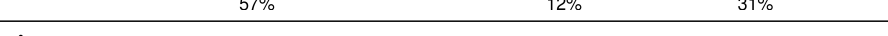
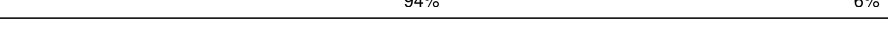
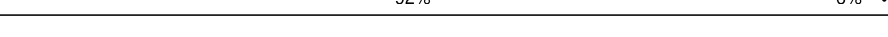
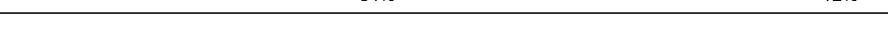
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 13236 ( 2.48 - 3.48 )                                    |

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    | <div><div></div><div>57%</div><div>41%</div></div>               |
| 2   | 1     | 65     | <div><div></div><div>71%</div><div>15%</div><div>14%</div></div> |
| 3   | 2     | 92     | <div><div></div><div>49%</div><div>50%</div></div>               |

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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  | A     | 1558   |    |
| 12  | C     | 297    |    |
| 13  | D     | 305    |    |
| 14  | E     | 348    |    |
| 15  | F     | 311    |   |
| 16  | H     | 267    |  |
| 17  | I     | 261    |  |
| 18  | J     | 192    |  |
| 19  | K     | 178    |  |
| 20  | L     | 145    |  |
| 21  | M     | 296    |  |
| 22  | N     | 251    |  |
| 23  | O     | 175    |  |
| 24  | P     | 180    |  |
| 25  | Q     | 292    |  |
| 26  | R     | 149    |  |
| 27  | S     | 205    |  |
| 28  | T     | 206    |  |

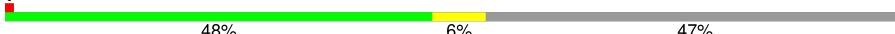
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | U     | 153    |                  |
| 30  | W     | 148    |                  |
| 31  | X     | 256    |                  |
| 32  | Y     | 250    |                  |
| 33  | Z     | 161    |                  |
| 34  | z     | 325    |                  |
| 35  | G     | 198    |                  |
| 35  | t     | 198    |                  |
| 35  | u     | 198    |                  |
| 36  | V     | 216    |                  |
| 37  | b     | 215    |                  |
| 38  | d     | 306    |                  |
| 39  | e     | 279    |                  |
| 40  | g     | 166    |                  |
| 41  | h     | 158    |                  |
| 42  | i     | 128    |                  |
| 43  | j     | 123    |                  |
| 44  | k     | 112    |                  |
| 45  | l     | 138    |                  |
| 46  | m     | 128    |                  |
| 47  | n     | 43     |                  |
| 48  | o     | 102    |                  |
| 49  | q     | 222    |                  |
| 50  | r     | 196    |                  |
| 51  | AB    | 296    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 52  | AC    | 167    |    |
| 53  | AD    | 430    |    |
| 54  | AE    | 125    |    |
| 55  | AF    | 242    |    |
| 56  | AG    | 396    |    |
| 57  | AH    | 201    |    |
| 58  | AJ    | 138    |    |
| 59  | AK    | 128    |    |
| 60  | AL    | 257    |    |
| 61  | AM    | 137    |    |
| 62  | AN    | 130    |    |
| 63  | AO    | 258    |   |
| 64  | AP    | 142    |  |
| 65  | AR    | 360    |  |
| 66  | AS    | 190    |  |
| 67  | AT    | 173    |  |
| 68  | AU    | 205    |  |
| 69  | AV    | 414    |  |
| 70  | AW    | 187    |  |
| 71  | AZ    | 106    |  |
| 72  | A0    | 217    |  |
| 73  | A1    | 323    |  |
| 74  | A3    | 199    |  |
| 75  | Az    | 34     |  |
| 76  | AY    | 395    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 77  | AA    | 954    |    |
| 78  | AI    | 194    |    |
| 79  | A4    | 689    |    |
| 80  | AX    | 398    |    |
| 81  | A2    | 118    |    |
| 82  | AQ    | 87     |    |
| 83  | c     | 332    |    |
| 84  | f     | 212    |    |
| 85  | p     | 206    |    |
| 86  | s     | 439    |    |
| 87  | OX    | 435    |    |
| 88  | a     | 142    |    |
| 89  | Aw    | 76     |  |
| 90  | Ax    | 76     |  |
| 91  | B     | 72     |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 102 | VAL  | B     | 101 | -         | -        | X       | -                |

## 2 Entry composition

There are 102 unique types of molecules in this entry. The entry contains 181859 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 0     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 898   | 554 | 176 | 162 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 464   | 296 | 89 | 77 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | 2     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 233 | 83 | 60 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | 3     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 539 | 162 | 128 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 4     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 342   | 217 | 72 | 49 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | 5     | 394      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3210  | 2073 | 560 | 566 | 11 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | 6     | 354      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2948  | 1881 | 525 | 533 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | 7     | 294      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2390  | 1529 | 405 | 438 | 18 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | 8     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1327  | 844 | 235 | 246 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | 9     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 997   | 644 | 170 | 181 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 11  | A     | 1558     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33070 | 14843 | 5963 | 10706 | 1558 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| A     | ?       | -        | A      | deletion | GB 2756414513 |
| A     | ?       | -        | C      | deletion | GB 2756414513 |
| A     | ?       | -        | U      | deletion | GB 2756414513 |

- Molecule 12 is a protein called Translational activator of cytochrome c oxidase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | C     | 223      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1732  | 1072 | 310 | 340 | 10 |         |       |

- Molecule 13 is a protein called 39S ribosomal protein L2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | D     | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1859  | 1157 | 376 | 317 | 9 |         |       |

- Molecule 14 is a protein called 39S ribosomal protein L3, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | E     | 305      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2406  | 1545 | 418 | 432 | 11 |         |       |

- Molecule 15 is a protein called 39S ribosomal protein L4, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | F     | 252      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2031  | 1305 | 370 | 350 | 6 |         |       |

- Molecule 16 is a protein called 39S ribosomal protein L9, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | H     | 202      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1661  | 1067 | 304 | 286 | 4 |         |       |

- Molecule 17 is a protein called 39S ribosomal protein L10, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 17  | I     | 181      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1446  | 932 | 260 | 244 | 10 |         |       |

- Molecule 18 is a protein called 39S ribosomal protein L11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | J     | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1330  | 847 | 237 | 244 | 2 |         |       |

- Molecule 19 is a protein called Large ribosomal subunit protein uL13m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | K     | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1455  | 936 | 259 | 253 | 7 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| K     | 1       | ACE      | -      | acetylation | UNP H2QWN0 |
| K     | 132     | TYR      | ASP    | conflict    | UNP H2QWN0 |

- Molecule 20 is a protein called 39S ribosomal protein L14, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | L     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 890   | 559 | 171 | 155 | 5 |         |       |

- Molecule 21 is a protein called 39S ribosomal protein L15, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | M     | 291      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2327  | 1483 | 430 | 408 | 6 |         |       |

- Molecule 22 is a protein called 39S ribosomal protein L16, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | N     | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1786  | 1143 | 326 | 307 | 10 |         |       |

- Molecule 23 is a protein called 39S ribosomal protein L17, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | O     | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1259  | 792 | 241 | 219 | 7 |         |       |

- Molecule 24 is a protein called 39S ribosomal protein L18, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | P     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1173  | 733 | 224 | 211 | 5 |         |       |

- Molecule 25 is a protein called 39S ribosomal protein L19, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 25  | Q     | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1878  | 1202 | 332 | 335 | 9 |         |       |

- Molecule 26 is a protein called 39S ribosomal protein L20, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | R     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1154  | 732 | 231 | 187 | 4 |         |       |

- Molecule 27 is a protein called 39S ribosomal protein L21, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | S     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1293  | 835 | 227 | 227 | 4 |         |       |

- Molecule 28 is a protein called 39S ribosomal protein L22, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | T     | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1369  | 875 | 254 | 233 | 7 |         |       |

- Molecule 29 is a protein called 39S ribosomal protein L23, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | U     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1248  | 786 | 234 | 225 | 3 |         |       |

- Molecule 30 is a protein called 39S ribosomal protein L27, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | W     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 904   | 577 | 171 | 153 | 3 |         |       |

- Molecule 31 is a protein called 39S ribosomal protein L28, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31  | X     | 244      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2044  | 1322 | 352 | 365 | 5 |         |       |

- Molecule 32 is a protein called 39S ribosomal protein L47, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | Y     | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1556  | 995 | 298 | 259 | 4 |         |       |

- Molecule 33 is a protein called 39S ribosomal protein L30, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | Z     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 996   | 636 | 186 | 171 | 3 |         |       |

- Molecule 34 is a protein called Large ribosomal subunit protein uL1m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | z     | 252      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2027  | 1304 | 336 | 381 | 6 |         |       |

- Molecule 35 is a protein called 39S ribosomal protein L12, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|--|---------|-------|
| 35  | G     | 72       | Total | C   | N  | O   |  | 0       | 0     |
|     |       |          | 558   | 358 | 97 | 103 |  |         |       |
| 35  | t     | 46       | Total | C   | N  | O   |  | 0       | 0     |
|     |       |          | 354   | 228 | 56 | 70  |  |         |       |
| 35  | u     | 32       | Total | C   | N  | O   |  | 0       | 0     |
|     |       |          | 257   | 168 | 40 | 49  |  |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | V     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1676  | 1068 | 298 | 302 | 8 |         |       |

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | b     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1193  | 742 | 231 | 217 | 3 |         |       |

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 38  | d     | 259      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2124  | 1357 | 369 | 384 | 14 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | e     | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1222 | 339 | 364 | 6 |         |       |

- Molecule 40 is a protein called 39S ribosomal protein L49, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | g     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1113  | 719 | 193 | 199 | 2 |         |       |

- Molecule 41 is a protein called 39S ribosomal protein L50, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | h     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 895   | 568 | 156 | 168 | 3 |         |       |

- Molecule 42 is a protein called 39S ribosomal protein L51, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | i     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 828   | 532 | 165 | 127 | 4 |         |       |

- Molecule 43 is a protein called 39S ribosomal protein L52, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | j     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 745   | 463 | 144 | 136 | 2 |         |       |

- Molecule 44 is a protein called Large ribosomal subunit protein mL53.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | k     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 774   | 479 | 148 | 142 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| k     | 1       | ACE      | -      | acetylation | UNP Q96EL3 |

- Molecule 45 is a protein called 39S ribosomal protein L54, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | l     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 688   | 437 | 120 | 128 | 3 |         |       |

- Molecule 46 is a protein called 39S ribosomal protein L55, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 46  | m     | 68       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 567   | 349 | 117 | 99 | 2 |         |       |

- Molecule 47 is a protein called Nascent polypeptide.

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 47  | n     | 43       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 215   | 129 | 43 | 43 |  |         |       |

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | o     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 798   | 501 | 165 | 129 | 3 |         |       |

- Molecule 49 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | q     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 929 | 292 | 269 | 5 |         |       |

- Molecule 50 is a protein called 39S ribosomal protein S18a, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | r     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1322  | 839 | 252 | 223 | 8 |         |       |

- Molecule 51 is a protein called 28S ribosomal protein S2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 51  | AB    | 225      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1828  | 1164 | 331 | 323 | 10 |         |       |

- Molecule 52 is a protein called 28S ribosomal protein S24, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | AC    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1083  | 699 | 195 | 185 | 4 |         |       |

- Molecule 53 is a protein called 28S ribosomal protein S5, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | AD    | 343      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2731  | 1713 | 518 | 487 | 13 |         |       |

- Molecule 54 is a protein called 28S ribosomal protein S6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | AE    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 972   | 614 | 177 | 177 | 4 |         |       |

- Molecule 55 is a protein called 28S ribosomal protein S7, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | AF    | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1725  | 1104 | 312 | 298 | 11 |         |       |

- Molecule 56 is a protein called 28S ribosomal protein S9, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56  | AG    | 327      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2688  | 1710 | 477 | 487 | 14 |         |       |

- Molecule 57 is a protein called 28S ribosomal protein S10, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | AH    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 745 | 194 | 210 | 3 |         |       |

- Molecule 58 is a protein called 28S ribosomal protein S12, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | AJ    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 839   | 521 | 169 | 143 | 6 |         |       |

- Molecule 59 is a protein called 28S ribosomal protein S14, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | AK    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 537 | 179 | 141 | 5 |         |       |

- Molecule 60 is a protein called 28S ribosomal protein S15, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | AL    | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1453  | 925 | 270 | 251 | 7 |         |       |

- Molecule 61 is a protein called 28S ribosomal protein S16, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | AM    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 942   | 594 | 185 | 157 | 6 |         |       |

- Molecule 62 is a protein called 28S ribosomal protein S17, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | AN    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 868   | 562 | 156 | 147 | 3 |         |       |

- Molecule 63 is a protein called 28S ribosomal protein S18b, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 63  | AO    | 193      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1592  | 1014 | 294 | 277 | 7 |         |       |

- Molecule 64 is a protein called 28S ribosomal protein S18c, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | AP    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 781   | 501 | 134 | 138 | 8 |         |       |

- Molecule 65 is a protein called 28S ribosomal protein S22, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 65  | AR    | 295      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2409  | 1533 | 413 | 455 | 8 |         |       |

- Molecule 66 is a protein called 28S ribosomal protein S23, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | AS    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 716 | 198 | 196 | 1 |         |       |

- Molecule 67 is a protein called 28S ribosomal protein S25, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 67  | AT    | 168      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1371  | 877 | 239 | 244 | 11 |         |       |

- Molecule 68 is a protein called 28S ribosomal protein S26, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | AU    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1488  | 916 | 301 | 267 | 4 |         |       |

- Molecule 69 is a protein called 28S ribosomal protein S27, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 69  | AV    | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2969  | 1904 | 495 | 558 | 12 |         |       |

- Molecule 70 is a protein called 28S ribosomal protein S28, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | AW    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 789   | 498 | 141 | 146 | 4 |         |       |

- Molecule 71 is a protein called 28S ribosomal protein S33, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | AZ    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 839   | 534 | 153 | 148 | 4 |         |       |

- Molecule 72 is a protein called Small ribosomal subunit protein mS34.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 72  | A0    | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1787  | 1130 | 339 | 313 | 5 |         |       |

- Molecule 73 is a protein called 28S ribosomal protein S35, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 73  | A1    | 279      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2265  | 1435 | 387 | 432 | 11 |         |       |

- Molecule 74 is a protein called Aurora kinase A-interacting protein.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 74  | A3    | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 625   | 401 | 134 | 89 | 1 |         |       |

- Molecule 75 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 75  | Az    | 34       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 719   | 324 | 123 | 238 | 34 |         |       |

- Molecule 76 is a protein called 28S ribosomal protein S31, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | AY    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1010  | 654 | 166 | 188 | 2 |         |       |

- Molecule 77 is a RNA chain called 12S mitochondrial rRNA.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 77  | AA    | 954      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 20260 | 9088 | 3647 | 6571 | 954 |         |       |

- Molecule 78 is a protein called 28S ribosomal protein S11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | AI    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1019  | 641 | 193 | 181 | 4 |         |       |

- Molecule 79 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 79  | A4    | 588      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4768  | 3053 | 808 | 879 | 28 |         |       |

- Molecule 80 is a protein called 28S ribosomal protein S29, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 80  | AX    | 352      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2849  | 1822 | 499 | 517 | 11 |         |       |

- Molecule 81 is a protein called Small ribosomal subunit protein mS37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | A2    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 935   | 579 | 182 | 166 | 8 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| A2    | 1       | ACE      | -      | acetylation | UNP Q96BP2 |

- Molecule 82 is a protein called Small ribosomal subunit protein bS21m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 82  | AQ    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 744   | 460 | 150 | 126 | 8 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| AQ    | 1       | ACE      | -      | acetylation | UNP P82921 |
| AQ    | 50      | ARG      | CYS    | variant     | UNP P82921 |

- Molecule 83 is a protein called 39S ribosomal protein L44, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 83  | c     | 286      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2299  | 1470 | 397 | 423 | 9 |         |       |

- Molecule 84 is a protein called 39S ribosomal protein L48, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 84  | f     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1252  | 799 | 207 | 242 | 4 |         |       |

- Molecule 85 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 85  | p     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1205  | 748 | 228 | 225 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 86  | s     | 385      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3148  | 2018 | 558 | 558 | 14 |         |       |

- Molecule 87 is a protein called Mitochondrial inner membrane protein OXA1L.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 87  | OX    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 468   | 292 | 93 | 81 | 2 |         |       |

- Molecule 88 is a protein called 39S ribosomal protein L42, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 88  | a     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 865   | 543 | 155 | 162 | 5 |         |       |

- Molecule 89 is a RNA chain called A/P-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 89  | Aw    | 68       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1434  | 646 | 248 | 472 | 68 |         |       |

- Molecule 90 is a RNA chain called P/E-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 90  | Ax    | 70       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1482  | 665 | 260 | 487 | 70 |         |       |

- Molecule 91 is a RNA chain called mitochondrial tRNA<sup>Val</sup>.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 91  | B     | 72       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1524  | 685 | 269 | 498 | 72 |         |       |

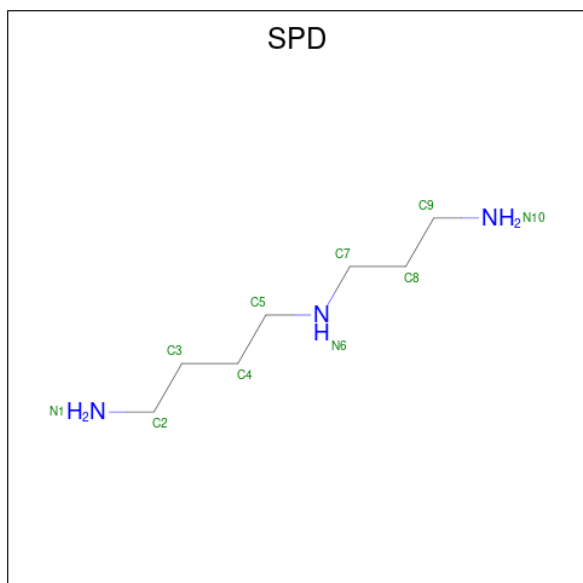
- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 92  | 0     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 92  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 92  | AO    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 93 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 93  | 6     | 1        | Total K<br>1 1   | 0       |
| 93  | A     | 30       | Total K<br>30 30 | 0       |
| 93  | D     | 1        | Total K<br>1 1   | 0       |
| 93  | M     | 2        | Total K<br>2 2   | 0       |
| 93  | N     | 1        | Total K<br>1 1   | 0       |
| 93  | o     | 1        | Total K<br>1 1   | 0       |
| 93  | AJ    | 1        | Total K<br>1 1   | 0       |
| 93  | AA    | 17       | Total K<br>17 17 | 0       |

- Molecule 94 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



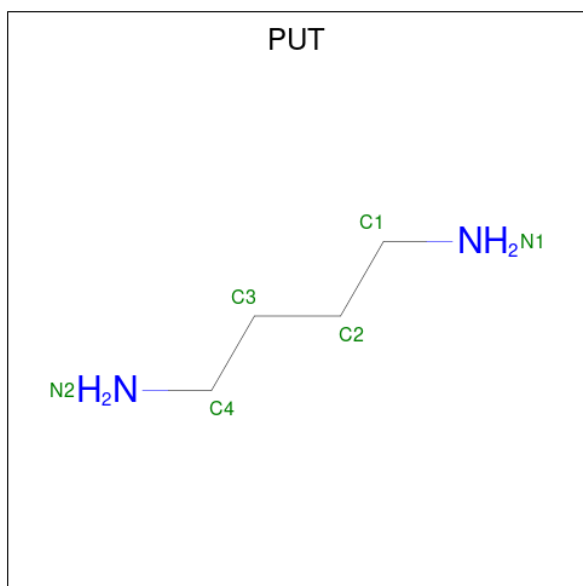
| Mol | Chain | Residues | Atoms               | AltConf |
|-----|-------|----------|---------------------|---------|
| 94  | A     | 1        | Total C N<br>10 7 3 | 0       |
| 94  | A     | 1        | Total C N<br>10 7 3 | 0       |

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| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 94  | A     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 94  | A     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 94  | A     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 94  | AA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 94  | AA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 94  | AA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 95 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula:  $C_4H_{12}N_2$ ).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 95  | A     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |

- Molecule 96 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

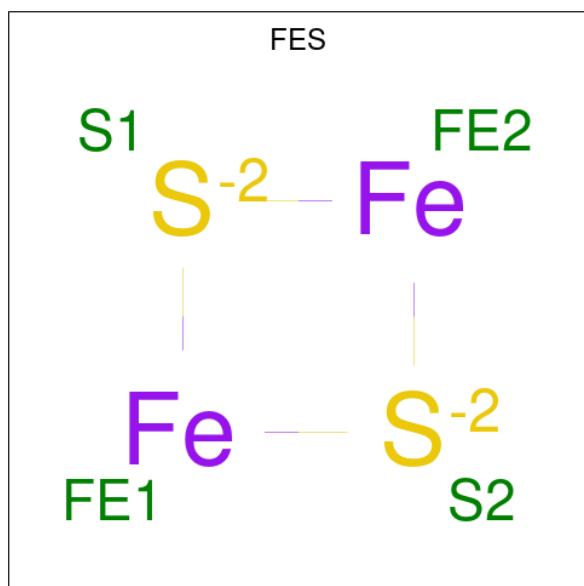
| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 96  | A     | 137      | Total | Mg  | 0       |
|     |       |          | 137   | 137 |         |
| 96  | D     | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |

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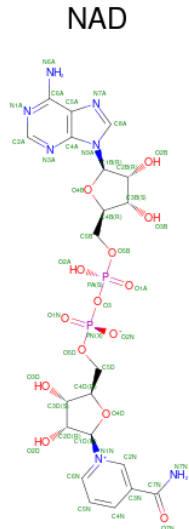
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 96  | E     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 96  | g     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 96  | AB    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 96  | A3    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 96  | AA    | 60       | Total | Mg | 0       |
|     |       |          | 60    | 60 |         |
| 96  | AX    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 97 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



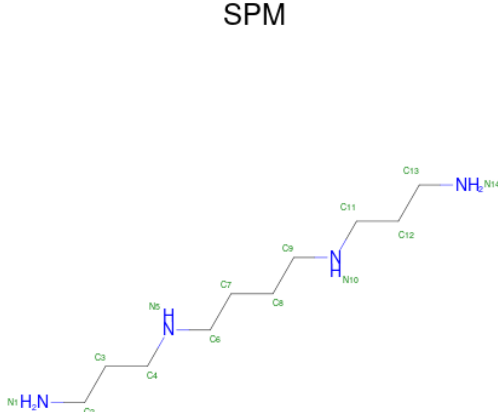
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 97  | r     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 97  | AP    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 97  | AT    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 98 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:  $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



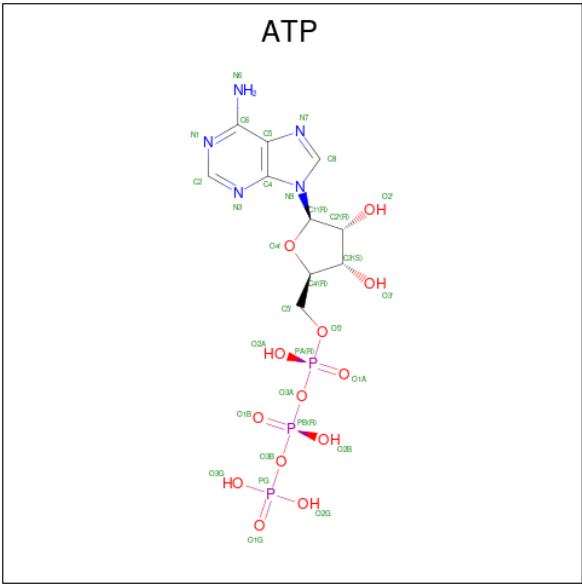
| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 98  | AA    | 1        | Total<br>44 | C<br>21 | N<br>7 | O<br>14 | P<br>2 | 0       |

- Molecule 99 is SPERMINE (CCD ID: SPM) (formula:  $\text{C}_{10}\text{H}_{26}\text{N}_4$ ) (labeled as "Ligand of Interest" by depositor).



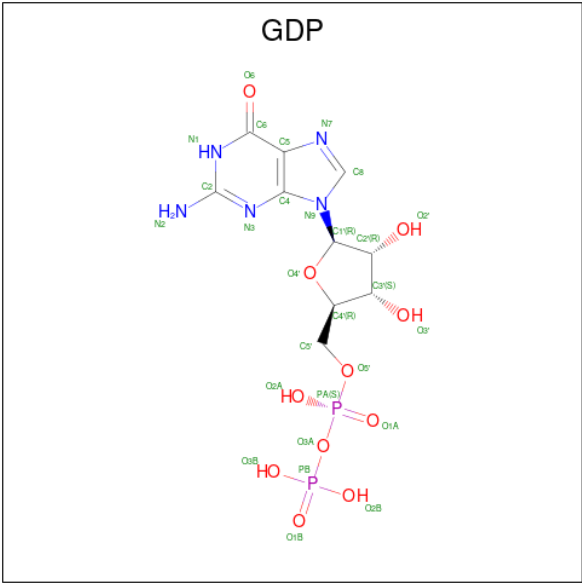
| Mol | Chain | Residues | Atoms       |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|
| 99  | AA    | 1        | Total<br>14 | C<br>10 | N<br>4 | 0       |
| 99  | AA    | 1        | Total<br>14 | C<br>10 | N<br>4 | 0       |

- Molecule 100 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



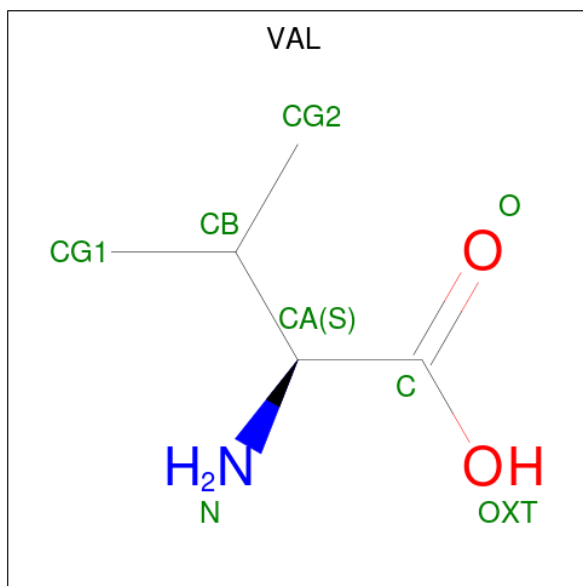
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 100 | AX    | 1        | 31    | 10 | 5 | 13 | 3 | 0       |

- Molecule 101 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



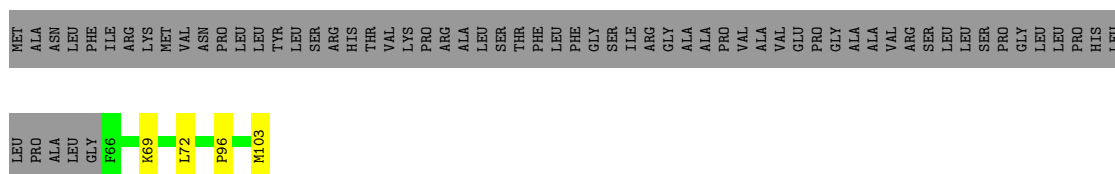
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 101 | AX    | 1        | 28    | 10 | 5 | 11 | 2 | 0       |

- Molecule 102 is VALINE (CCD ID: VAL) (formula:  $C_5H_{11}NO_2$ ).



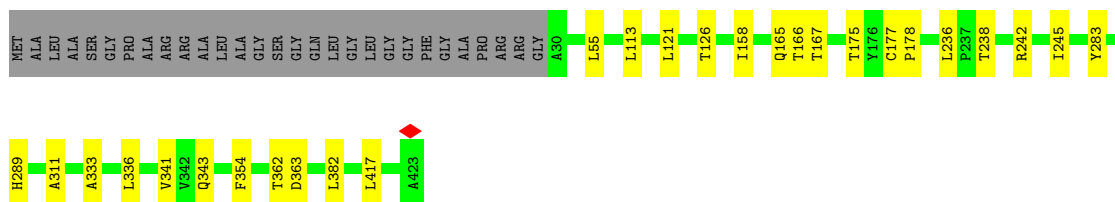
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
|     |       |          | Total | C | N | O |         |
| 102 | B     | 1        | 7     | 5 | 1 | 1 | 0       |





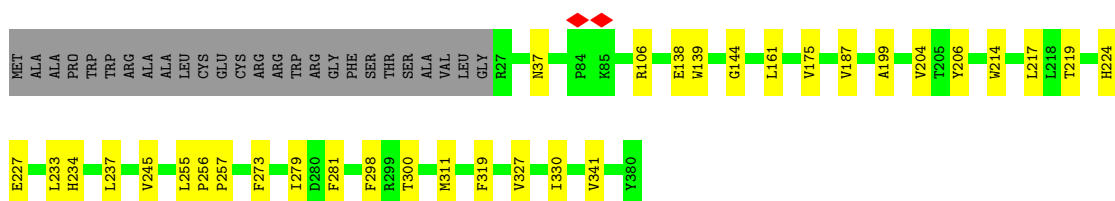
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5: 87% 6% 7%



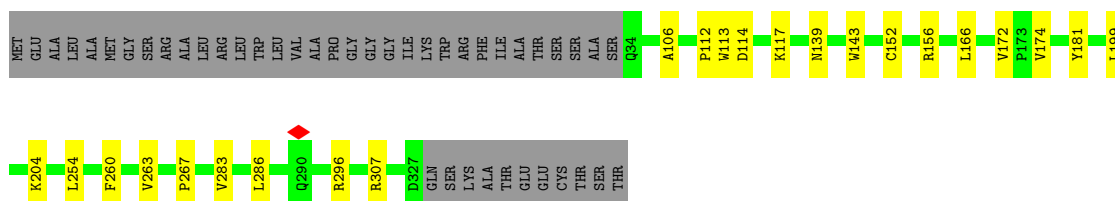
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6: 84% 9% 7%



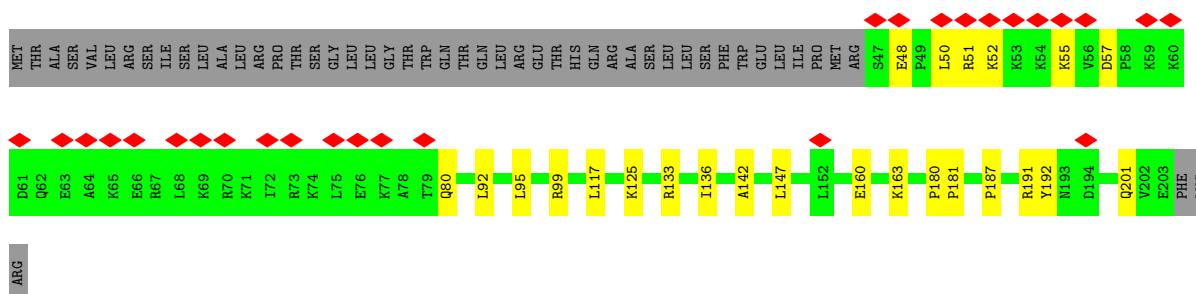
- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7: 80% 7% 13%

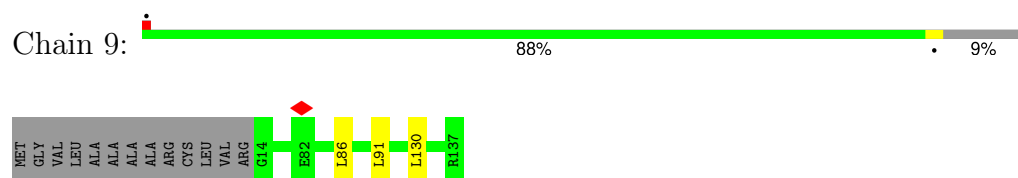


- Molecule 9: 39S ribosomal protein L40, mitochondrial

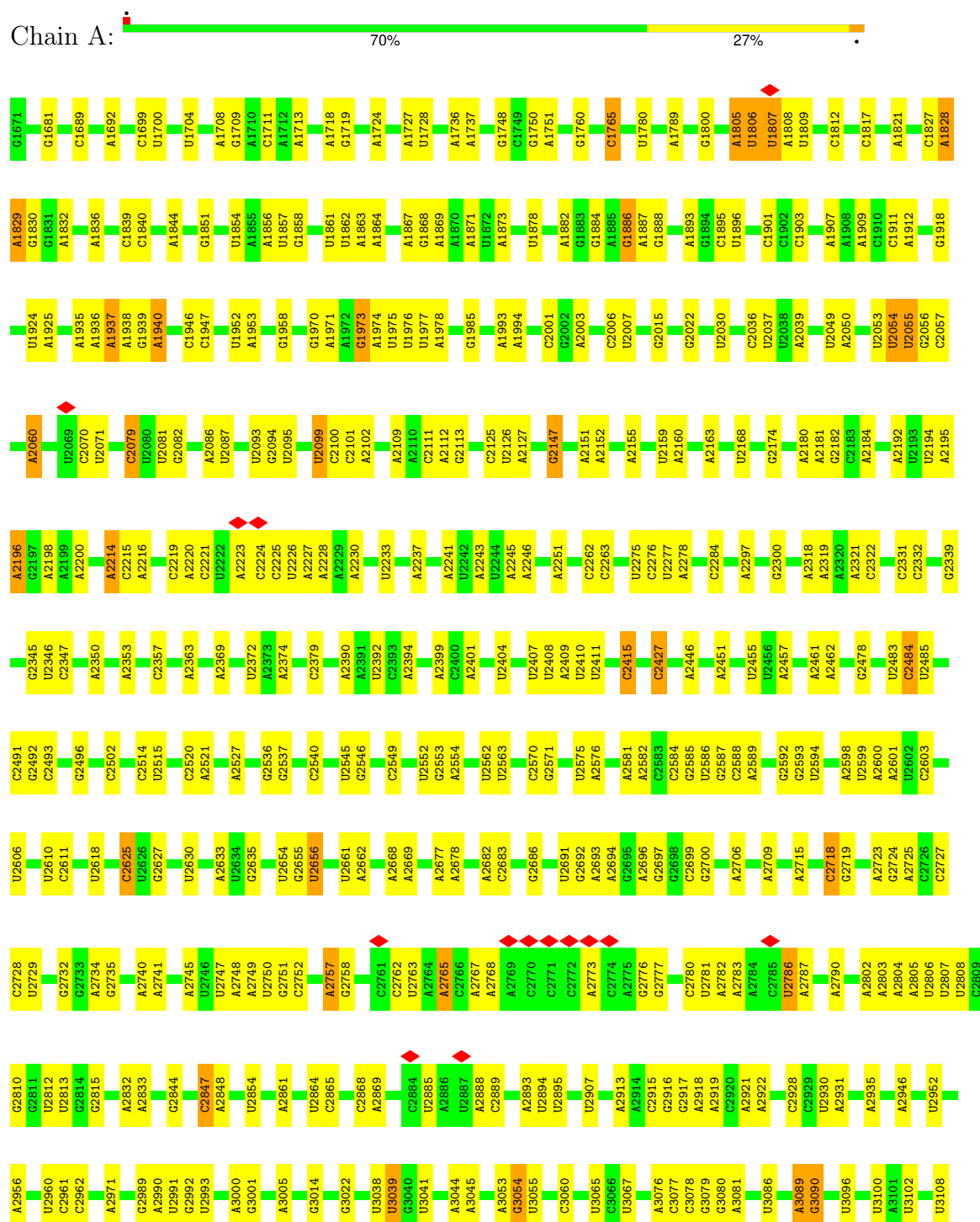
Chain 8: 13% 65% 12% 24%



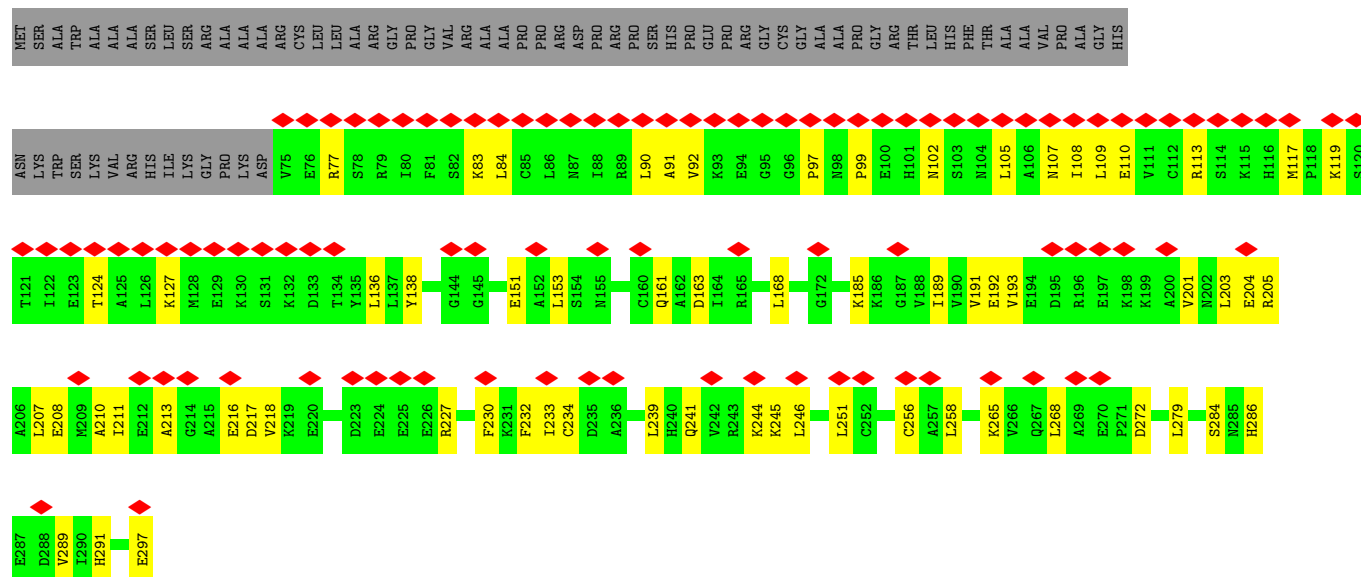
- Molecule 10: 39S ribosomal protein L41, mitochondrial



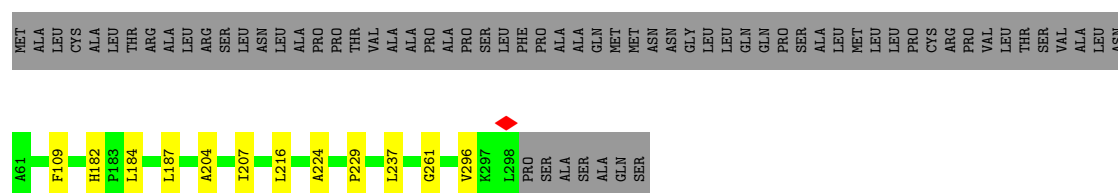
- Molecule 11: 16S mitochondrial rRNA



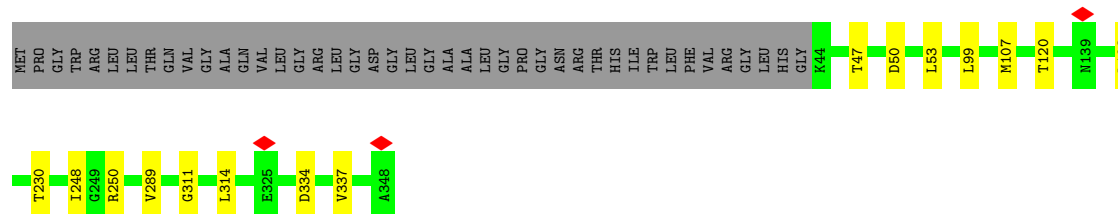
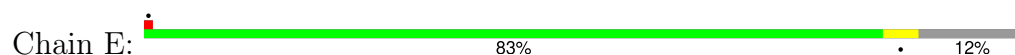
- Molecule 12: Translational activator of cytochrome c oxidase 1



- Molecule 13: 39S ribosomal protein L2, mitochondrial

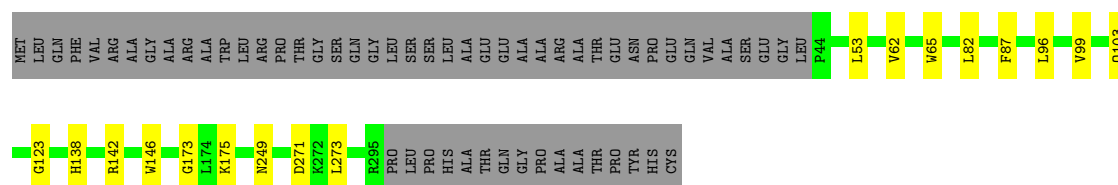


- Molecule 14: 39S ribosomal protein L3, mitochondrial



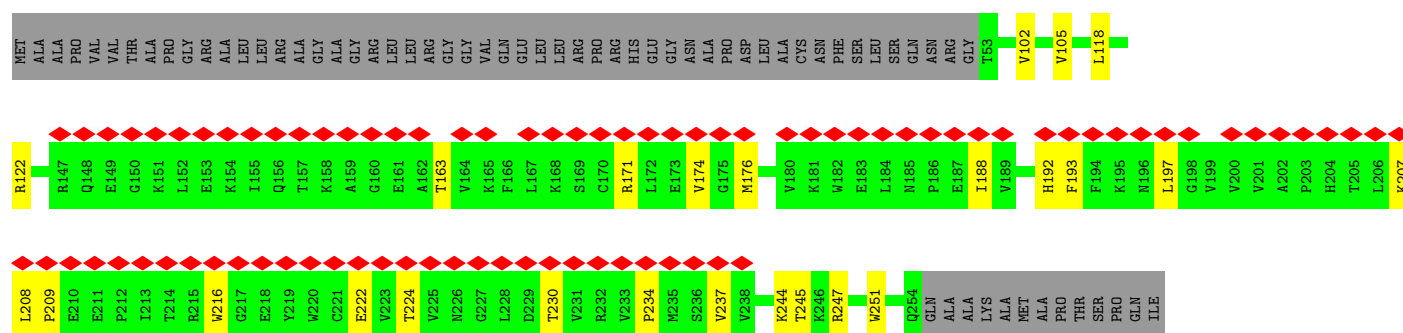
- Molecule 15: 39S ribosomal protein L4, mitochondrial

Chain F: 



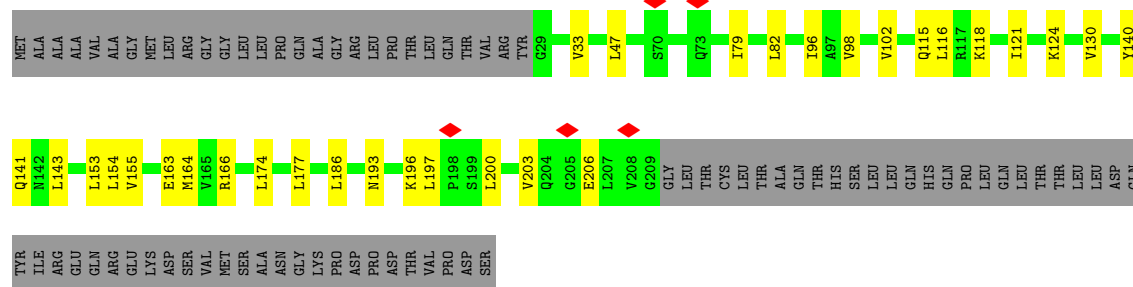
- Molecule 16: 39S ribosomal protein L9, mitochondrial

Chain H: 



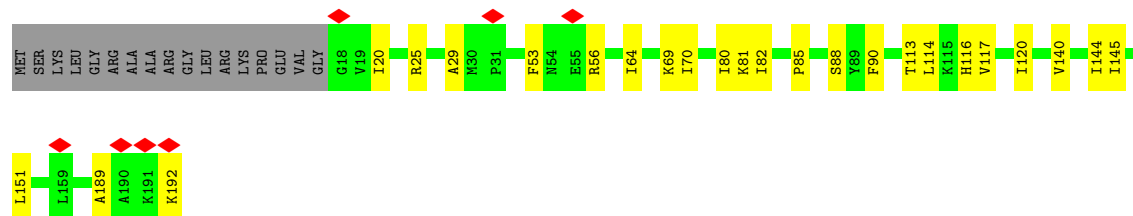
- Molecule 17: 39S ribosomal protein L10, mitochondrial

Chain I: 

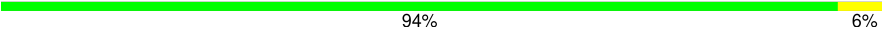


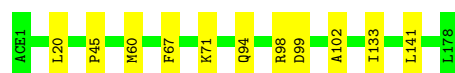
- Molecule 18: 39S ribosomal protein L11, mitochondrial

Chain J: 



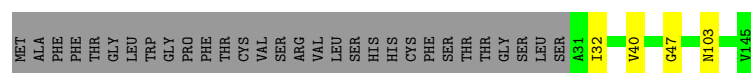
- Molecule 19: Large ribosomal subunit protein uL13m

Chain K:  94% 6%



- Molecule 20: 39S ribosomal protein L14, mitochondrial

Chain L:  77% 21%



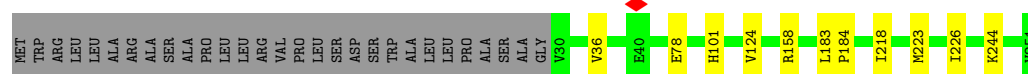
- Molecule 21: 39S ribosomal protein L15, mitochondrial

Chain M:  92% 6%



- Molecule 22: 39S ribosomal protein L16, mitochondrial

Chain N:  84% 12%



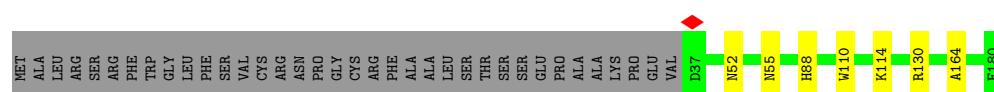
- Molecule 23: 39S ribosomal protein L17, mitochondrial

Chain O:  83% 5% 12%



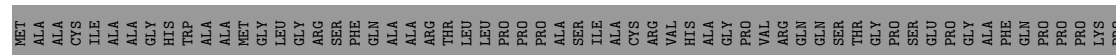
- Molecule 24: 39S ribosomal protein L18, mitochondrial

Chain P:  76% 20%



- Molecule 25: 39S ribosomal protein L19, mitochondrial

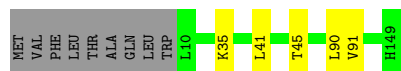
Chain Q:  72% 5% 23%





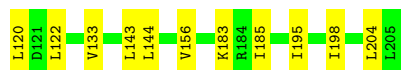
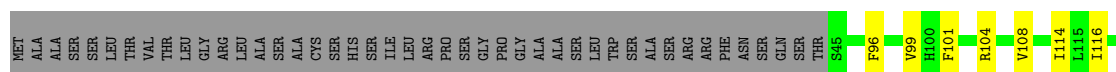
- Molecule 26: 39S ribosomal protein L20, mitochondrial

Chain R: 91% 6%



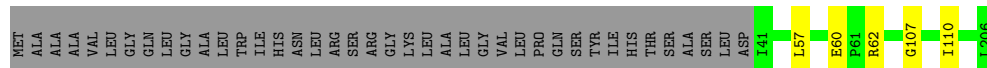
- Molecule 27: 39S ribosomal protein L21, mitochondrial

Chain S: 70% 9% 21%



- Molecule 28: 39S ribosomal protein L22, mitochondrial

Chain T: 78% 19%



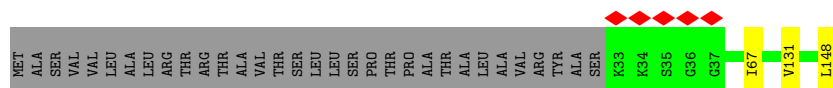
- Molecule 29: 39S ribosomal protein L23, mitochondrial

Chain U: 12% 95% 5%



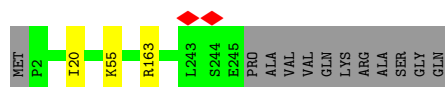
- Molecule 30: 39S ribosomal protein L27, mitochondrial

Chain W: 76% 22%

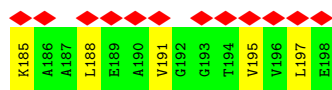


- Molecule 31: 39S ribosomal protein L28, mitochondrial

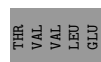
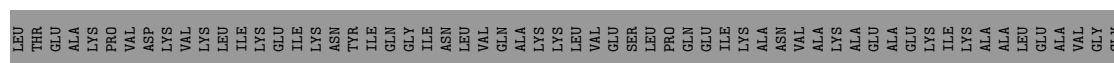
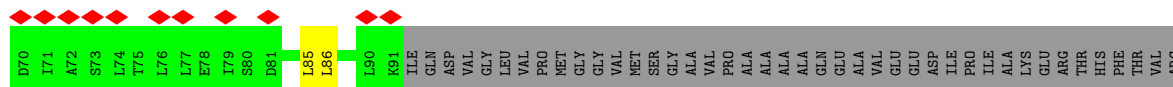
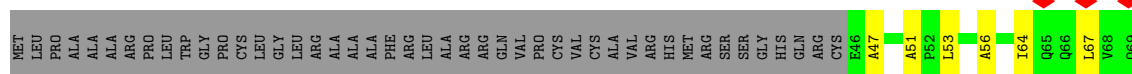
Chain X: 94% 5%



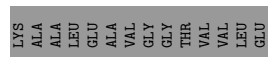
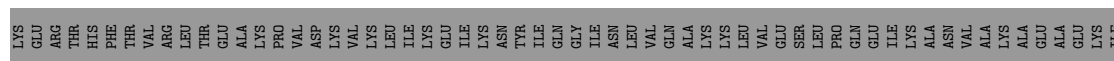
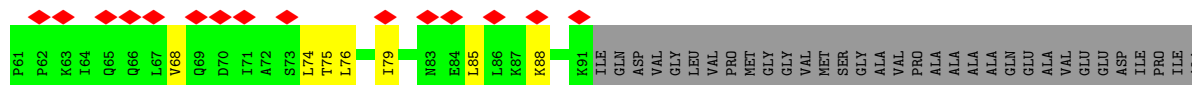
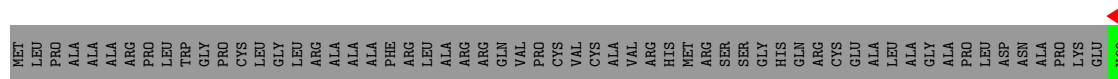




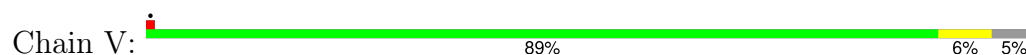
- Molecule 35: 39S ribosomal protein L12, mitochondrial



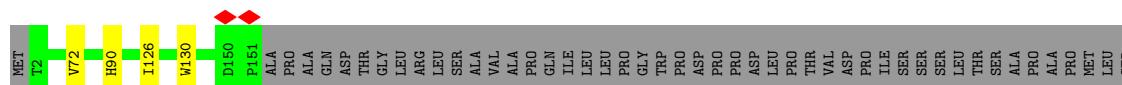
- Molecule 35: 39S ribosomal protein L12, mitochondrial



- Molecule 36: 39S ribosomal protein L24, mitochondrial



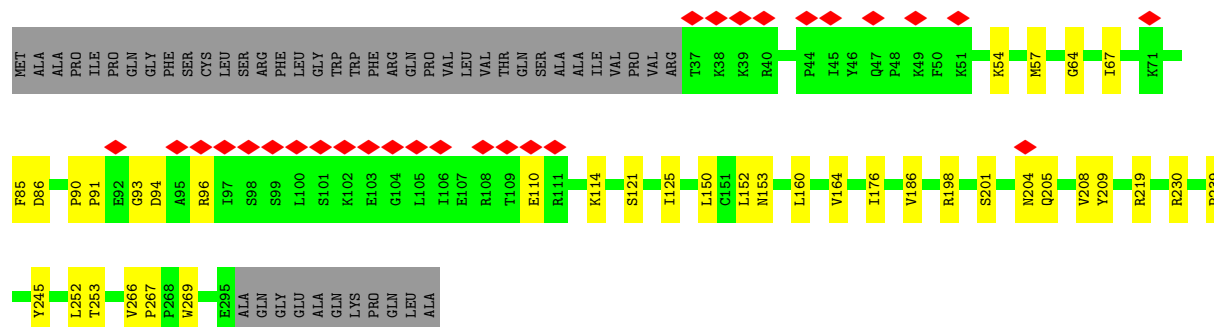
- Molecule 37: 39S ribosomal protein L43, mitochondrial



ALA  
VAL  
SER  
CYS  
LEU  
PRO  
PRO  
ILE  
VAL  
PHE  
SER  
ALA  
LEU  
THR  
THR  
VAL  
CYS  
SER  
ALA

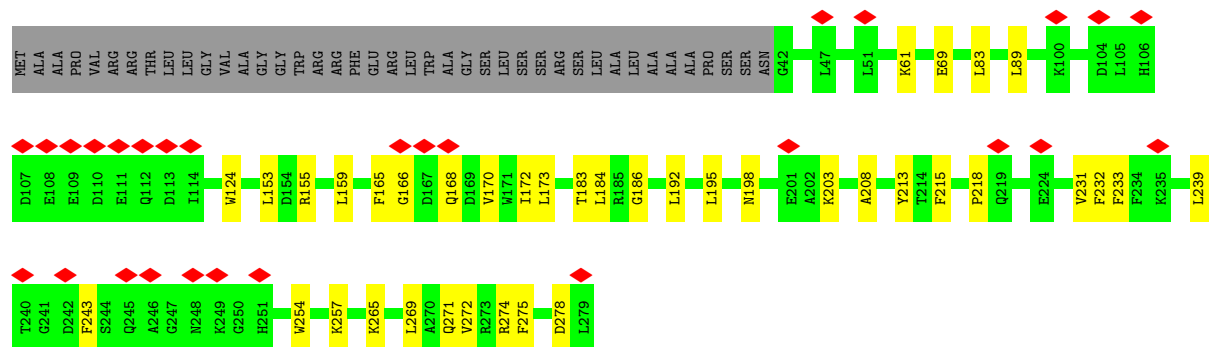
- Molecule 38: 39S ribosomal protein L45, mitochondrial

Chain d: 



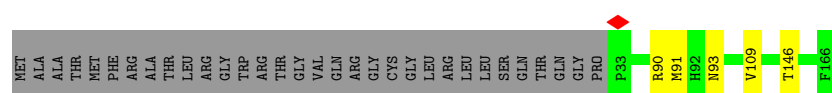
- Molecule 39: 39S ribosomal protein L46, mitochondrial

Chain e: 



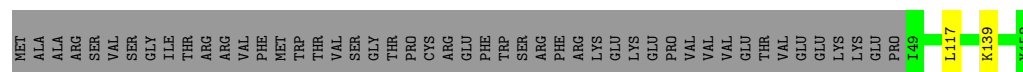
- Molecule 40: 39S ribosomal protein L49, mitochondrial

Chain g: 



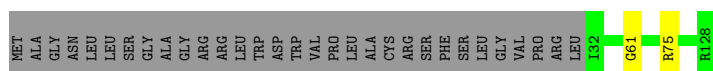
- Molecule 41: 39S ribosomal protein L50, mitochondrial

Chain h: 

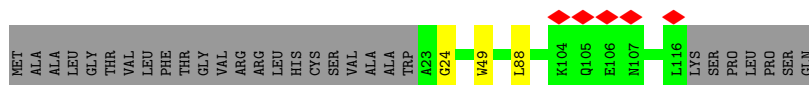


- Molecule 42: 39S ribosomal protein L51, mitochondrial

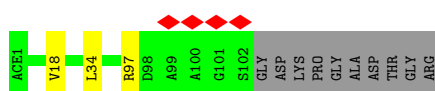
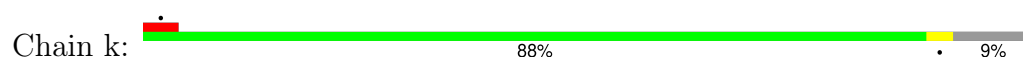
Chain i: 



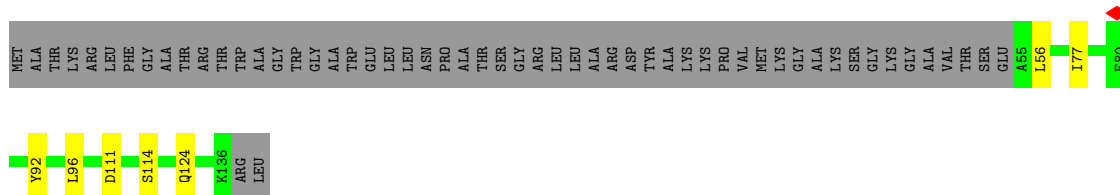
- Molecule 43: 39S ribosomal protein L52, mitochondrial



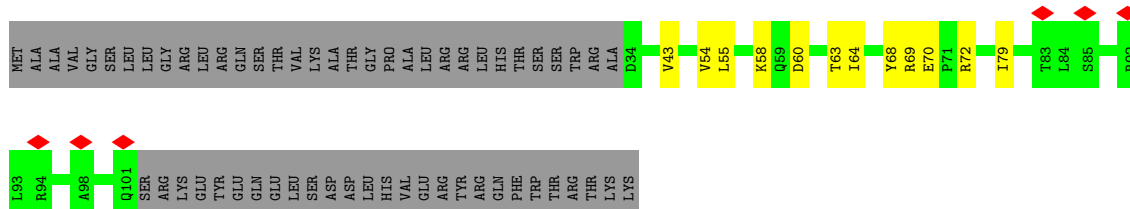
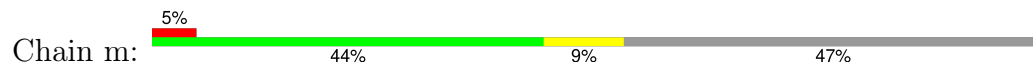
- Molecule 44: Large ribosomal subunit protein mL53



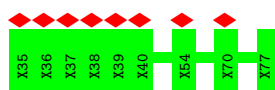
- Molecule 45: 39S ribosomal protein L54, mitochondrial



- Molecule 46: 39S ribosomal protein L55, mitochondrial



- Molecule 47: Nascent polypeptide



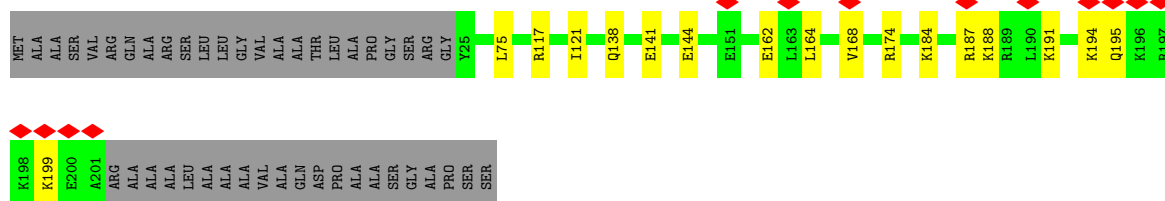
- Molecule 48: Ribosomal protein 63, mitochondrial

Chain o:  86% 6% 8%



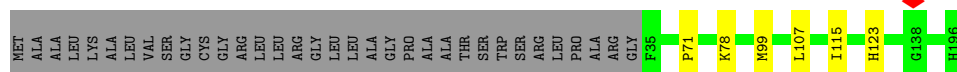
- Molecule 49: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:  6% 72% 8% 20%



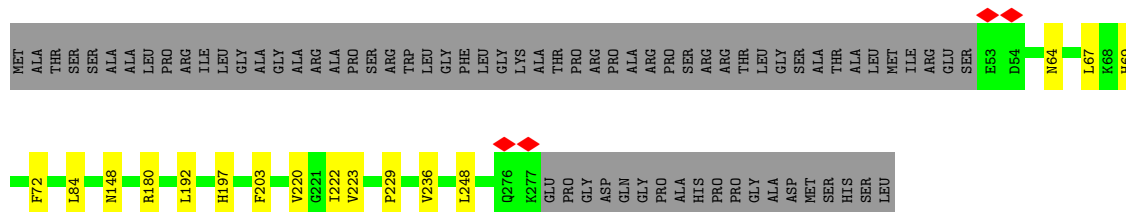
- Molecule 50: 39S ribosomal protein S18a, mitochondrial

Chain r:  80% 17%



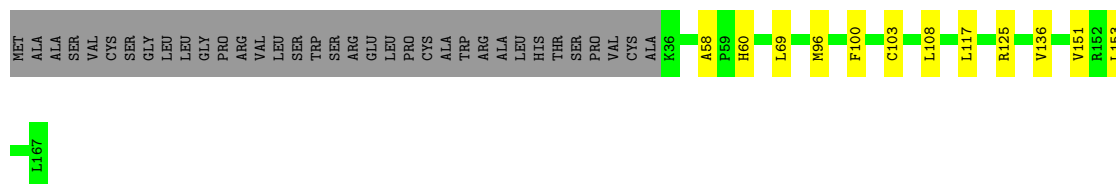
- Molecule 51: 28S ribosomal protein S2, mitochondrial

Chain AB:  71% 5% 24%



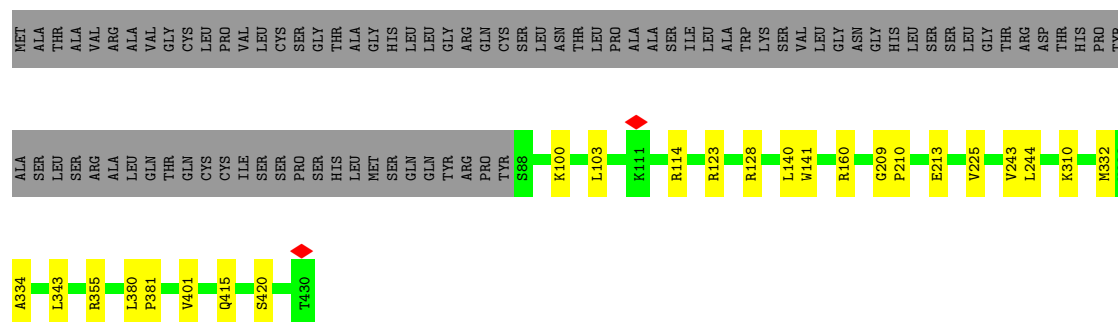
- Molecule 52: 28S ribosomal protein S24, mitochondrial

Chain AC:  72% 7% 21%



- Molecule 53: 28S ribosomal protein S5, mitochondrial

Chain AD:  74% 6% 20%



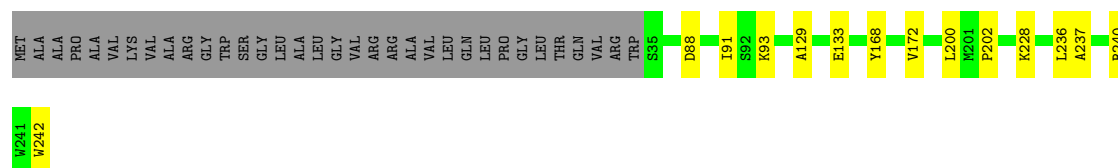
- Molecule 54: 28S ribosomal protein S6, mitochondrial

Chain AE: 85% 13% .



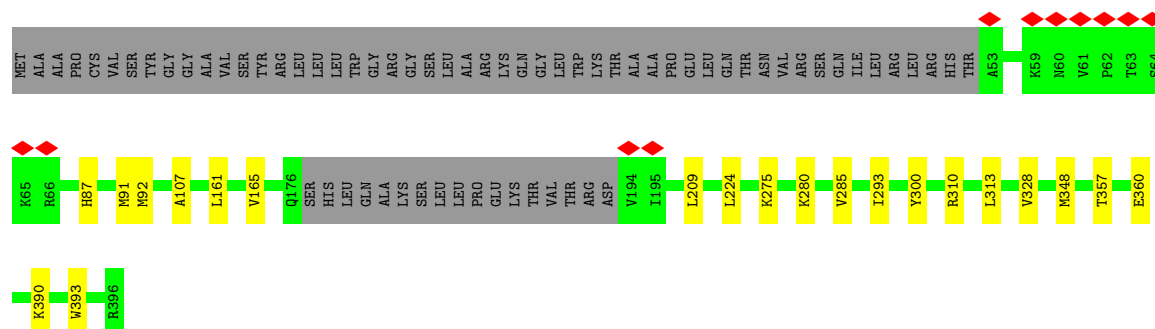
- Molecule 55: 28S ribosomal protein S7, mitochondrial

Chain AF: 80% 6% 14%



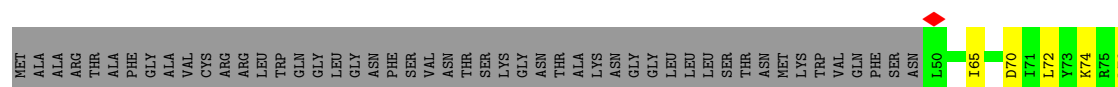
- Molecule 56: 28S ribosomal protein S9, mitochondrial

Chain AG: 77% 5% 17%



- Molecule 57: 28S ribosomal protein S10, mitochondrial

Chain AH: 55% 14% 30%

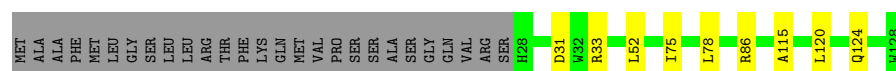




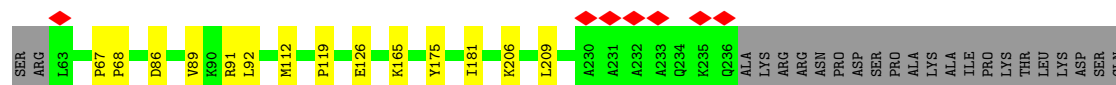
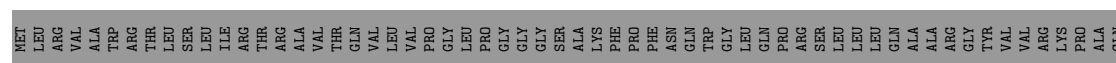
- Molecule 58: 28S ribosomal protein S12, mitochondrial



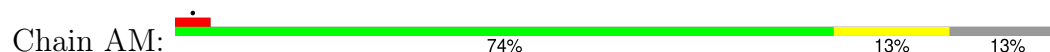
- Molecule 59: 28S ribosomal protein S14, mitochondrial



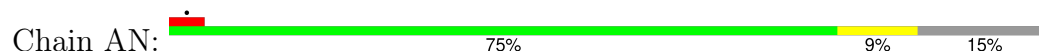
- Molecule 60: 28S ribosomal protein S15, mitochondrial



- Molecule 61: 28S ribosomal protein S16, mitochondrial

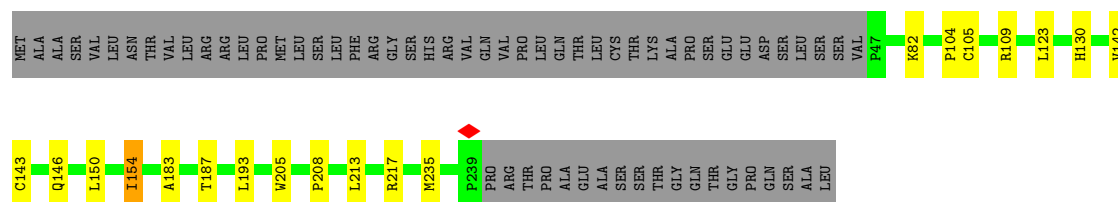


- Molecule 62: 28S ribosomal protein S17, mitochondrial

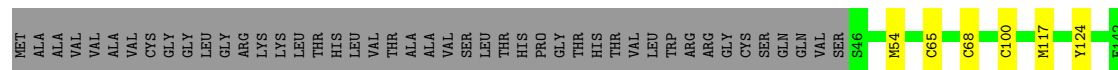


- Molecule 63: 28S ribosomal protein S18b, mitochondrial

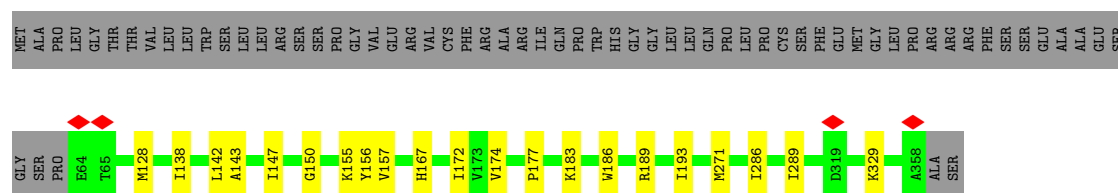
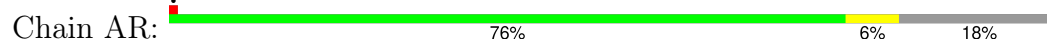




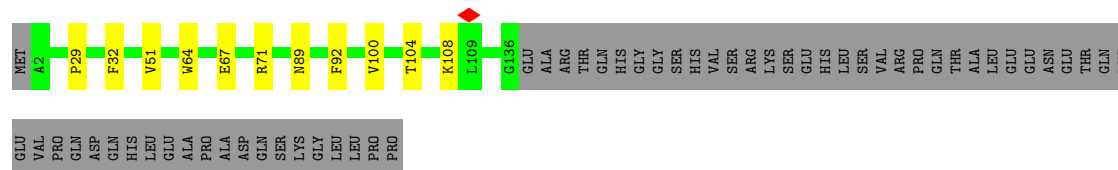
- Molecule 64: 28S ribosomal protein S18c, mitochondrial



- Molecule 65: 28S ribosomal protein S22, mitochondrial



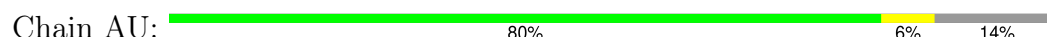
- Molecule 66: 28S ribosomal protein S23, mitochondrial



- Molecule 67: 28S ribosomal protein S25, mitochondrial

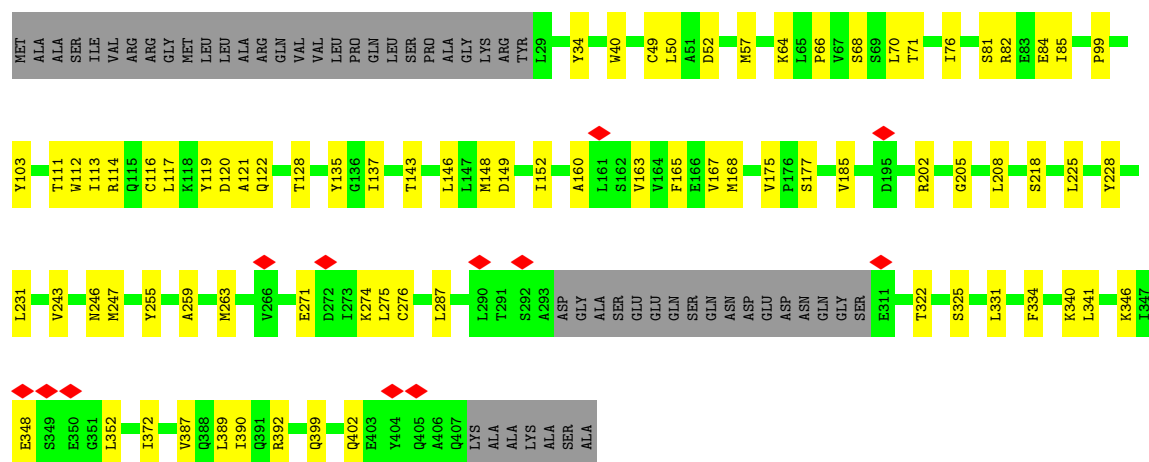


- Molecule 68: 28S ribosomal protein S26, mitochondrial

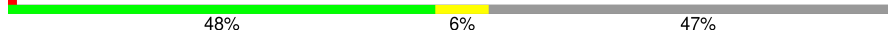


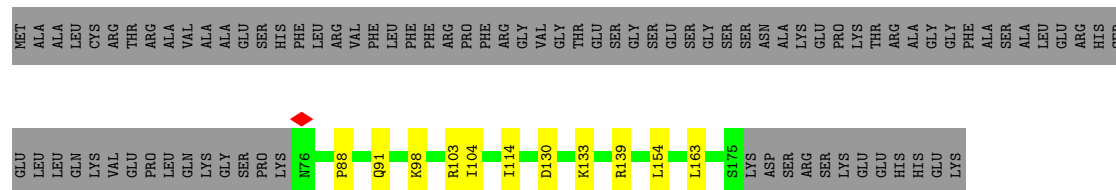
- Molecule 69: 28S ribosomal protein S27, mitochondrial

Chain AV: 



- Molecule 70: 28S ribosomal protein S28, mitochondrial

Chain AW: 



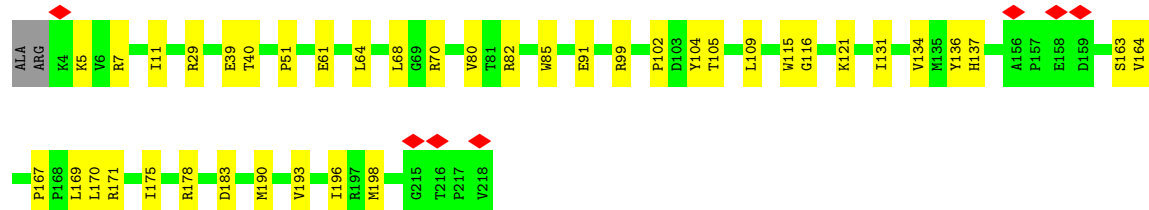
- Molecule 71: 28S ribosomal protein S33, mitochondrial

Chain AZ: 



- Molecule 72: Small ribosomal subunit protein mS34

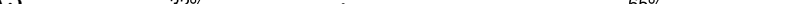
Chain A0: 

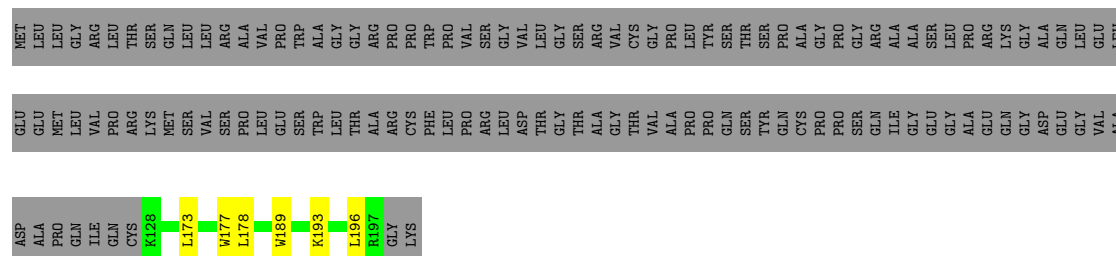


- Molecule 73: 28S ribosomal protein S35, mitochondrial

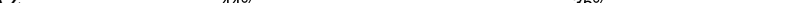
Chain A1: 

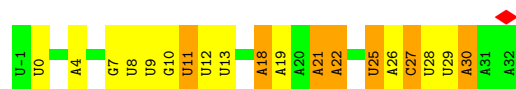
- Molecule 74: Aurora kinase A-interacting protein

Chain A3:  32% 0% 65%



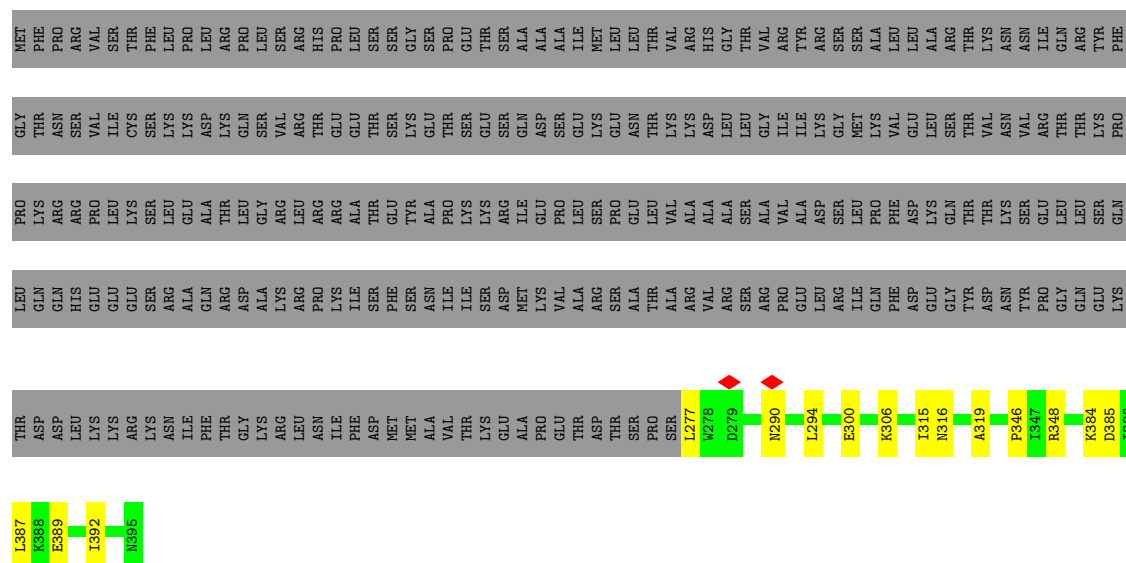
- Molecule 75: mRNA

Chain Az: 



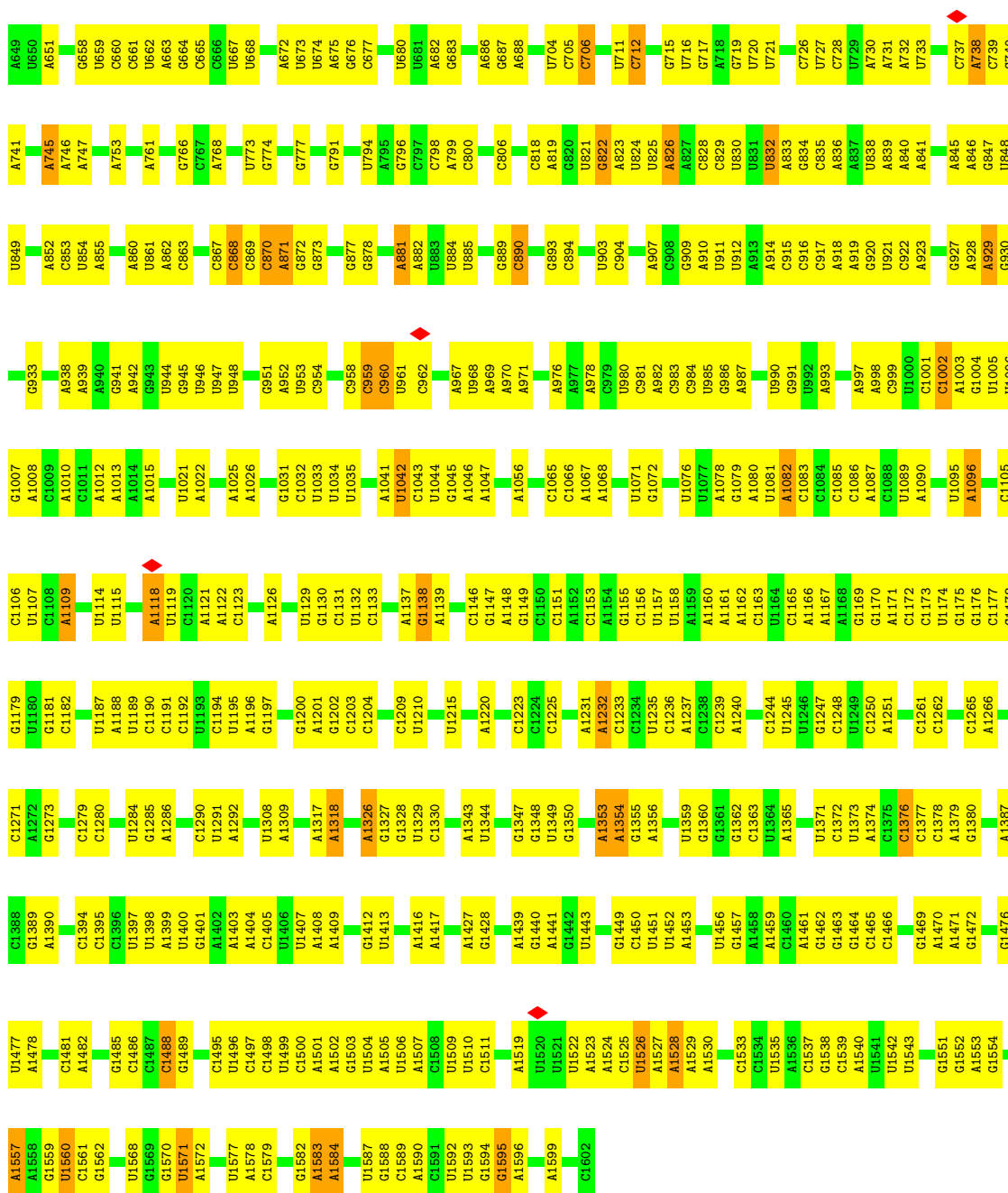
- Molecule 76: 28S ribosomal protein S31, mitochondrial

Chain AY:  26% 70%



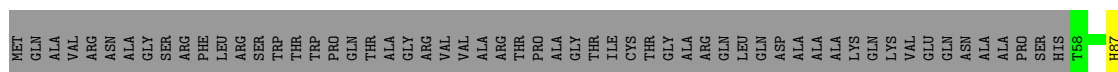
- Molecule 77: 12S mitochondrial rRNA

Chain AA:  51% 45%



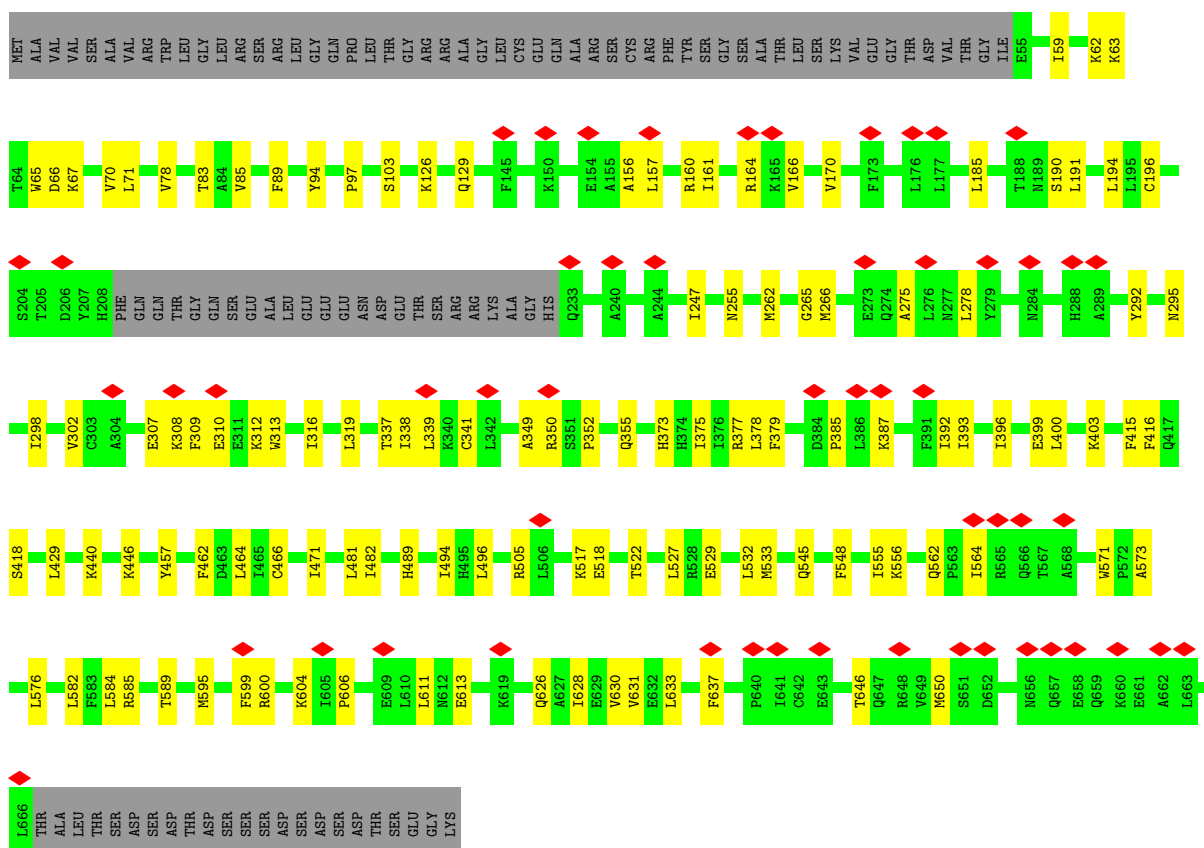
- Molecule 78: 28S ribosomal protein S11, mitochondrial

Chain AI: 68% 29%



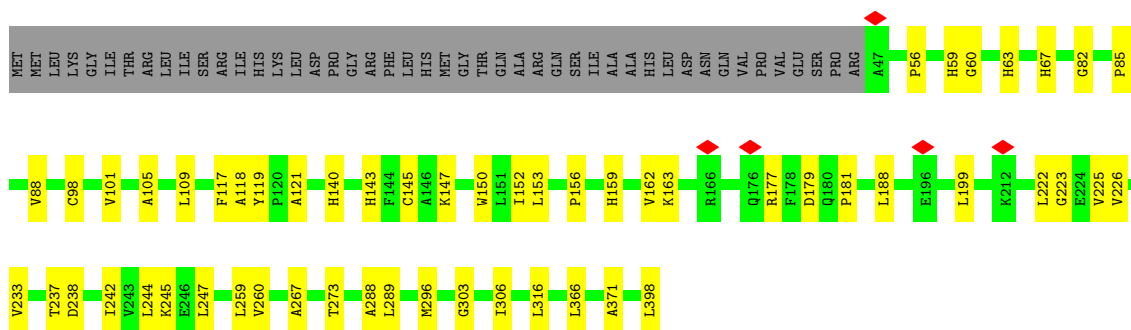
- Molecule 79: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain A4: 

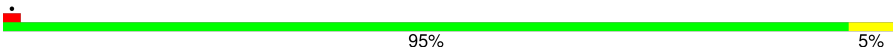


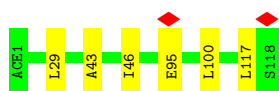
- Molecule 80: 28S ribosomal protein S29, mitochondrial

Chain AX: 



- Molecule 81: Small ribosomal subunit protein mS37

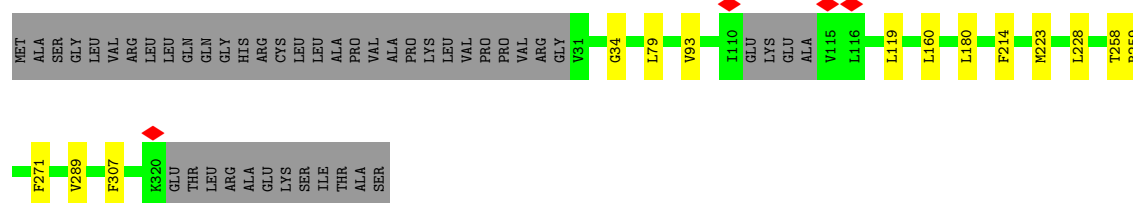
Chain A2: 

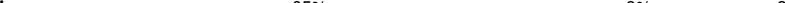


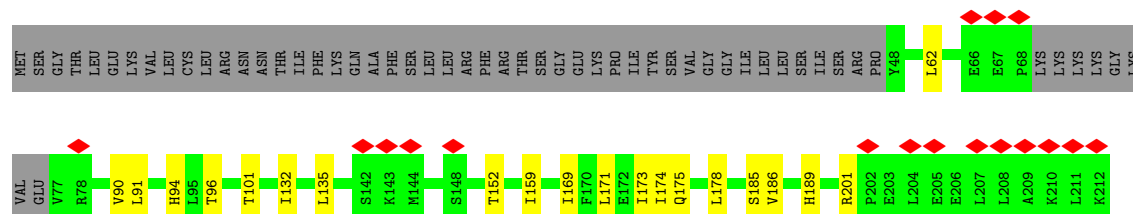
- Molecule 82: Small ribosomal subunit protein bS21m

Diagram illustrating the 1000 Genomes Project, showing a sequence of populations: ACE1, H4, T11, M66, E67, M68, and C87. The populations are represented by colored blocks (yellow and green) connected by lines, indicating a genetic lineage or relationship.

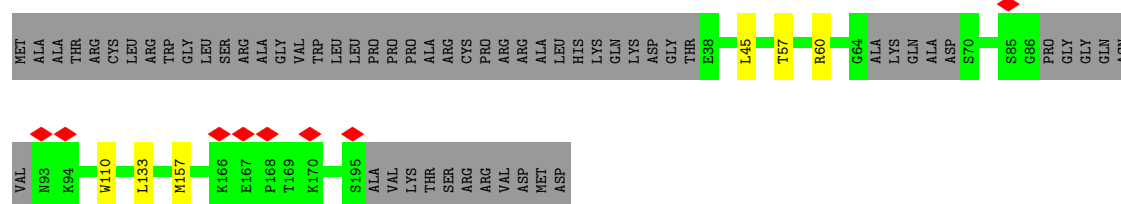
- Chain c:  82% 14%



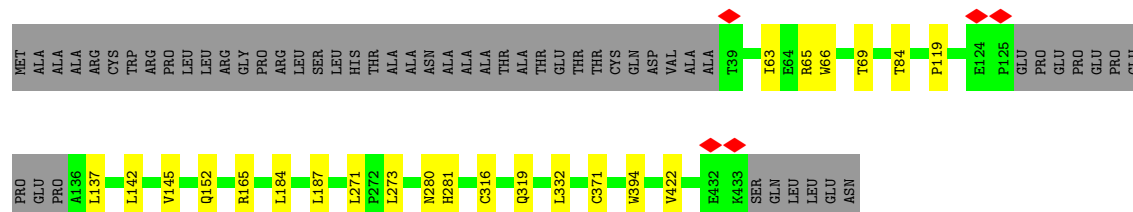
- Chain f: 



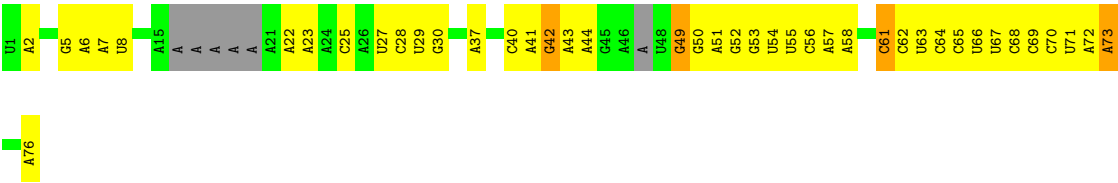
- Chain p:  68% 29%



- Chain s:  82% 5% 12%







• Molecule 91: mitochondrial tRNAVal



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 64516                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 55                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 5000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.622                                   | Depositor |
| Minimum map value                    | -0.193                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.020                                   | Depositor |
| Recommended contour level            | 0.05                                    | Depositor |
| Map size (Å)                         | 512.63995, 512.63995, 512.63995         | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.068, 1.068, 1.068                     | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 0.24         | 0/913       | 0.25        | 0/1224      |
| 2   | 1     | 0.22         | 0/469       | 0.29        | 0/621       |
| 3   | 2     | 0.29         | 0/383       | 0.26        | 0/507       |
| 4   | 3     | 0.29         | 0/853       | 0.28        | 0/1136      |
| 5   | 4     | 0.28         | 0/350       | 0.26        | 0/461       |
| 6   | 5     | 0.22         | 0/3305      | 0.29        | 0/4502      |
| 7   | 6     | 0.20         | 0/3043      | 0.29        | 0/4140      |
| 8   | 7     | 0.19         | 0/2447      | 0.28        | 0/3310      |
| 9   | 8     | 0.14         | 0/1354      | 0.34        | 0/1819      |
| 10  | 9     | 0.22         | 0/1025      | 0.27        | 0/1379      |
| 11  | A     | 0.28         | 0/36876     | 0.30        | 0/57402     |
| 12  | C     | 0.14         | 0/1754      | 0.33        | 0/2357      |
| 13  | D     | 0.23         | 0/1896      | 0.28        | 0/2549      |
| 14  | E     | 0.25         | 0/2475      | 0.30        | 0/3355      |
| 15  | F     | 0.27         | 0/2090      | 0.29        | 0/2842      |
| 16  | H     | 0.16         | 0/1698      | 0.31        | 0/2292      |
| 17  | I     | 0.17         | 0/1478      | 0.30        | 0/1999      |
| 18  | J     | 0.15         | 0/1348      | 0.30        | 0/1813      |
| 19  | K     | 0.27         | 0/1497      | 0.28        | 0/2031      |
| 20  | L     | 0.22         | 0/905       | 0.28        | 0/1218      |
| 21  | M     | 0.26         | 0/2381      | 0.29        | 0/3212      |
| 22  | N     | 0.24         | 0/1833      | 0.28        | 0/2468      |
| 23  | O     | 0.26         | 0/1283      | 0.29        | 0/1727      |
| 24  | P     | 0.21         | 0/1199      | 0.26        | 0/1623      |
| 25  | Q     | 0.22         | 0/1921      | 0.26        | 0/2588      |
| 26  | R     | 0.27         | 0/1175      | 0.26        | 0/1572      |
| 27  | S     | 0.26         | 0/1320      | 0.29        | 0/1789      |
| 28  | T     | 0.26         | 0/1403      | 0.27        | 0/1886      |
| 29  | U     | 0.25         | 0/1279      | 0.35        | 0/1730      |
| 30  | W     | 0.26         | 0/926       | 0.26        | 0/1244      |
| 31  | X     | 0.23         | 0/2099      | 0.24        | 0/2837      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 32  | Y     | 0.25         | 0/1593  | 0.25        | 0/2136  |
| 33  | Z     | 0.26         | 0/1021  | 0.30        | 0/1378  |
| 34  | z     | 0.15         | 0/2067  | 0.36        | 0/2793  |
| 35  | G     | 0.19         | 0/562   | 0.50        | 0/754   |
| 35  | t     | 0.13         | 0/358   | 0.30        | 0/486   |
| 35  | u     | 0.19         | 0/259   | 0.40        | 0/350   |
| 36  | V     | 0.20         | 0/1721  | 0.27        | 0/2333  |
| 37  | b     | 0.25         | 0/1218  | 0.29        | 0/1649  |
| 38  | d     | 0.19         | 0/2181  | 0.35        | 0/2949  |
| 39  | e     | 0.15         | 0/1970  | 0.33        | 0/2658  |
| 40  | g     | 0.25         | 0/1151  | 0.29        | 0/1569  |
| 41  | h     | 0.18         | 0/918   | 0.26        | 0/1249  |
| 42  | i     | 0.28         | 0/850   | 0.28        | 0/1135  |
| 43  | j     | 0.22         | 0/760   | 0.25        | 0/1023  |
| 44  | k     | 0.16         | 0/783   | 0.22        | 0/1057  |
| 45  | l     | 0.14         | 0/707   | 0.29        | 0/960   |
| 46  | m     | 0.12         | 0/575   | 0.31        | 0/772   |
| 48  | o     | 0.26         | 0/819   | 0.30        | 0/1097  |
| 49  | q     | 0.18         | 0/1529  | 0.29        | 0/2055  |
| 50  | r     | 0.24         | 0/1362  | 0.29        | 0/1846  |
| 51  | AB    | 0.19         | 0/1871  | 0.27        | 0/2531  |
| 52  | AC    | 0.20         | 0/1113  | 0.30        | 0/1505  |
| 53  | AD    | 0.20         | 0/2783  | 0.27        | 0/3724  |
| 54  | AE    | 0.15         | 0/989   | 0.27        | 0/1335  |
| 55  | AF    | 0.15         | 0/1767  | 0.24        | 0/2373  |
| 56  | AG    | 0.17         | 0/2746  | 0.26        | 0/3681  |
| 57  | AH    | 0.20         | 0/1178  | 0.29        | 0/1598  |
| 58  | AJ    | 0.19         | 0/855   | 0.29        | 0/1148  |
| 59  | AK    | 0.19         | 0/880   | 0.29        | 0/1182  |
| 60  | AL    | 0.16         | 0/1477  | 0.22        | 0/1974  |
| 61  | AM    | 0.18         | 0/963   | 0.32        | 0/1295  |
| 62  | AN    | 0.19         | 0/886   | 0.26        | 0/1199  |
| 63  | AO    | 0.18         | 0/1648  | 0.30        | 0/2243  |
| 64  | AP    | 0.17         | 0/798   | 0.27        | 0/1070  |
| 65  | AR    | 0.16         | 0/2456  | 0.28        | 0/3317  |
| 66  | AS    | 0.17         | 0/1138  | 0.25        | 0/1533  |
| 67  | AT    | 0.18         | 0/1402  | 0.28        | 0/1883  |
| 68  | AU    | 0.15         | 0/1510  | 0.25        | 0/2025  |
| 69  | AV    | 0.17         | 0/3030  | 0.36        | 0/4093  |
| 70  | AW    | 0.17         | 0/801   | 0.25        | 0/1079  |
| 71  | AZ    | 0.16         | 0/857   | 0.26        | 0/1141  |
| 72  | A0    | 0.15         | 0/1834  | 0.32        | 0/2484  |
| 73  | A1    | 0.15         | 0/2313  | 0.28        | 0/3129  |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 74  | A3    | 0.20         | 0/636    | 0.31        | 0/839    |
| 75  | Az    | 0.16         | 0/804    | 0.33        | 0/1248   |
| 76  | AY    | 0.17         | 0/1040   | 0.27        | 0/1402   |
| 77  | AA    | 0.23         | 0/22537  | 0.28        | 0/35085  |
| 78  | AI    | 0.18         | 0/1039   | 0.27        | 0/1400   |
| 79  | A4    | 0.16         | 0/4877   | 0.33        | 0/6598   |
| 80  | AX    | 0.15         | 0/2921   | 0.33        | 0/3954   |
| 81  | A2    | 0.17         | 0/947    | 0.28        | 0/1266   |
| 82  | AQ    | 0.18         | 0/754    | 0.25        | 0/1003   |
| 83  | c     | 0.22         | 0/2347   | 0.26        | 0/3171   |
| 84  | f     | 0.16         | 0/1273   | 0.34        | 0/1716   |
| 85  | p     | 0.17         | 0/1223   | 0.26        | 0/1641   |
| 86  | s     | 0.25         | 0/3231   | 0.30        | 0/4389   |
| 87  | OX    | 0.18         | 0/478    | 0.42        | 0/639    |
| 88  | a     | 0.23         | 0/891    | 0.33        | 0/1208   |
| 89  | Aw    | 0.16         | 0/1600   | 0.36        | 0/2476   |
| 90  | Ax    | 0.16         | 0/1654   | 0.32        | 0/2565   |
| 91  | B     | 0.16         | 0/1626   | 0.27        | 0/2523   |
| All | All   | 0.22         | 0/190555 | 0.30        | 0/270547 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 898   | 0        | 916      | 2       | 0            |
| 2   | 1     | 464   | 0        | 511      | 6       | 0            |
| 3   | 2     | 377   | 0        | 406      | 1       | 0            |
| 4   | 3     | 832   | 0        | 883      | 3       | 0            |
| 5   | 4     | 342   | 0        | 361      | 3       | 0            |
| 6   | 5     | 3210  | 0        | 3204     | 20      | 0            |
| 7   | 6     | 2948  | 0        | 2841     | 19      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | 7     | 2390  | 0        | 2397     | 14      | 0            |
| 9   | 8     | 1327  | 0        | 1368     | 25      | 0            |
| 10  | 9     | 997   | 0        | 987      | 2       | 0            |
| 11  | A     | 33070 | 0        | 16795    | 172     | 0            |
| 12  | C     | 1732  | 0        | 1740     | 43      | 0            |
| 13  | D     | 1859  | 0        | 1920     | 8       | 0            |
| 14  | E     | 2406  | 0        | 2415     | 9       | 0            |
| 15  | F     | 2031  | 0        | 2065     | 10      | 0            |
| 16  | H     | 1661  | 0        | 1734     | 14      | 0            |
| 17  | I     | 1446  | 0        | 1532     | 19      | 0            |
| 18  | J     | 1330  | 0        | 1407     | 19      | 0            |
| 19  | K     | 1455  | 0        | 1452     | 6       | 0            |
| 20  | L     | 890   | 0        | 941      | 2       | 0            |
| 21  | M     | 2327  | 0        | 2395     | 13      | 0            |
| 22  | N     | 1786  | 0        | 1817     | 8       | 0            |
| 23  | O     | 1259  | 0        | 1294     | 6       | 0            |
| 24  | P     | 1173  | 0        | 1165     | 5       | 0            |
| 25  | Q     | 1878  | 0        | 1909     | 9       | 0            |
| 26  | R     | 1154  | 0        | 1214     | 4       | 0            |
| 27  | S     | 1293  | 0        | 1365     | 11      | 0            |
| 28  | T     | 1369  | 0        | 1410     | 3       | 0            |
| 29  | U     | 1248  | 0        | 1228     | 4       | 0            |
| 30  | W     | 904   | 0        | 935      | 2       | 0            |
| 31  | X     | 2044  | 0        | 2060     | 4       | 0            |
| 32  | Y     | 1556  | 0        | 1597     | 5       | 0            |
| 33  | Z     | 996   | 0        | 1044     | 2       | 0            |
| 34  | z     | 2027  | 0        | 2076     | 32      | 0            |
| 35  | G     | 558   | 0        | 612      | 24      | 0            |
| 35  | t     | 354   | 0        | 377      | 6       | 0            |
| 35  | u     | 257   | 0        | 283      | 7       | 0            |
| 36  | V     | 1676  | 0        | 1687     | 7       | 0            |
| 37  | b     | 1193  | 0        | 1191     | 3       | 0            |
| 38  | d     | 2124  | 0        | 2125     | 23      | 0            |
| 39  | e     | 1931  | 0        | 1916     | 38      | 0            |
| 40  | g     | 1113  | 0        | 1097     | 3       | 0            |
| 41  | h     | 895   | 0        | 881      | 2       | 0            |
| 42  | i     | 828   | 0        | 857      | 2       | 0            |
| 43  | j     | 745   | 0        | 746      | 3       | 0            |
| 44  | k     | 774   | 0        | 784      | 2       | 0            |
| 45  | l     | 688   | 0        | 674      | 9       | 0            |
| 46  | m     | 567   | 0        | 591      | 8       | 0            |
| 47  | n     | 215   | 0        | 52       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48  | o     | 798   | 0        | 804      | 5       | 0            |
| 49  | q     | 1495  | 0        | 1492     | 13      | 0            |
| 50  | r     | 1322  | 0        | 1348     | 4       | 0            |
| 51  | AB    | 1828  | 0        | 1815     | 9       | 0            |
| 52  | AC    | 1083  | 0        | 1088     | 8       | 0            |
| 53  | AD    | 2731  | 0        | 2802     | 18      | 0            |
| 54  | AE    | 972   | 0        | 1000     | 11      | 0            |
| 55  | AF    | 1725  | 0        | 1769     | 9       | 0            |
| 56  | AG    | 2688  | 0        | 2687     | 13      | 0            |
| 57  | AH    | 1152  | 0        | 1183     | 20      | 0            |
| 58  | AJ    | 839   | 0        | 887      | 17      | 0            |
| 59  | AK    | 862   | 0        | 885      | 8       | 0            |
| 60  | AL    | 1453  | 0        | 1540     | 12      | 0            |
| 61  | AM    | 942   | 0        | 965      | 14      | 0            |
| 62  | AN    | 868   | 0        | 928      | 8       | 0            |
| 63  | AO    | 1592  | 0        | 1557     | 16      | 0            |
| 64  | AP    | 781   | 0        | 806      | 5       | 0            |
| 65  | AR    | 2409  | 0        | 2428     | 15      | 0            |
| 66  | AS    | 1111  | 0        | 1115     | 7       | 0            |
| 67  | AT    | 1371  | 0        | 1393     | 10      | 0            |
| 68  | AU    | 1488  | 0        | 1499     | 11      | 0            |
| 69  | AV    | 2969  | 0        | 2961     | 52      | 0            |
| 70  | AW    | 789   | 0        | 802      | 8       | 0            |
| 71  | AZ    | 839   | 0        | 858      | 5       | 0            |
| 72  | A0    | 1787  | 0        | 1796     | 28      | 0            |
| 73  | A1    | 2265  | 0        | 2294     | 21      | 0            |
| 74  | A3    | 625   | 0        | 698      | 6       | 0            |
| 75  | Az    | 719   | 0        | 360      | 9       | 0            |
| 76  | AY    | 1010  | 0        | 957      | 10      | 0            |
| 77  | AA    | 20260 | 0        | 10288    | 328     | 0            |
| 78  | AI    | 1019  | 0        | 1059     | 6       | 0            |
| 79  | A4    | 4768  | 0        | 4766     | 79      | 0            |
| 80  | AX    | 2849  | 0        | 2843     | 36      | 0            |
| 81  | A2    | 935   | 0        | 969      | 6       | 0            |
| 82  | AQ    | 744   | 0        | 758      | 5       | 0            |
| 83  | c     | 2299  | 0        | 2320     | 10      | 0            |
| 84  | f     | 1252  | 0        | 1269     | 14      | 0            |
| 85  | p     | 1205  | 0        | 1223     | 4       | 0            |
| 86  | s     | 3148  | 0        | 3131     | 16      | 0            |
| 87  | OX    | 468   | 0        | 464      | 4       | 0            |
| 88  | a     | 865   | 0        | 829      | 7       | 0            |
| 89  | Aw    | 1434  | 0        | 728      | 32      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 90  | Ax    | 1482   | 0        | 753      | 29      | 0            |
| 91  | B     | 1524   | 0        | 779      | 22      | 0            |
| 92  | 0     | 1      | 0        | 0        | 0       | 0            |
| 92  | 4     | 1      | 0        | 0        | 0       | 0            |
| 92  | AO    | 1      | 0        | 0        | 0       | 0            |
| 93  | 6     | 1      | 0        | 0        | 0       | 0            |
| 93  | A     | 30     | 0        | 0        | 0       | 0            |
| 93  | AA    | 17     | 0        | 0        | 0       | 0            |
| 93  | AJ    | 1      | 0        | 0        | 0       | 0            |
| 93  | D     | 1      | 0        | 0        | 0       | 0            |
| 93  | M     | 2      | 0        | 0        | 0       | 0            |
| 93  | N     | 1      | 0        | 0        | 0       | 0            |
| 93  | o     | 1      | 0        | 0        | 0       | 0            |
| 94  | A     | 50     | 0        | 95       | 1       | 0            |
| 94  | AA    | 30     | 0        | 57       | 4       | 0            |
| 95  | A     | 6      | 0        | 12       | 0       | 0            |
| 96  | A     | 137    | 0        | 0        | 0       | 0            |
| 96  | A3    | 1      | 0        | 0        | 0       | 0            |
| 96  | AA    | 60     | 0        | 0        | 0       | 0            |
| 96  | AB    | 1      | 0        | 0        | 0       | 0            |
| 96  | AX    | 1      | 0        | 0        | 0       | 0            |
| 96  | D     | 2      | 0        | 0        | 0       | 0            |
| 96  | E     | 1      | 0        | 0        | 0       | 0            |
| 96  | g     | 1      | 0        | 0        | 0       | 0            |
| 97  | AP    | 4      | 0        | 0        | 0       | 0            |
| 97  | AT    | 4      | 0        | 0        | 0       | 0            |
| 97  | r     | 4      | 0        | 0        | 1       | 0            |
| 98  | AA    | 44     | 0        | 26       | 1       | 0            |
| 99  | AA    | 28     | 0        | 52       | 0       | 0            |
| 100 | AX    | 31     | 0        | 12       | 0       | 0            |
| 101 | AX    | 28     | 0        | 12       | 3       | 0            |
| 102 | B     | 7      | 0        | 8        | 4       | 0            |
| All | All   | 181859 | 0        | 154427   | 1396    | 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 4.

The worst 5 of 1396 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 35:G:148:GLU:O | 35:G:152:TYR:HB3 | 1.80                     | 0.82              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:e:218:PRO:HG2  | 102:B:101:VAL:HG22 | 1.60                     | 0.82              |
| 39:e:172:ILE:HD13 | 91:B:76:A:H2       | 1.46                     | 0.81              |
| 15:F:103:GLN:HE22 | 15:F:249:ASN:HD22  | 1.29                     | 0.79              |
| 77:AA:1587:U:H2'  | 77:AA:1588:G:H8    | 1.52                     | 0.75              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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     | 108/188 (57%) | 108 (100%) | 0       | 0        | 100         | 100 |
| 2   | 1     | 54/65 (83%)   | 53 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 3   | 2     | 44/92 (48%)   | 43 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 4   | 3     | 93/188 (50%)  | 92 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 5   | 4     | 36/103 (35%)  | 36 (100%)  | 0       | 0        | 100         | 100 |
| 6   | 5     | 392/423 (93%) | 386 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 7   | 6     | 352/380 (93%) | 344 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 8   | 7     | 292/338 (86%) | 284 (97%)  | 8 (3%)  | 0        | 100         | 100 |
| 9   | 8     | 155/206 (75%) | 149 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 10  | 9     | 122/137 (89%) | 120 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 12  | C     | 221/297 (74%) | 214 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 13  | D     | 236/305 (77%) | 229 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 14  | E     | 303/348 (87%) | 293 (97%)  | 10 (3%) | 0        | 100         | 100 |
| 15  | F     | 250/311 (80%) | 250 (100%) | 0       | 0        | 100         | 100 |
| 16  | H     | 200/267 (75%) | 192 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 17  | I     | 179/261 (69%) | 177 (99%)  | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 18  | J     | 173/192 (90%) | 171 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 19  | K     | 176/178 (99%) | 173 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 20  | L     | 113/145 (78%) | 108 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 21  | M     | 289/296 (98%) | 283 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 22  | N     | 220/251 (88%) | 219 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 23  | O     | 152/175 (87%) | 147 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 24  | P     | 142/180 (79%) | 136 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 25  | Q     | 224/292 (77%) | 219 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 26  | R     | 138/149 (93%) | 137 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 27  | S     | 159/205 (78%) | 158 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 28  | T     | 164/206 (80%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 29  | U     | 150/153 (98%) | 146 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 30  | W     | 114/148 (77%) | 111 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 31  | X     | 242/256 (94%) | 240 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 32  | Y     | 179/250 (72%) | 176 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 33  | Z     | 120/161 (74%) | 118 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 34  | z     | 250/325 (77%) | 231 (92%)  | 19 (8%) | 0        | 100         | 100 |
| 35  | G     | 70/198 (35%)  | 67 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 35  | t     | 44/198 (22%)  | 44 (100%)  | 0       | 0        | 100         | 100 |
| 35  | u     | 30/198 (15%)  | 30 (100%)  | 0       | 0        | 100         | 100 |
| 36  | V     | 203/216 (94%) | 200 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 37  | b     | 148/215 (69%) | 140 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 38  | d     | 257/306 (84%) | 239 (93%)  | 18 (7%) | 0        | 100         | 100 |
| 39  | e     | 236/279 (85%) | 226 (96%)  | 10 (4%) | 0        | 100         | 100 |
| 40  | g     | 132/166 (80%) | 131 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 41  | h     | 108/158 (68%) | 103 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 42  | i     | 95/128 (74%)  | 95 (100%)  | 0       | 0        | 100         | 100 |
| 43  | j     | 92/123 (75%)  | 90 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 44  | k     | 100/112 (89%) | 99 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 45  | l     | 80/138 (58%)  | 77 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 46  | m     | 66/128 (52%)  | 63 (96%)   | 3 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 48  | o     | 92/102 (90%)  | 91 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 49  | q     | 175/222 (79%) | 175 (100%) | 0       | 0        | 100         | 100 |
| 50  | r     | 160/196 (82%) | 157 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 51  | AB    | 223/296 (75%) | 215 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 52  | AC    | 130/167 (78%) | 126 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 53  | AD    | 341/430 (79%) | 332 (97%)  | 9 (3%)  | 0        | 100         | 100 |
| 54  | AE    | 120/125 (96%) | 118 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 55  | AF    | 206/242 (85%) | 204 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 56  | AG    | 323/396 (82%) | 314 (97%)  | 9 (3%)  | 0        | 100         | 100 |
| 57  | AH    | 138/201 (69%) | 132 (96%)  | 5 (4%)  | 1 (1%)   | 18          | 50  |
| 58  | AJ    | 106/138 (77%) | 101 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 59  | AK    | 99/128 (77%)  | 99 (100%)  | 0       | 0        | 100         | 100 |
| 60  | AL    | 172/257 (67%) | 171 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 61  | AM    | 117/137 (85%) | 114 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 62  | AN    | 108/130 (83%) | 103 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 63  | AO    | 191/258 (74%) | 187 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 64  | AP    | 95/142 (67%)  | 94 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 65  | AR    | 293/360 (81%) | 287 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 66  | AS    | 133/190 (70%) | 132 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 67  | AT    | 166/173 (96%) | 164 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 68  | AU    | 174/205 (85%) | 174 (100%) | 0       | 0        | 100         | 100 |
| 69  | AV    | 358/414 (86%) | 340 (95%)  | 18 (5%) | 0        | 100         | 100 |
| 70  | AW    | 98/187 (52%)  | 97 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 71  | AZ    | 98/106 (92%)  | 97 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 72  | A0    | 213/217 (98%) | 206 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 73  | A1    | 277/323 (86%) | 267 (96%)  | 10 (4%) | 0        | 100         | 100 |
| 74  | A3    | 68/199 (34%)  | 66 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 76  | AY    | 117/395 (30%) | 117 (100%) | 0       | 0        | 100         | 100 |
| 78  | AI    | 135/194 (70%) | 129 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 79  | A4    | 584/689 (85%) | 570 (98%)  | 14 (2%) | 0        | 100         | 100 |
| 80  | AX    | 350/398 (88%) | 334 (95%)  | 16 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 81  | A2    | 116/118 (98%)     | 112 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 82  | AQ    | 85/87 (98%)       | 83 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 83  | c     | 282/332 (85%)     | 276 (98%)   | 6 (2%)   | 0        | 100         | 100 |
| 84  | f     | 153/212 (72%)     | 148 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 85  | p     | 141/206 (68%)     | 139 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 86  | s     | 381/439 (87%)     | 372 (98%)   | 9 (2%)   | 0        | 100         | 100 |
| 87  | OX    | 51/435 (12%)      | 48 (94%)    | 3 (6%)   | 0        | 100         | 100 |
| 88  | a     | 99/142 (70%)      | 97 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| All | All   | 14871/19622 (76%) | 14498 (98%) | 372 (2%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | AH    | 126 | ILE  |

### 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     | 99/164 (60%)  | 99 (100%)  | 0        | 100         | 100 |
| 2   | 1     | 53/60 (88%)   | 53 (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     | 270/303 (89%) | 270 (100%) | 0        | 100         | 100 |
| 9   | 8     | 146/190 (77%) | 146 (100%) | 0        | 100         | 100 |
| 10  | 9     | 104/112 (93%) | 104 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 12  | C     | 193/245 (79%)  | 193 (100%) | 0        | 100         | 100 |
| 13  | D     | 192/245 (78%)  | 192 (100%) | 0        | 100         | 100 |
| 14  | E     | 260/290 (90%)  | 260 (100%) | 0        | 100         | 100 |
| 15  | F     | 219/262 (84%)  | 219 (100%) | 0        | 100         | 100 |
| 16  | H     | 182/228 (80%)  | 182 (100%) | 0        | 100         | 100 |
| 17  | I     | 165/232 (71%)  | 165 (100%) | 0        | 100         | 100 |
| 18  | J     | 138/150 (92%)  | 138 (100%) | 0        | 100         | 100 |
| 19  | K     | 155/155 (100%) | 155 (100%) | 0        | 100         | 100 |
| 20  | L     | 98/124 (79%)   | 98 (100%)  | 0        | 100         | 100 |
| 21  | M     | 246/249 (99%)  | 246 (100%) | 0        | 100         | 100 |
| 22  | N     | 189/211 (90%)  | 189 (100%) | 0        | 100         | 100 |
| 23  | O     | 134/150 (89%)  | 134 (100%) | 0        | 100         | 100 |
| 24  | P     | 126/155 (81%)  | 126 (100%) | 0        | 100         | 100 |
| 25  | Q     | 207/256 (81%)  | 207 (100%) | 0        | 100         | 100 |
| 26  | R     | 118/126 (94%)  | 118 (100%) | 0        | 100         | 100 |
| 27  | S     | 146/180 (81%)  | 146 (100%) | 0        | 100         | 100 |
| 28  | T     | 146/176 (83%)  | 146 (100%) | 0        | 100         | 100 |
| 29  | U     | 134/135 (99%)  | 134 (100%) | 0        | 100         | 100 |
| 30  | W     | 94/119 (79%)   | 94 (100%)  | 0        | 100         | 100 |
| 31  | X     | 220/229 (96%)  | 220 (100%) | 0        | 100         | 100 |
| 32  | Y     | 163/223 (73%)  | 163 (100%) | 0        | 100         | 100 |
| 33  | Z     | 113/147 (77%)  | 113 (100%) | 0        | 100         | 100 |
| 34  | z     | 226/287 (79%)  | 226 (100%) | 0        | 100         | 100 |
| 35  | G     | 60/158 (38%)   | 60 (100%)  | 0        | 100         | 100 |
| 35  | t     | 40/158 (25%)   | 40 (100%)  | 0        | 100         | 100 |
| 35  | u     | 31/158 (20%)   | 31 (100%)  | 0        | 100         | 100 |
| 36  | V     | 183/191 (96%)  | 183 (100%) | 0        | 100         | 100 |
| 37  | b     | 132/186 (71%)  | 132 (100%) | 0        | 100         | 100 |
| 38  | d     | 237/274 (86%)  | 237 (100%) | 0        | 100         | 100 |
| 39  | e     | 207/236 (88%)  | 207 (100%) | 0        | 100         | 100 |
| 40  | g     | 124/148 (84%)  | 124 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 41  | h     | 104/148 (70%)  | 104 (100%) | 0        | 100         | 100 |
| 42  | i     | 86/110 (78%)   | 86 (100%)  | 0        | 100         | 100 |
| 43  | j     | 74/97 (76%)    | 74 (100%)  | 0        | 100         | 100 |
| 44  | k     | 83/89 (93%)    | 83 (100%)  | 0        | 100         | 100 |
| 45  | l     | 76/116 (66%)   | 76 (100%)  | 0        | 100         | 100 |
| 46  | m     | 61/113 (54%)   | 61 (100%)  | 0        | 100         | 100 |
| 48  | o     | 80/87 (92%)    | 80 (100%)  | 0        | 100         | 100 |
| 49  | q     | 153/178 (86%)  | 153 (100%) | 0        | 100         | 100 |
| 50  | r     | 147/169 (87%)  | 147 (100%) | 0        | 100         | 100 |
| 51  | AB    | 198/249 (80%)  | 198 (100%) | 0        | 100         | 100 |
| 52  | AC    | 115/143 (80%)  | 115 (100%) | 0        | 100         | 100 |
| 53  | AD    | 286/357 (80%)  | 286 (100%) | 0        | 100         | 100 |
| 54  | AE    | 104/107 (97%)  | 104 (100%) | 0        | 100         | 100 |
| 55  | AF    | 185/209 (88%)  | 185 (100%) | 0        | 100         | 100 |
| 56  | AG    | 285/342 (83%)  | 285 (100%) | 0        | 100         | 100 |
| 57  | AH    | 130/180 (72%)  | 130 (100%) | 0        | 100         | 100 |
| 58  | AJ    | 93/118 (79%)   | 93 (100%)  | 0        | 100         | 100 |
| 59  | AK    | 91/113 (80%)   | 91 (100%)  | 0        | 100         | 100 |
| 60  | AL    | 158/226 (70%)  | 158 (100%) | 0        | 100         | 100 |
| 61  | AM    | 97/113 (86%)   | 97 (100%)  | 0        | 100         | 100 |
| 62  | AN    | 96/115 (84%)   | 96 (100%)  | 0        | 100         | 100 |
| 63  | AO    | 174/230 (76%)  | 173 (99%)  | 1 (1%)   | 78          | 88  |
| 64  | AP    | 88/123 (72%)   | 88 (100%)  | 0        | 100         | 100 |
| 65  | AR    | 264/318 (83%)  | 264 (100%) | 0        | 100         | 100 |
| 66  | AS    | 116/164 (71%)  | 116 (100%) | 0        | 100         | 100 |
| 67  | AT    | 153/157 (98%)  | 153 (100%) | 0        | 100         | 100 |
| 68  | AU    | 152/174 (87%)  | 152 (100%) | 0        | 100         | 100 |
| 69  | AV    | 325/364 (89%)  | 325 (100%) | 0        | 100         | 100 |
| 70  | AW    | 87/158 (55%)   | 87 (100%)  | 0        | 100         | 100 |
| 71  | AZ    | 90/95 (95%)    | 90 (100%)  | 0        | 100         | 100 |
| 72  | A0    | 188/189 (100%) | 188 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 73  | A1    | 257/291 (88%)     | 257 (100%)   | 0        | 100         | 100 |
| 74  | A3    | 65/166 (39%)      | 65 (100%)    | 0        | 100         | 100 |
| 76  | AY    | 110/357 (31%)     | 110 (100%)   | 0        | 100         | 100 |
| 78  | AI    | 105/147 (71%)     | 105 (100%)   | 0        | 100         | 100 |
| 79  | A4    | 526/609 (86%)     | 526 (100%)   | 0        | 100         | 100 |
| 80  | AX    | 311/351 (89%)     | 311 (100%)   | 0        | 100         | 100 |
| 81  | A2    | 100/100 (100%)    | 100 (100%)   | 0        | 100         | 100 |
| 82  | AQ    | 78/78 (100%)      | 78 (100%)    | 0        | 100         | 100 |
| 83  | c     | 251/288 (87%)     | 251 (100%)   | 0        | 100         | 100 |
| 84  | f     | 139/188 (74%)     | 139 (100%)   | 0        | 100         | 100 |
| 85  | p     | 135/181 (75%)     | 135 (100%)   | 0        | 100         | 100 |
| 86  | s     | 339/381 (89%)     | 339 (100%)   | 0        | 100         | 100 |
| 87  | OX    | 49/372 (13%)      | 49 (100%)    | 0        | 100         | 100 |
| 88  | a     | 99/133 (74%)      | 99 (100%)    | 0        | 100         | 100 |
| All | All   | 13284/16932 (78%) | 13283 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | AO    | 154 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | AD    | 361 | GLN  |
| 65  | AR    | 86  | ASN  |
| 88  | a     | 126 | HIS  |
| 54  | AE    | 56  | GLN  |
| 56  | AG    | 384 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 11  | A     | 1556/1558 (99%) | 261 (16%)         | 3 (0%)          |
| 75  | Az    | 33/34 (97%)     | 13 (39%)          | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 77  | AA    | 953/954 (99%)   | 143 (15%)         | 0               |
| 89  | Aw    | 64/76 (84%)     | 34 (53%)          | 0               |
| 90  | Ax    | 67/76 (88%)     | 14 (20%)          | 0               |
| 91  | B     | 70/72 (97%)     | 16 (22%)          | 0               |
| All | All   | 2743/2770 (99%) | 481 (17%)         | 3 (0%)          |

5 of 481 RNA backbone outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1681 | G    |
| 11  | A     | 1689 | C    |
| 11  | A     | 1692 | A    |
| 11  | A     | 1699 | C    |
| 11  | A     | 1700 | U    |

All (3) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 2194 | U    |
| 11  | A     | 2245 | A    |
| 11  | A     | 2484 | C    |

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

13 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 | $\# Z  > 2$ |
| 77  | B8T  | AA    | 1486 | 96,77 | 19,22,23     | 0.41 | 0           | 25,31,34    | 0.31 | 0           |
| 11  | OMG  | A     | 2815 | 11,93 | 23,26,27     | 0.38 | 0           | 32,38,41    | 0.42 | 0           |
| 11  | OMU  | A     | 3039 | 11,93 | 19,22,23     | 0.33 | 0           | 25,31,34    | 0.74 | 1 (4%)      |
| 77  | MA6  | AA    | 1584 | 77    | 23,26,27     | 0.34 | 0           | 33,38,41    | 0.74 | 1 (3%)      |
| 91  | 1MA  | B     | 9    | 91    | 21,25,26     | 0.38 | 0           | 30,37,40    | 0.65 | 0           |
| 77  | MA6  | AA    | 1583 | 77    | 23,26,27     | 0.34 | 0           | 33,38,41    | 0.72 | 1 (3%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 91  | 2MG  | B     | 10   | 91   | 23,26,27     | 0.36 | 0        | 33,38,41    | 0.41 | 0        |
| 91  | PSU  | B     | 39   | 91   | 18,21,22     | 1.05 | 1 (5%)   | 21,30,33    | 0.72 | 0        |
| 11  | PSU  | A     | 3067 | 11   | 18,21,22     | 1.13 | 2 (11%)  | 21,30,33    | 0.80 | 1 (4%)   |
| 11  | OMG  | A     | 3040 | 11   | 23,26,27     | 0.35 | 0        | 32,38,41    | 0.45 | 0        |
| 77  | 5MU  | AA    | 1076 | 77   | 19,22,23     | 0.38 | 0        | 27,32,35    | 0.59 | 0        |
| 11  | 1MA  | A     | 2617 | 11   | 21,25,26     | 0.42 | 0        | 30,37,40    | 0.60 | 0        |
| 77  | 5MC  | AA    | 1488 | 77   | 19,22,23     | 0.84 | 1 (5%)   | 26,32,35    | 0.52 | 0        |

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

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 77  | B8T  | AA    | 1486 | 96,77 | -       | 0/7/27/28  | 0/2/2/2 |
| 11  | OMG  | A     | 2815 | 11,93 | -       | 0/9/27/28  | 0/3/3/3 |
| 11  | OMU  | A     | 3039 | 11,93 | -       | 0/9/27/28  | 0/2/2/2 |
| 77  | MA6  | AA    | 1584 | 77    | -       | 1/11/29/30 | 0/3/3/3 |
| 91  | 1MA  | B     | 9    | 91    | -       | 1/7/25/26  | 0/3/3/3 |
| 77  | MA6  | AA    | 1583 | 77    | -       | 0/11/29/30 | 0/3/3/3 |
| 91  | 2MG  | B     | 10   | 91    | -       | 0/9/27/28  | 0/3/3/3 |
| 91  | PSU  | B     | 39   | 91    | -       | 0/7/25/26  | 0/2/2/2 |
| 11  | PSU  | A     | 3067 | 11    | -       | 1/7/25/26  | 0/2/2/2 |
| 11  | OMG  | A     | 3040 | 11    | -       | 0/9/27/28  | 0/3/3/3 |
| 77  | 5MU  | AA    | 1076 | 77    | -       | 4/7/25/26  | 0/2/2/2 |
| 11  | 1MA  | A     | 2617 | 11    | -       | 0/7/25/26  | 0/3/3/3 |
| 77  | 5MC  | AA    | 1488 | 77    | -       | 0/7/25/26  | 0/2/2/2 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 91  | B     | 39   | PSU  | C6-C5   | 3.65  | 1.39        | 1.35     |
| 11  | A     | 3067 | PSU  | C6-C5   | 3.43  | 1.39        | 1.35     |
| 77  | AA    | 1488 | 5MC  | C5-C4   | -3.33 | 1.41        | 1.44     |
| 11  | A     | 3067 | PSU  | O4'-C1' | -2.75 | 1.40        | 1.43     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 77  | AA    | 1584 | MA6  | C2-N1-C6 | 2.94 | 119.02      | 111.83   |
| 77  | AA    | 1583 | MA6  | C2-N1-C6 | 2.94 | 119.02      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | A     | 3039 | OMU  | C2'-C1'-N1  | -2.62 | 109.26      | 114.24   |
| 11  | A     | 3067 | PSU  | O4'-C1'-C2' | 2.40  | 108.47      | 105.15   |

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 77  | AA    | 1076 | 5MU  | O4'-C4'-C5'-O5' |
| 77  | AA    | 1076 | 5MU  | C3'-C4'-C5'-O5' |
| 77  | AA    | 1584 | MA6  | C4'-C5'-O5'-P   |
| 77  | AA    | 1076 | 5MU  | C2'-C1'-N1-C6   |
| 77  | AA    | 1076 | 5MU  | C2'-C1'-N1-C2   |

There are no ring outliers.

5 monomers are involved in 6 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 77  | AA    | 1486 | B8T  | 1       | 0            |
| 11  | A     | 2815 | OMG  | 1       | 0            |
| 11  | A     | 3039 | OMU  | 1       | 0            |
| 77  | AA    | 1583 | MA6  | 2       | 0            |
| 77  | AA    | 1488 | 5MC  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 279 ligands modelled in this entry, 261 are monoatomic - leaving 18 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 |
| 99  | SPM  | AA    | 1702 | -     | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.25 | 0        |
| 94  | SPD  | A     | 3301 | -     | 9,9,9        | 0.14 | 0        | 8,8,8       | 0.17 | 0        |
| 98  | NAD  | AA    | 1701 | 96    | 46,48,48     | 1.22 | 3 (6%)   | 64,73,73    | 0.85 | 4 (6%)   |
| 94  | SPD  | AA    | 1703 | -     | 9,9,9        | 0.15 | 0        | 8,8,8       | 0.24 | 0        |
| 94  | SPD  | AA    | 1783 | -     | 9,9,9        | 0.15 | 0        | 8,8,8       | 0.19 | 0        |
| 97  | FES  | AT    | 201  | 67,61 | 0,4,4        | -    | -        | -           | -    | -        |
| 94  | SPD  | A     | 3472 | -     | 9,9,9        | 0.14 | 0        | 8,8,8       | 0.34 | 0        |
| 95  | PUT  | A     | 3303 | -     | 5,5,5        | 0.13 | 0        | 4,4,4       | 0.24 | 0        |
| 99  | SPM  | AA    | 1780 | -     | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.17 | 0        |
| 94  | SPD  | A     | 3302 | -     | 9,9,9        | 0.15 | 0        | 8,8,8       | 0.20 | 0        |
| 97  | FES  | r     | 201  | 50,17 | 0,4,4        | -    | -        | -           | -    | -        |
| 101 | GDP  | AX    | 503  | -     | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.74 | 7 (15%)  |
| 94  | SPD  | A     | 3471 | -     | 9,9,9        | 0.17 | 0        | 8,8,8       | 0.18 | 0        |
| 97  | FES  | AP    | 201  | 54,64 | 0,4,4        | -    | -        | -           | -    | -        |
| 102 | VAL  | B     | 101  | 91    | 4,6,7        | 0.79 | 0        | 6,7,9       | 1.02 | 1 (16%)  |
| 94  | SPD  | AA    | 1782 | -     | 9,9,9        | 0.14 | 0        | 8,8,8       | 0.16 | 0        |
| 100 | ATP  | AX    | 501  | 96    | 32,33,33     | 0.38 | 0        | 48,52,52    | 0.35 | 0        |
| 94  | SPD  | A     | 3473 | -     | 9,9,9        | 0.17 | 0        | 8,8,8       | 0.23 | 0        |

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

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 99  | SPM  | AA    | 1702 | -     | -       | 0/11/11/11 | -       |
| 94  | SPD  | A     | 3301 | -     | -       | 0/7/7/7    | -       |
| 97  | FES  | AP    | 201  | 54,64 | -       | -          | 0/1/1/1 |
| 98  | NAD  | AA    | 1701 | 96    | -       | 4/30/62/62 | 0/5/5/5 |
| 94  | SPD  | AA    | 1703 | -     | -       | 0/7/7/7    | -       |
| 94  | SPD  | AA    | 1783 | -     | -       | 0/7/7/7    | -       |
| 97  | FES  | AT    | 201  | 67,61 | -       | -          | 0/1/1/1 |
| 94  | SPD  | A     | 3472 | -     | -       | 1/7/7/7    | -       |
| 95  | PUT  | A     | 3303 | -     | -       | 0/3/3/3    | -       |
| 99  | SPM  | AA    | 1780 | -     | -       | 1/11/11/11 | -       |
| 94  | SPD  | A     | 3302 | -     | -       | 1/7/7/7    | -       |
| 101 | GDP  | AX    | 503  | -     | -       | 0/16/32/32 | 0/3/3/3 |
| 102 | VAL  | B     | 101  | 91    | -       | 2/5/6/8    | -       |
| 94  | SPD  | A     | 3471 | -     | -       | 0/7/7/7    | -       |
| 97  | FES  | r     | 201  | 50,17 | -       | -          | 0/1/1/1 |
| 94  | SPD  | AA    | 1782 | -     | -       | 0/7/7/7    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 100 | ATP  | AX    | 501  | 96   | -       | 0/22/38/38 | 0/3/3/3 |
| 94  | SPD  | A     | 3473 | -    | -       | 0/7/7/7    | -       |

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

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 98  | AA    | 1701 | NAD  | PA-O3   | 5.11  | 1.65        | 1.59     |
| 98  | AA    | 1701 | NAD  | PN-O3   | 3.05  | 1.62        | 1.59     |
| 101 | AX    | 503  | GDP  | C5-C4   | 3.04  | 1.47        | 1.38     |
| 98  | AA    | 1701 | NAD  | O4D-C1D | -2.70 | 1.37        | 1.40     |
| 101 | AX    | 503  | GDP  | C6-N1   | -2.53 | 1.34        | 1.38     |

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

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 101 | AX    | 503 | GDP  | C5-C4-N3 | -5.87 | 119.05      | 128.39   |
| 101 | AX    | 503 | GDP  | C2-N3-C4 | 4.76  | 120.50      | 112.30   |
| 101 | AX    | 503 | GDP  | N9-C4-N3 | 4.36  | 134.68      | 125.95   |
| 101 | AX    | 503 | GDP  | C6-C5-N7 | 3.18  | 136.08      | 130.29   |
| 101 | AX    | 503 | GDP  | C4-C5-N7 | -2.48 | 106.75      | 110.67   |

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 102 | B     | 101  | VAL  | O-C-CA-CB       |
| 102 | B     | 101  | VAL  | C-CA-CB-CG2     |
| 98  | AA    | 1701 | NAD  | O4D-C4D-C5D-O5D |
| 98  | AA    | 1701 | NAD  | C3D-C4D-C5D-O5D |
| 94  | A     | 3302 | SPD  | N1-C2-C3-C4     |

There are no ring outliers.

7 monomers are involved in 14 short contacts:

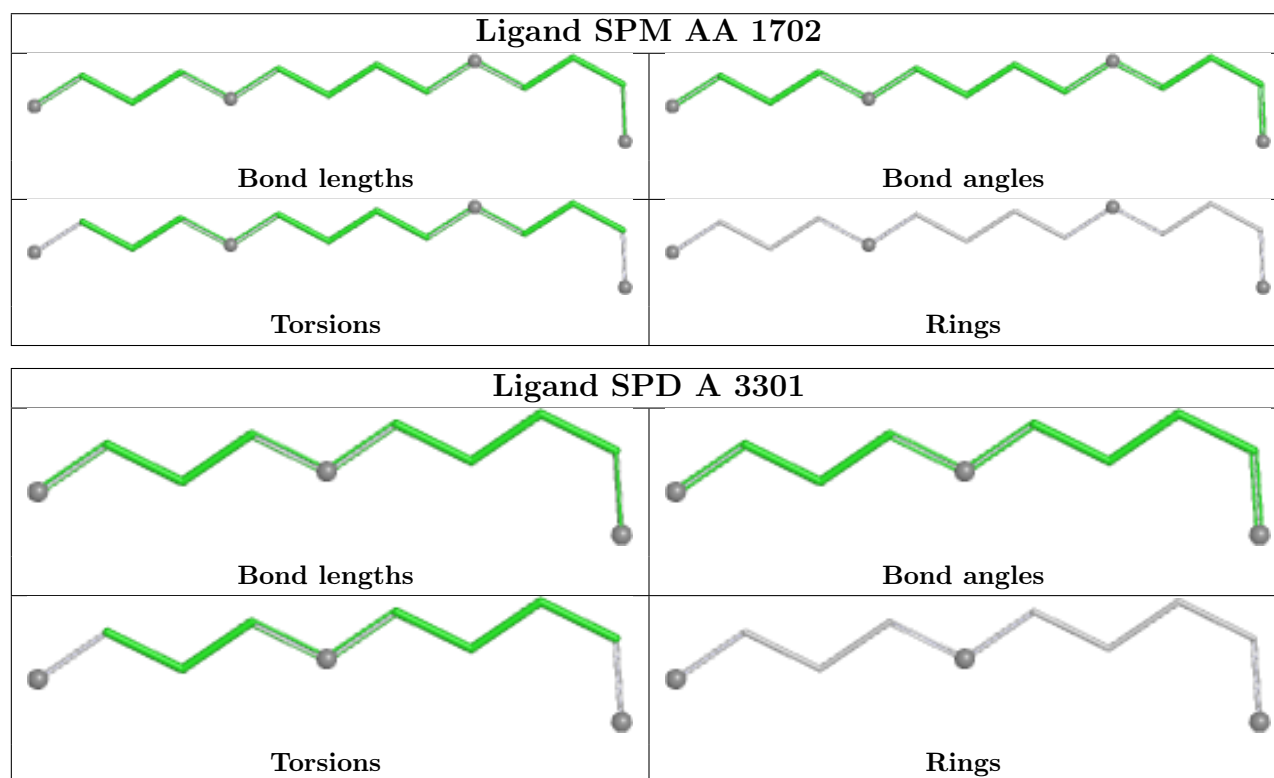
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 98  | AA    | 1701 | NAD  | 1       | 0            |
| 94  | AA    | 1703 | SPD  | 1       | 0            |
| 94  | A     | 3302 | SPD  | 1       | 0            |
| 97  | r     | 201  | FES  | 1       | 0            |
| 101 | AX    | 503  | GDP  | 3       | 0            |
| 102 | B     | 101  | VAL  | 4       | 0            |

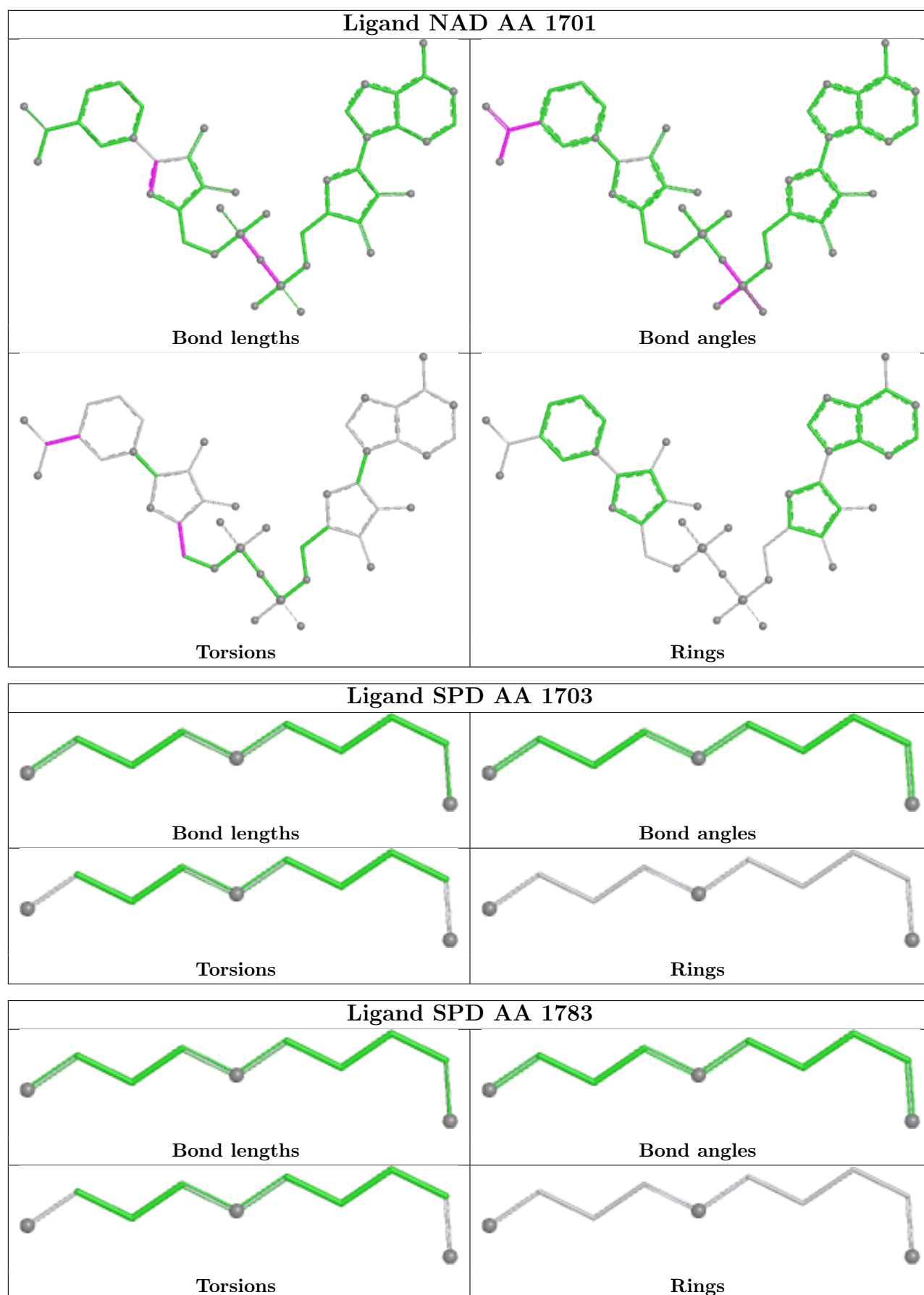
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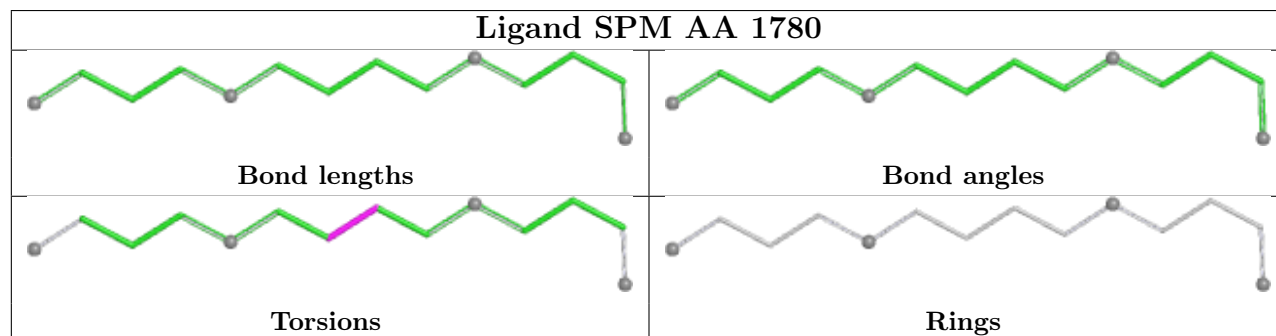
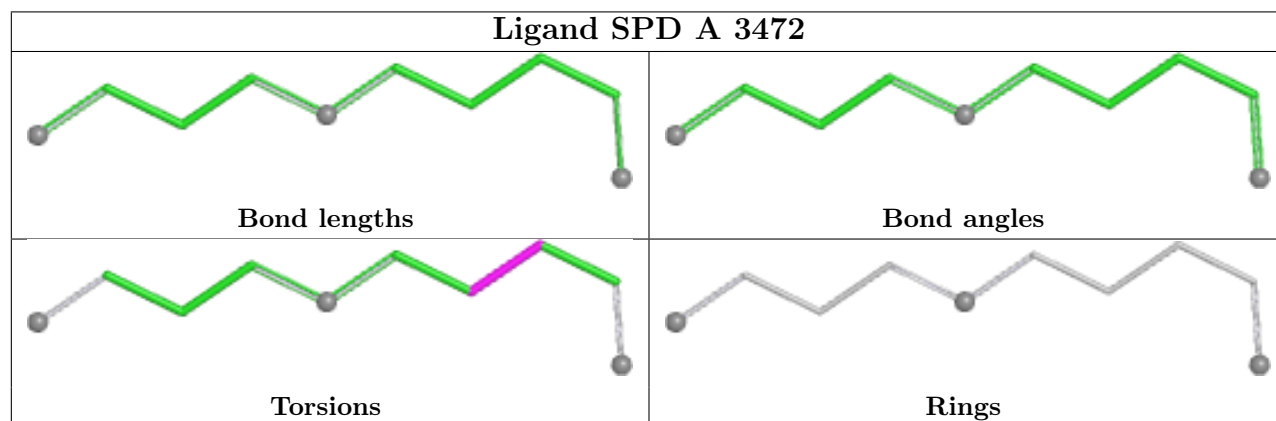
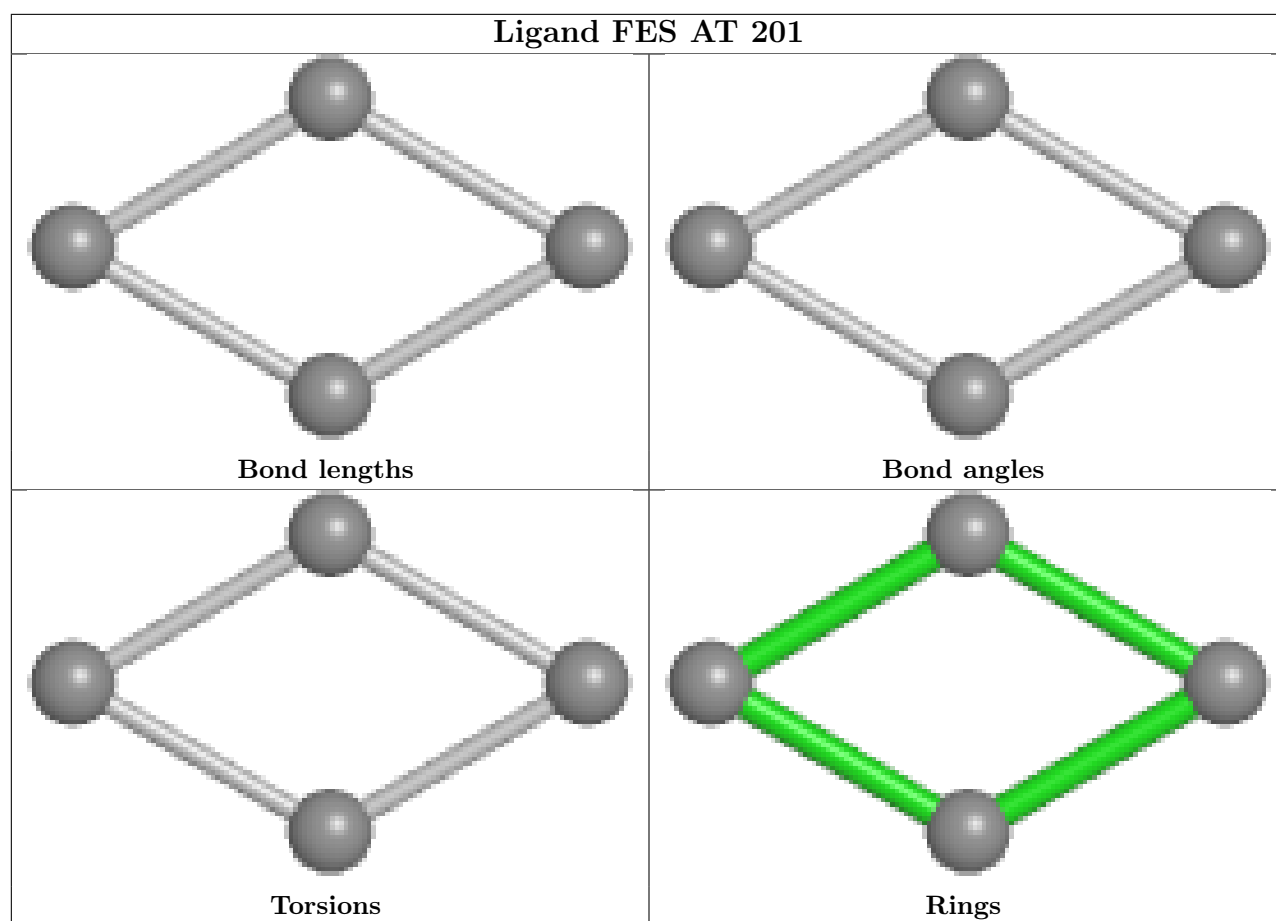
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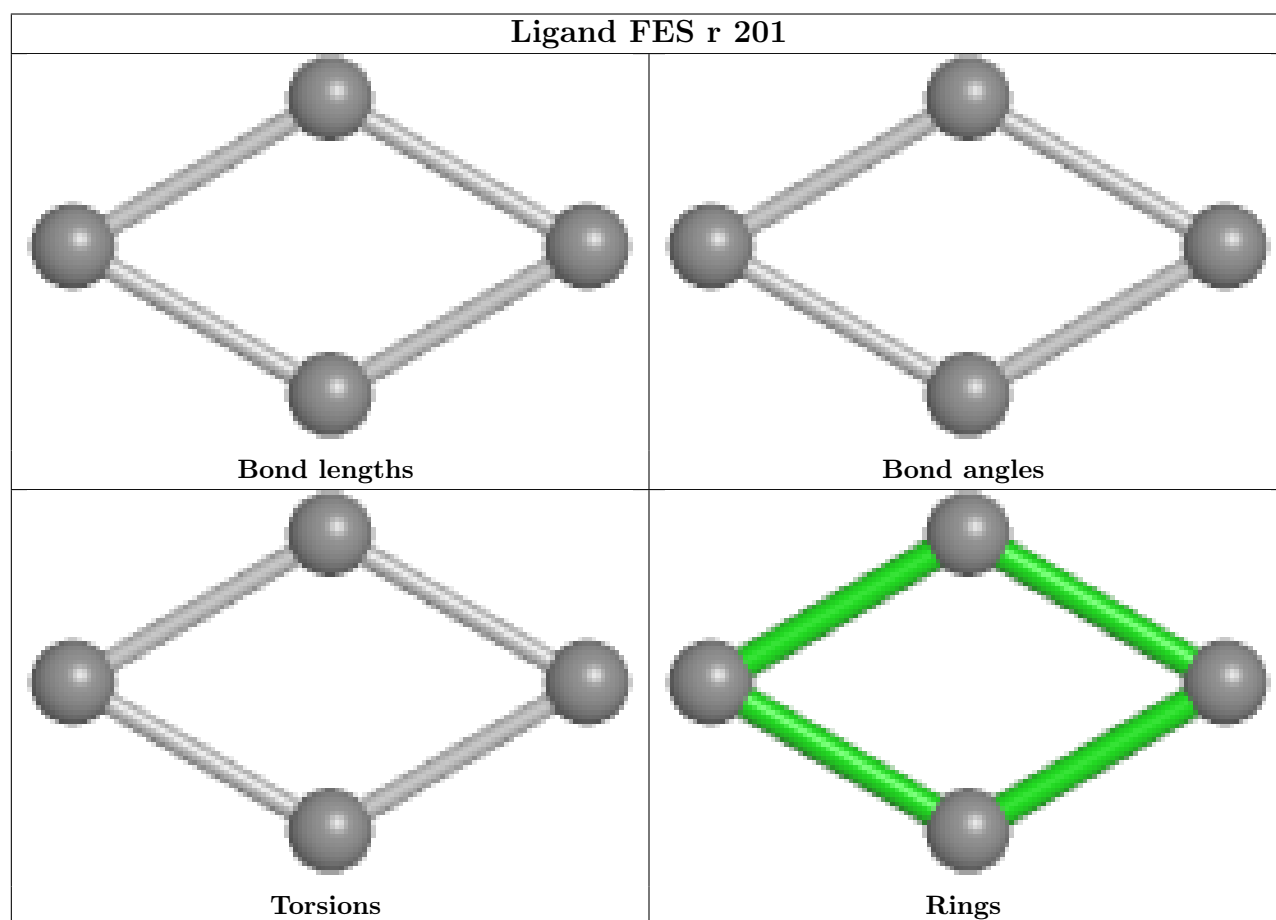
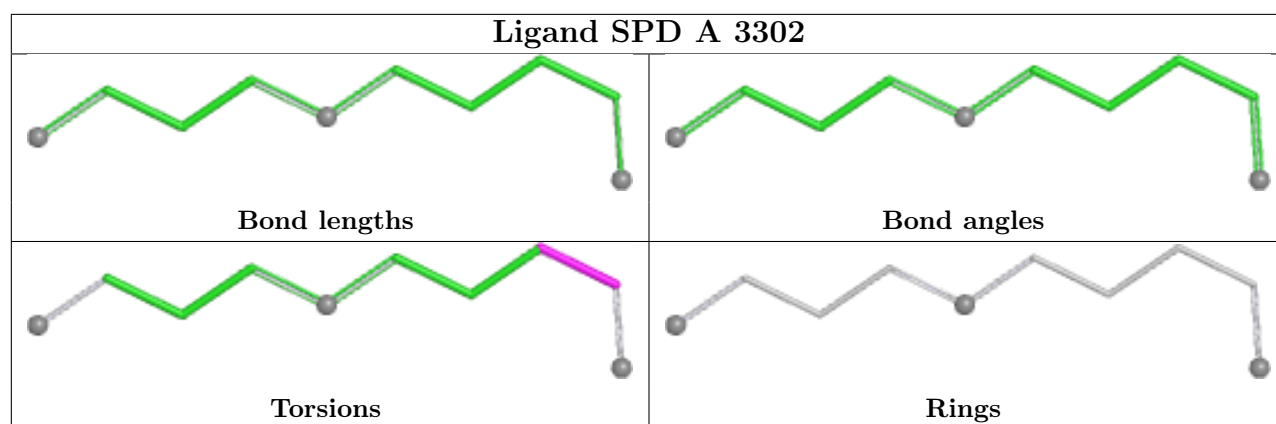
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 94  | AA    | 1782 | SPD  | 3       | 0            |

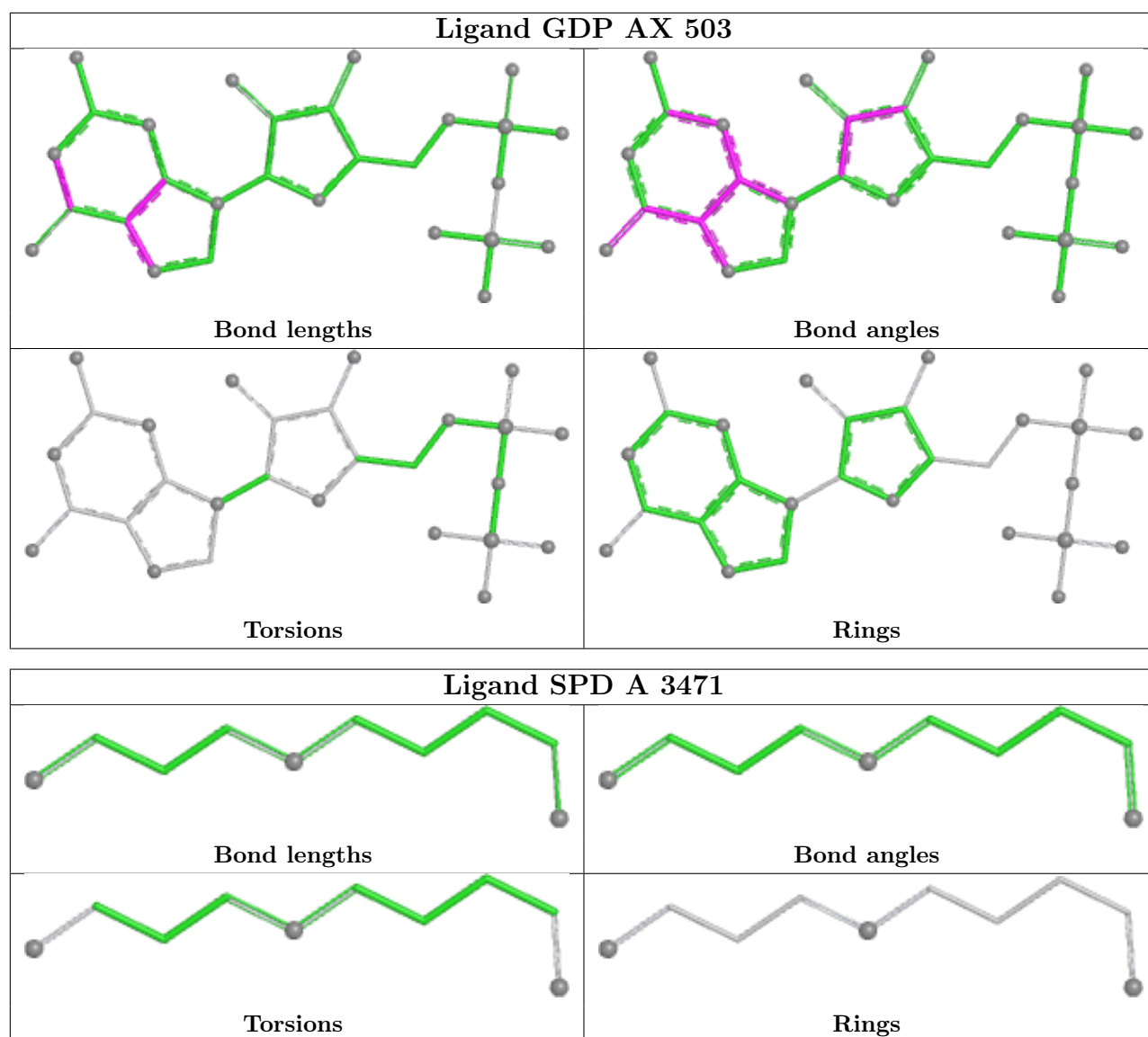
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

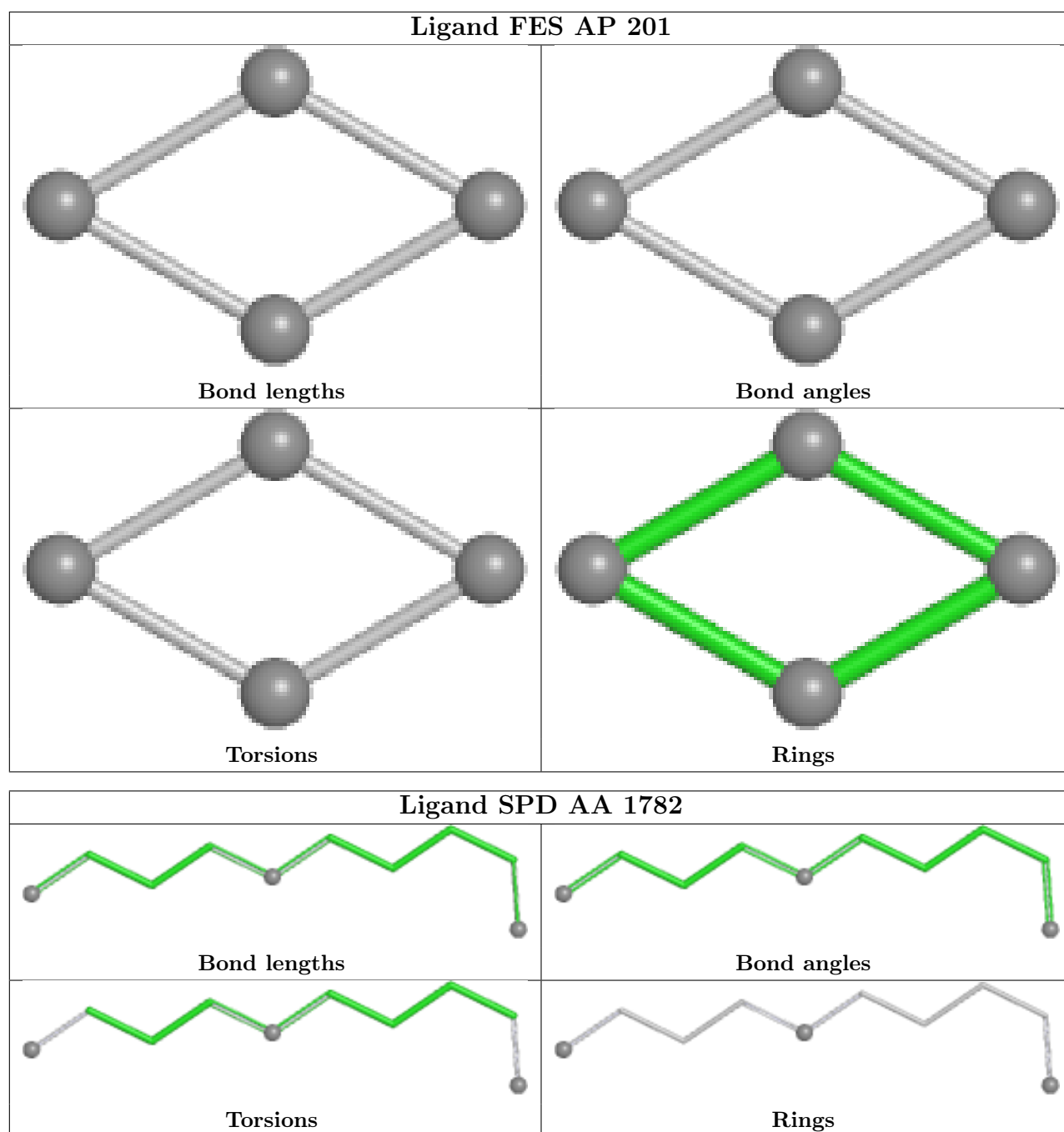


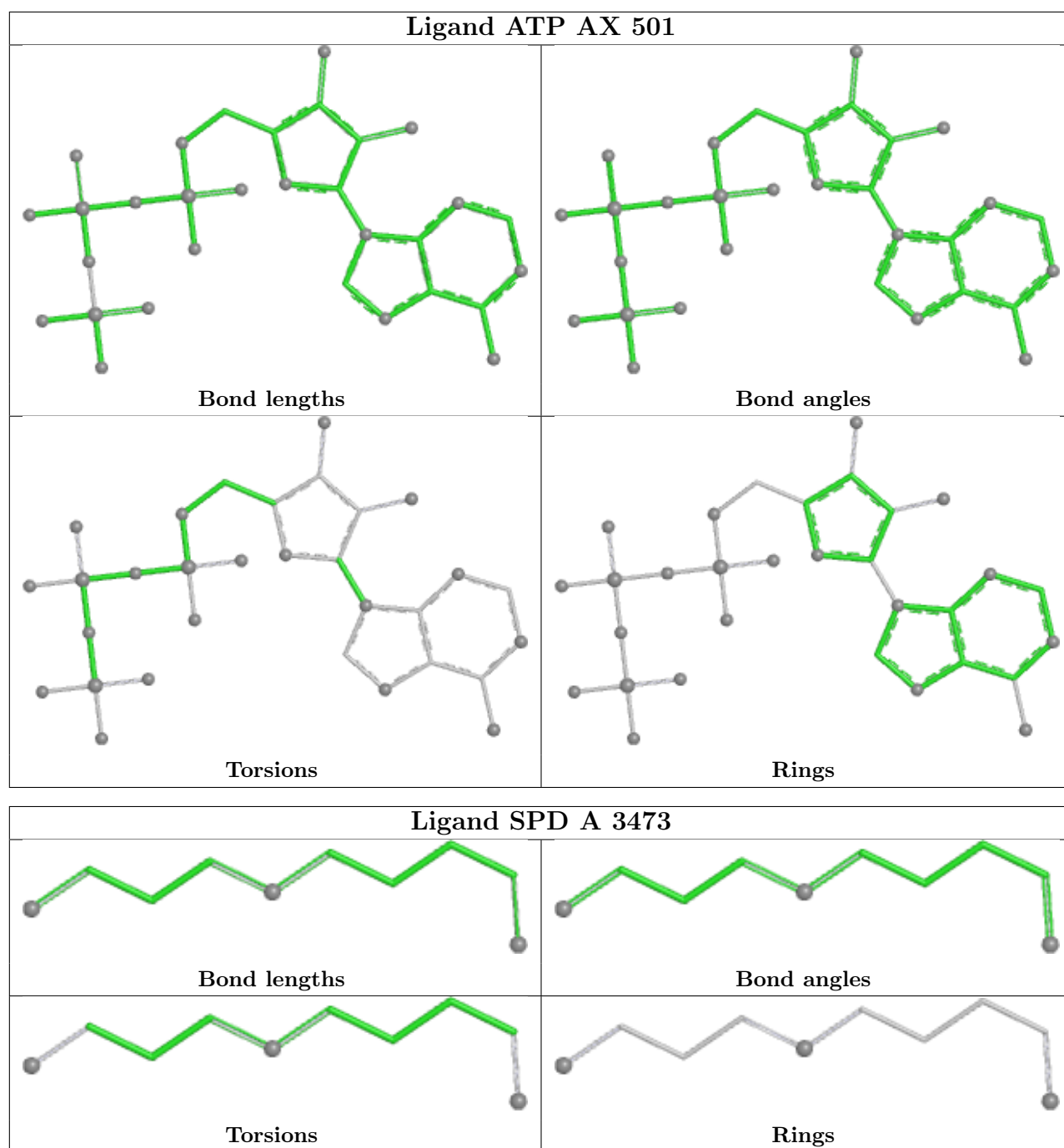












## 5.7 Other polymers [i](#)

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 |
|-----|-------|------------------|
| 11  | A     | 1                |
| 91  | B     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 2357:C    | O3'    | 2361:G    | P      | 9.73         |
| 1     | B     | 46:A      | O3'    | 48:U      | P      | 4.60         |

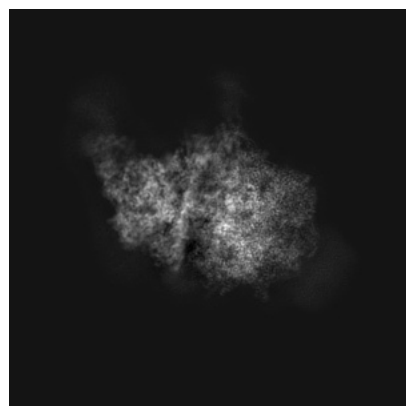
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71829. These allow visual inspection of the internal detail of the map and identification of artifacts.

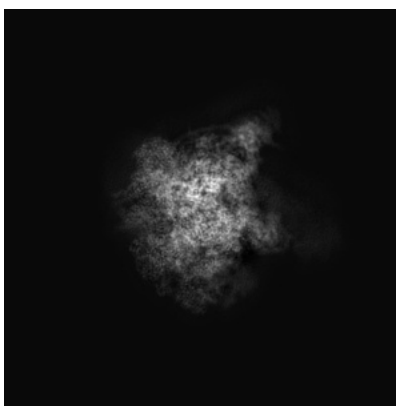
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

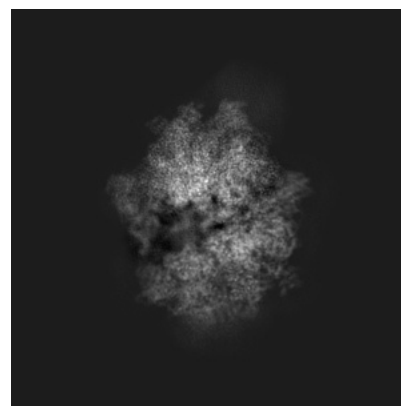
#### 6.1.1 Primary map



X

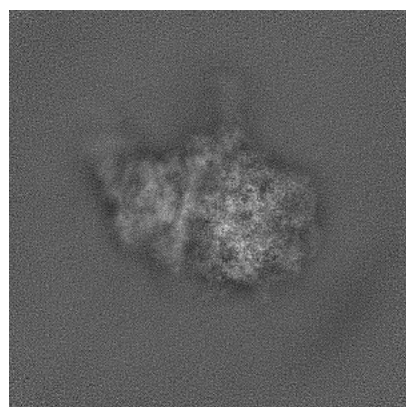


Y

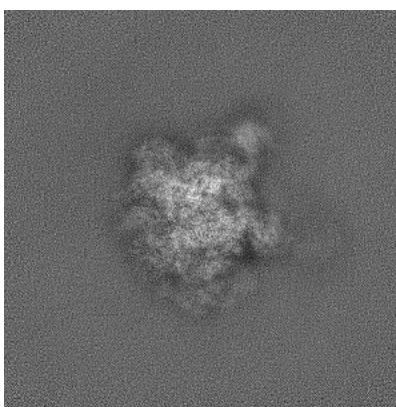


Z

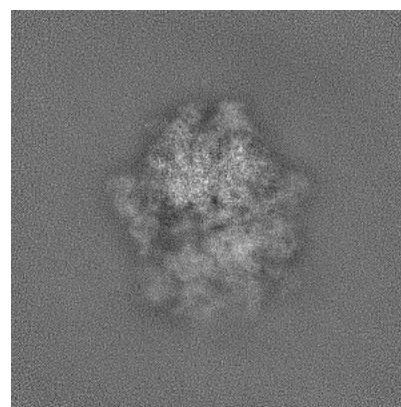
#### 6.1.2 Raw map



X



Y

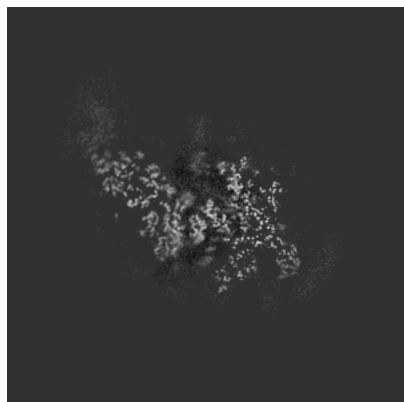


Z

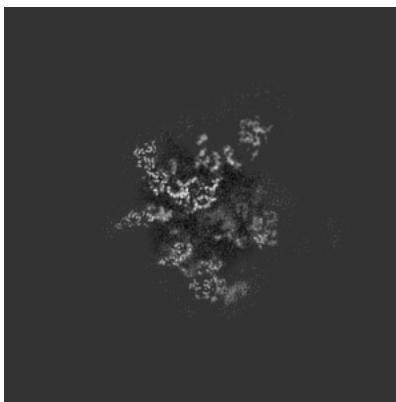
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

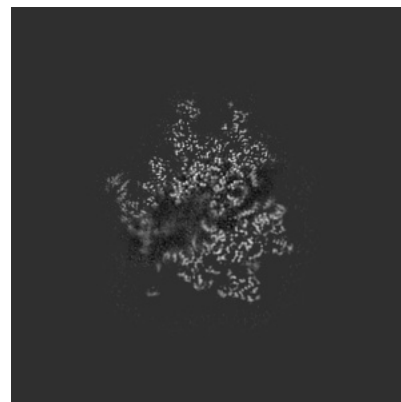
### 6.2.1 Primary map



X Index: 240

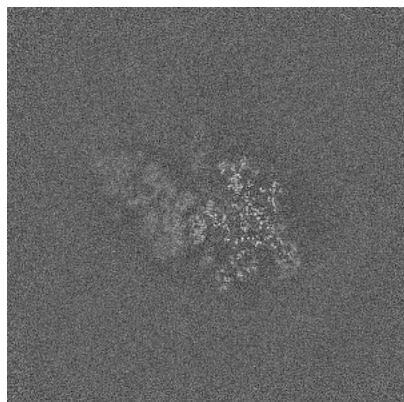


Y Index: 240

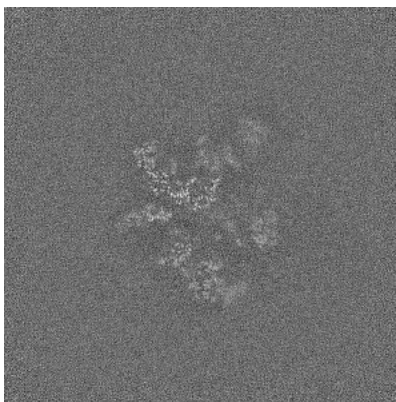


Z Index: 240

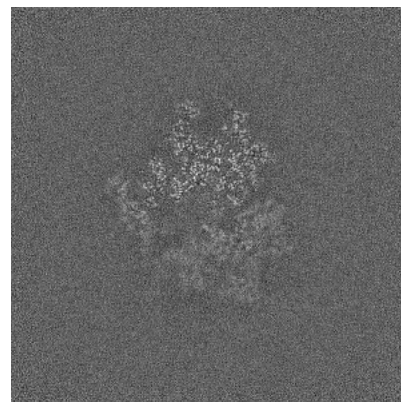
### 6.2.2 Raw map



X Index: 240



Y Index: 240

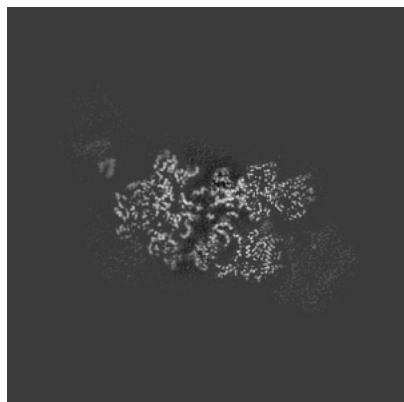


Z Index: 240

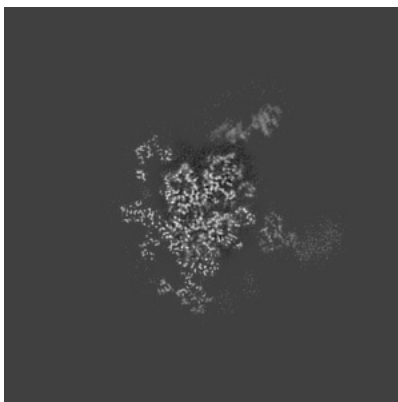
The images above show central slices of the map in three orthogonal directions.

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

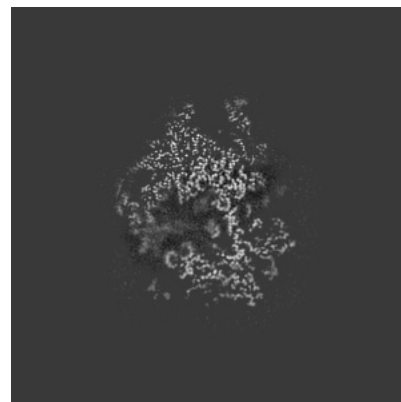
### 6.3.1 Primary map



X Index: 275

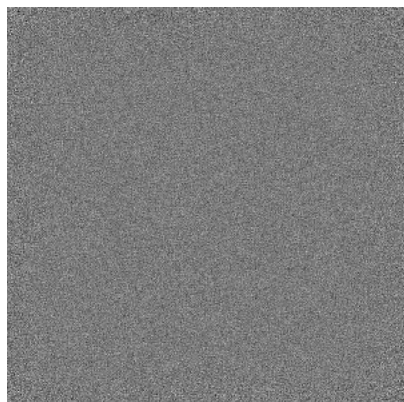


Y Index: 263

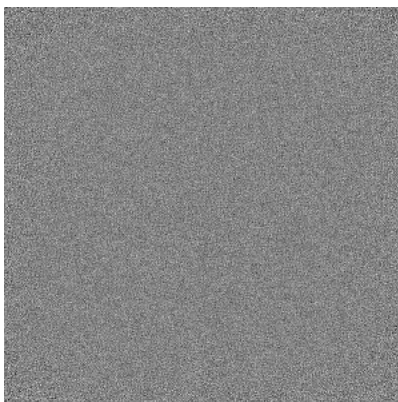


Z Index: 249

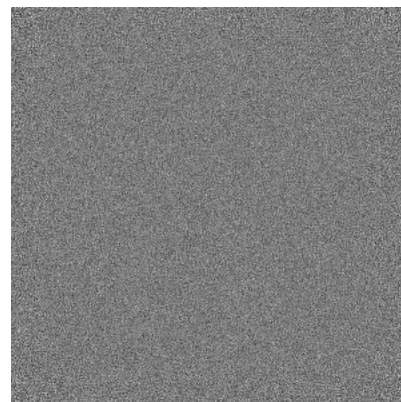
### 6.3.2 Raw map



X Index: 0



Y Index: 0

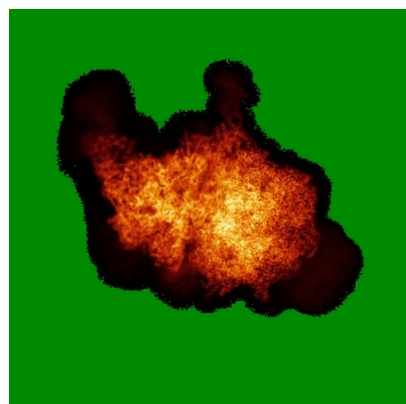


Z Index: 0

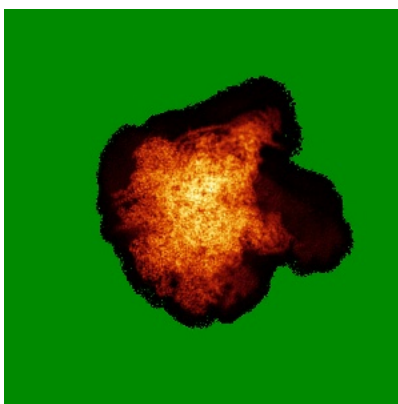
The images above show the largest variance slices of the map in three orthogonal directions.

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

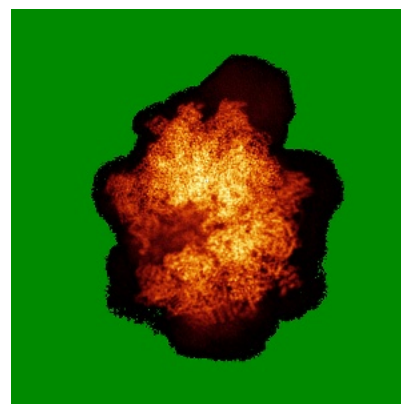
### 6.4.1 Primary map



X

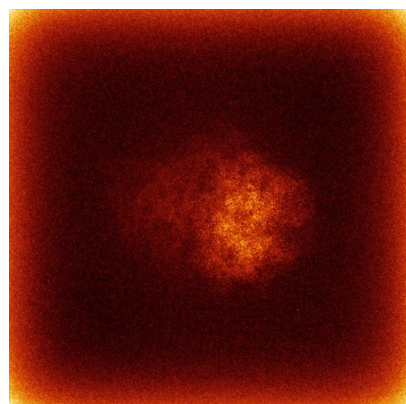


Y

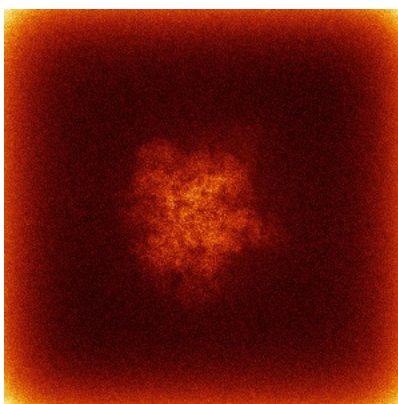


Z

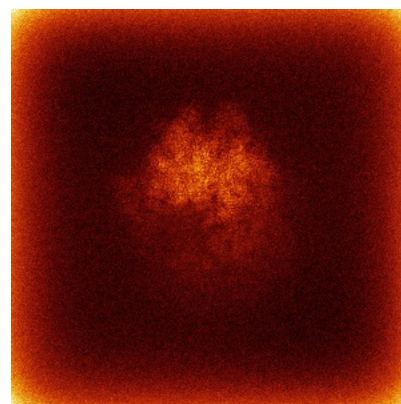
### 6.4.2 Raw map



X



Y

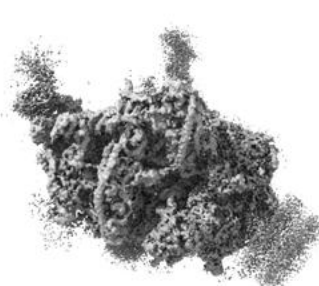


Z

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

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

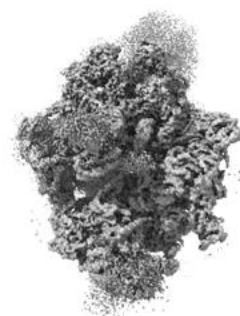
### 6.5.1 Primary map



X



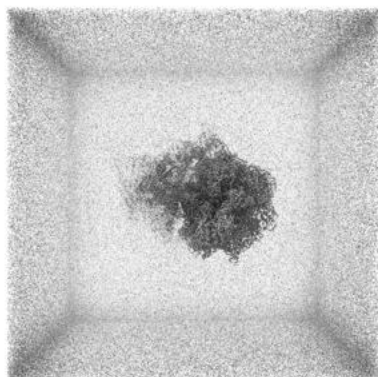
Y



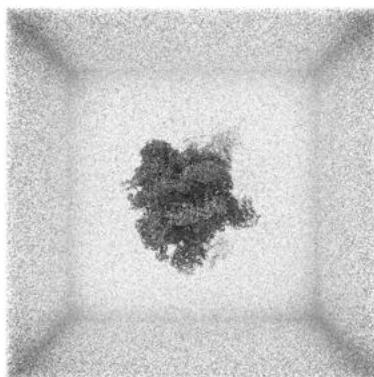
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

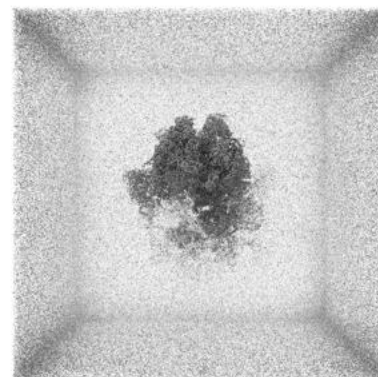
### 6.5.2 Raw map



X



Y



Z

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

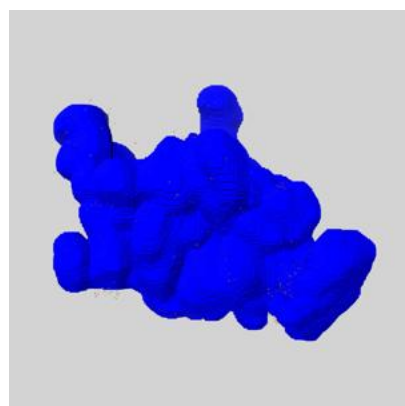
## 6.6 Mask visualisation [i](#)

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

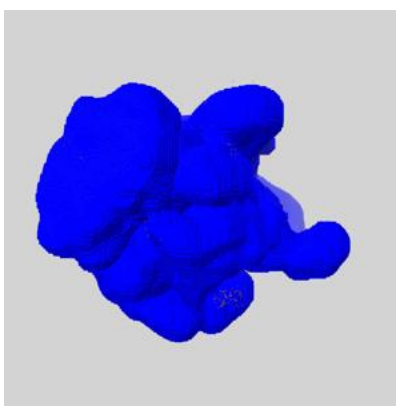
A mask typically either:

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

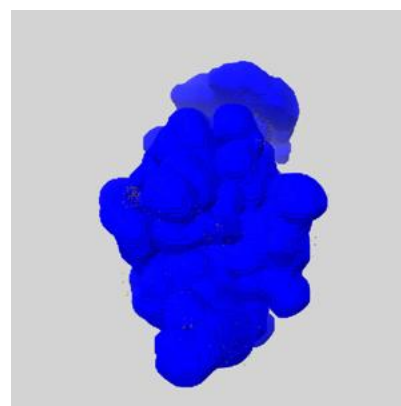
### 6.6.1 emd\_71829\_msk\_1.map [i](#)



X



Y

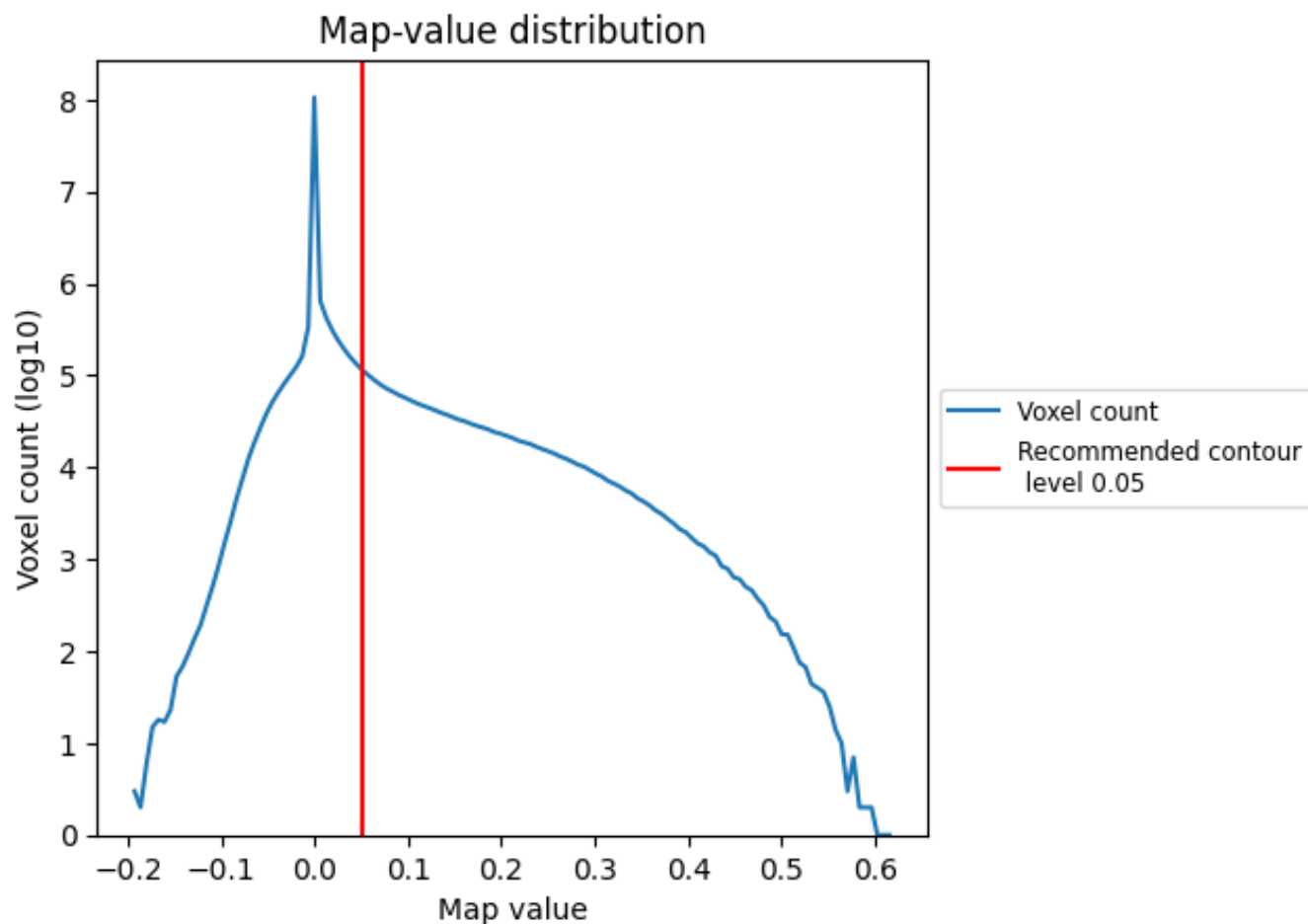


Z

## 7 Map analysis [i](#)

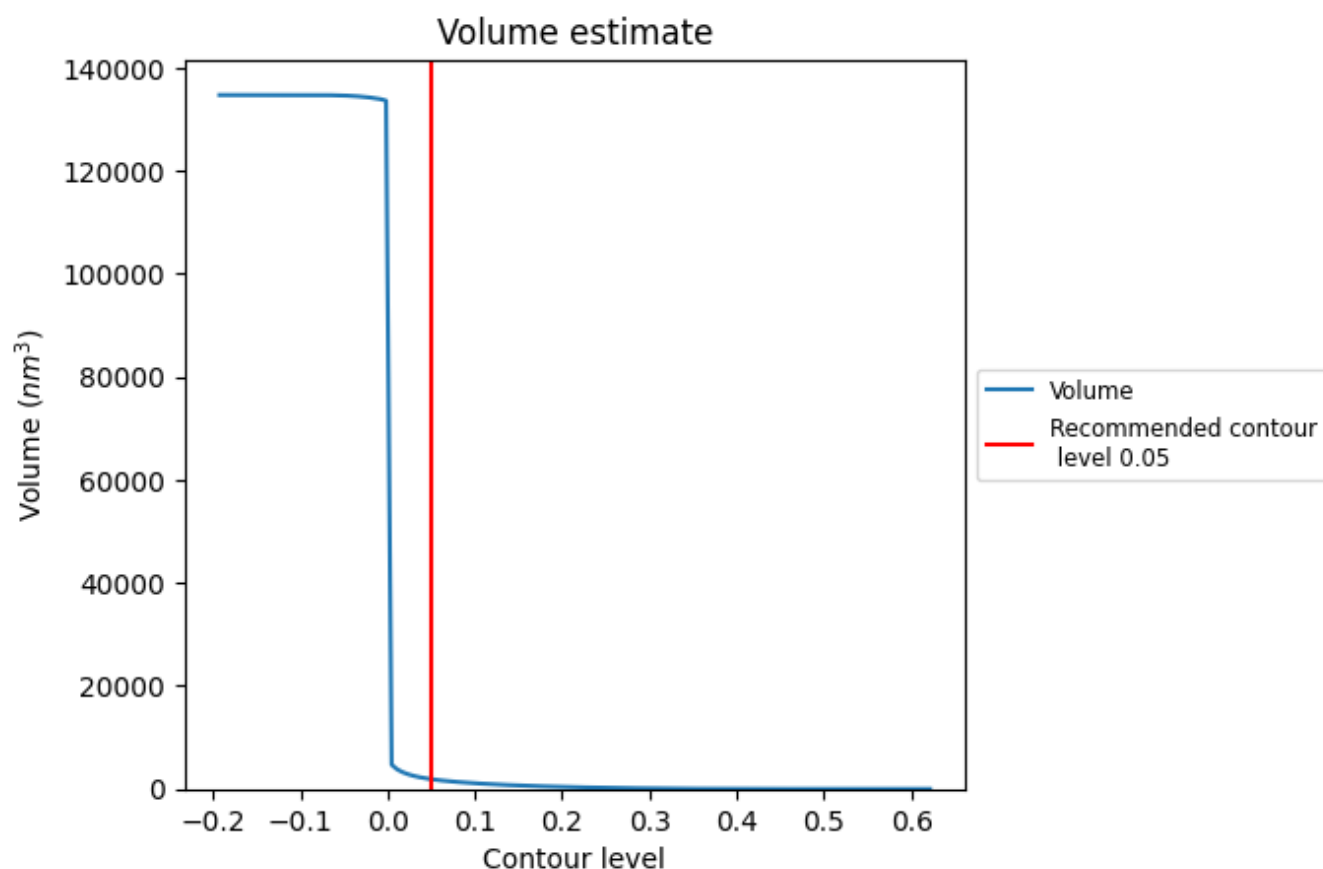
This section contains the results of statistical analysis of the map.

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



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

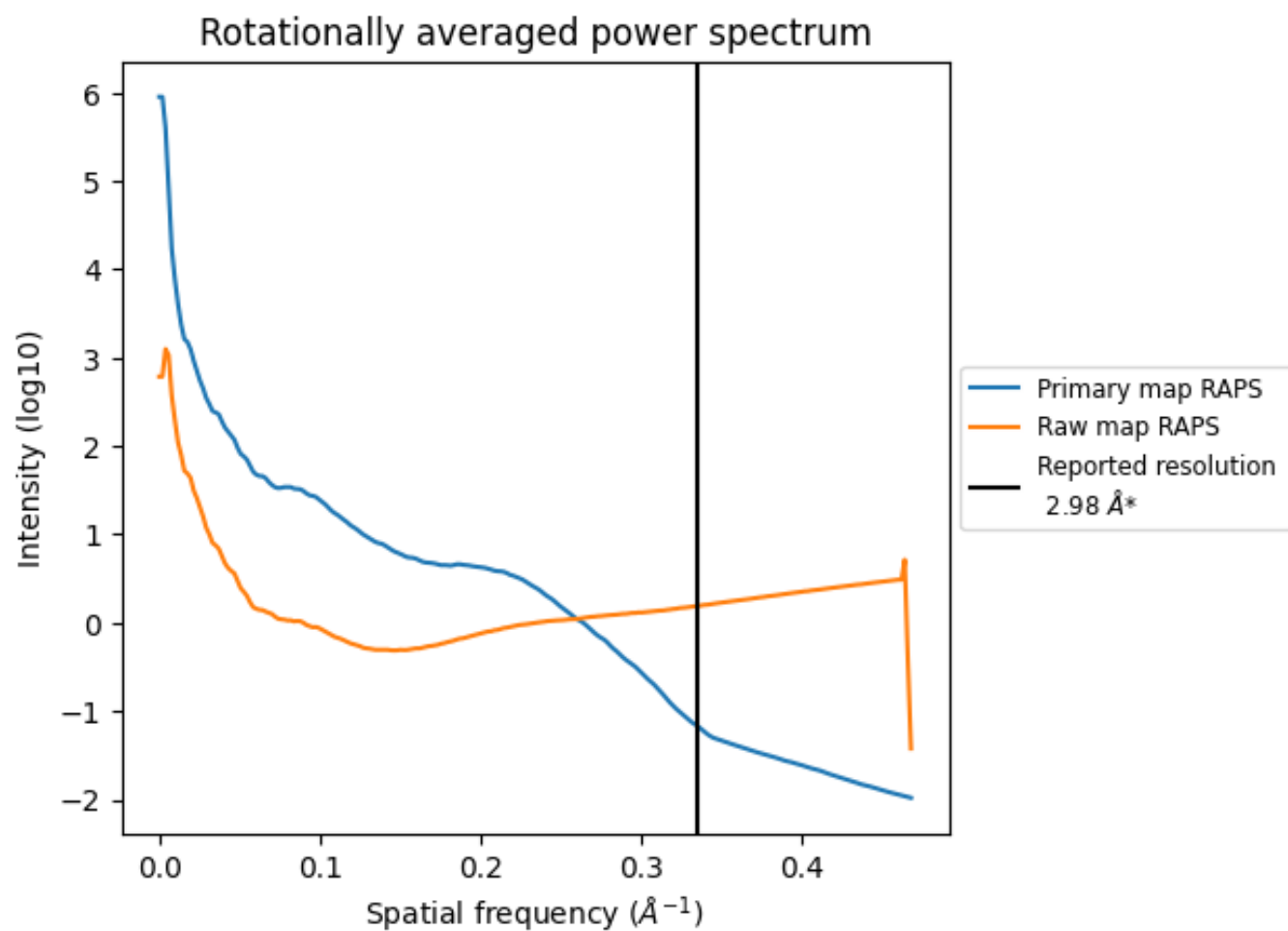
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1895  $\text{nm}^3$ ; this corresponds to an approximate mass of 1712 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 ⓘ

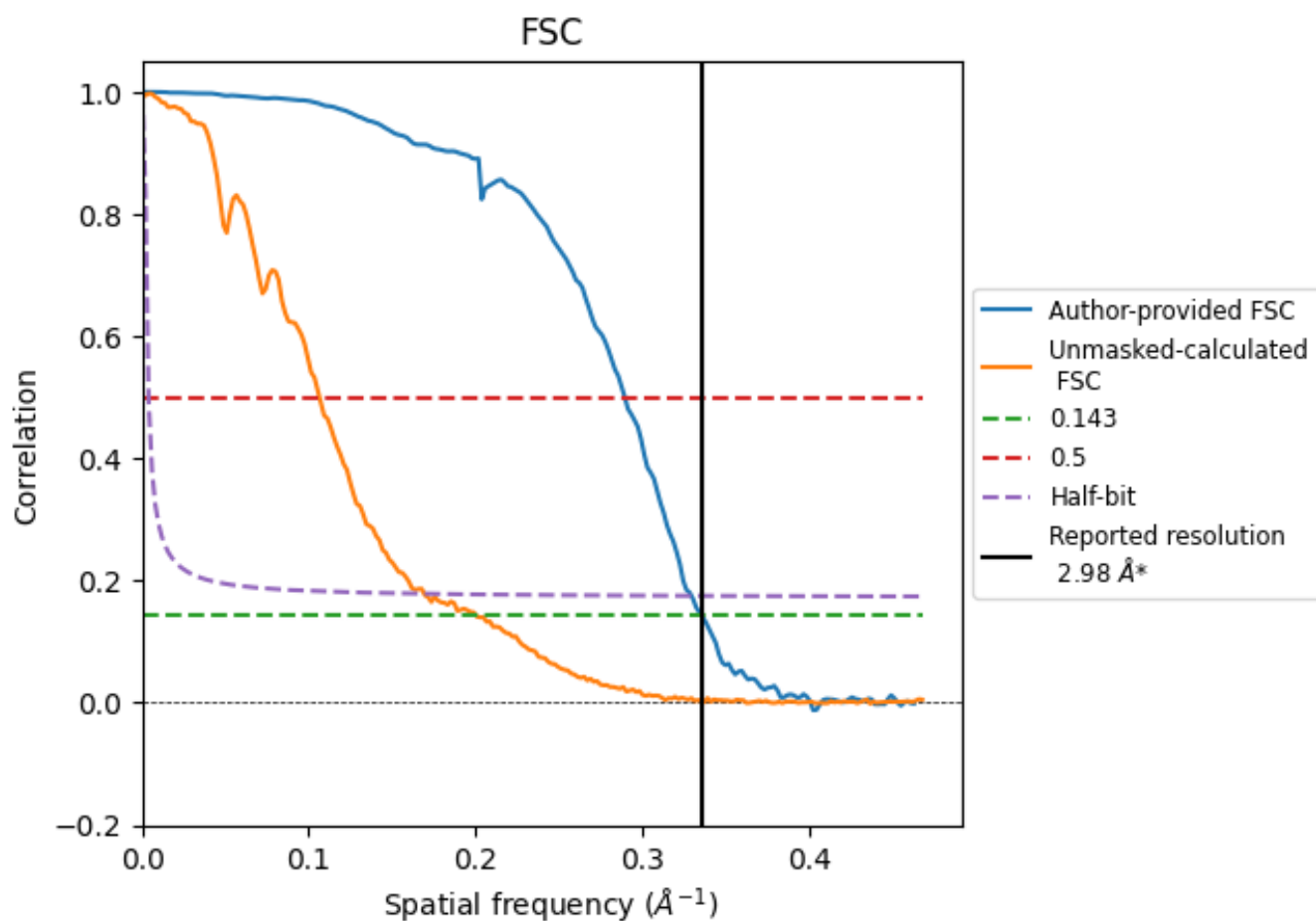


\*Reported resolution corresponds to spatial frequency of 0.336  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.336 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

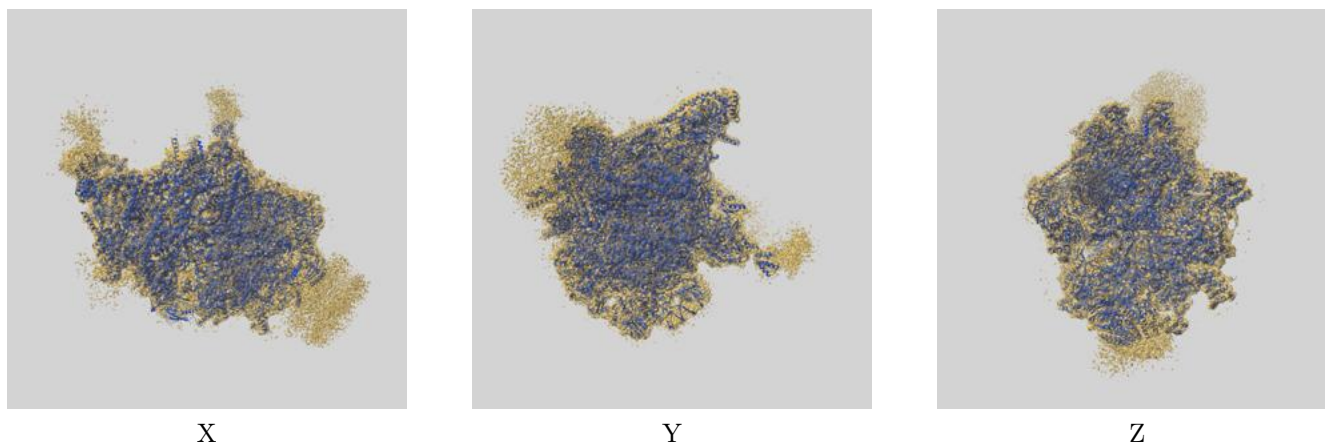
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.98                               | -    | -        |
| Author-provided FSC curve | 2.98                               | 3.45 | 3.03     |
| Unmasked-calculated*      | 4.99                               | 9.39 | 5.91     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.99 differs from the reported value 2.98 by more than 10 %

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

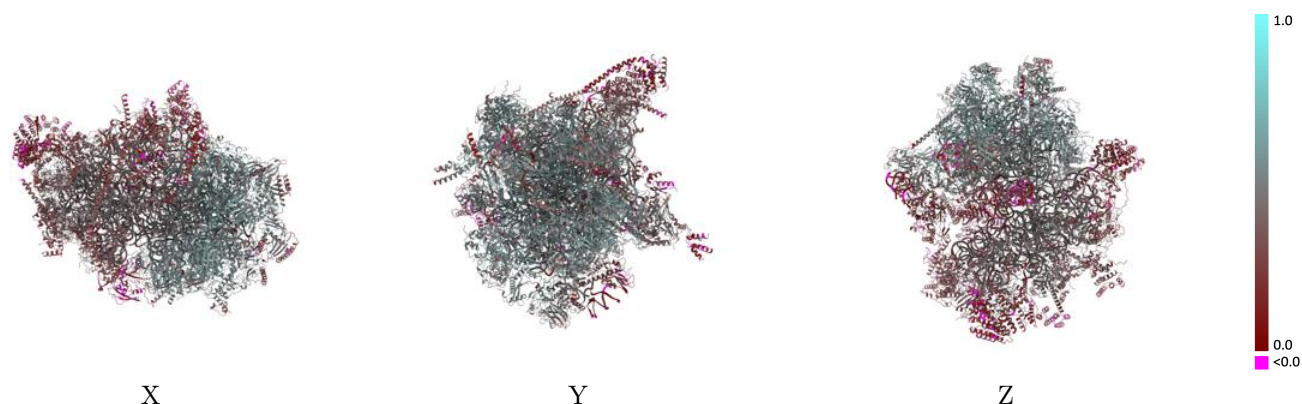
This section contains information regarding the fit between EMDB map EMD-71829 and PDB model 9PSM. Per-residue inclusion information can be found in section [3](#) on page [27](#).

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



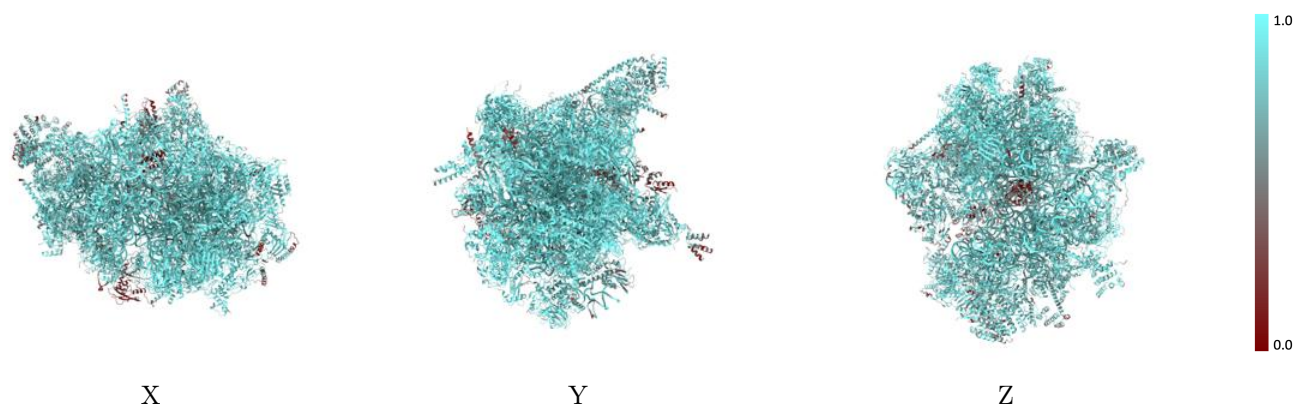
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



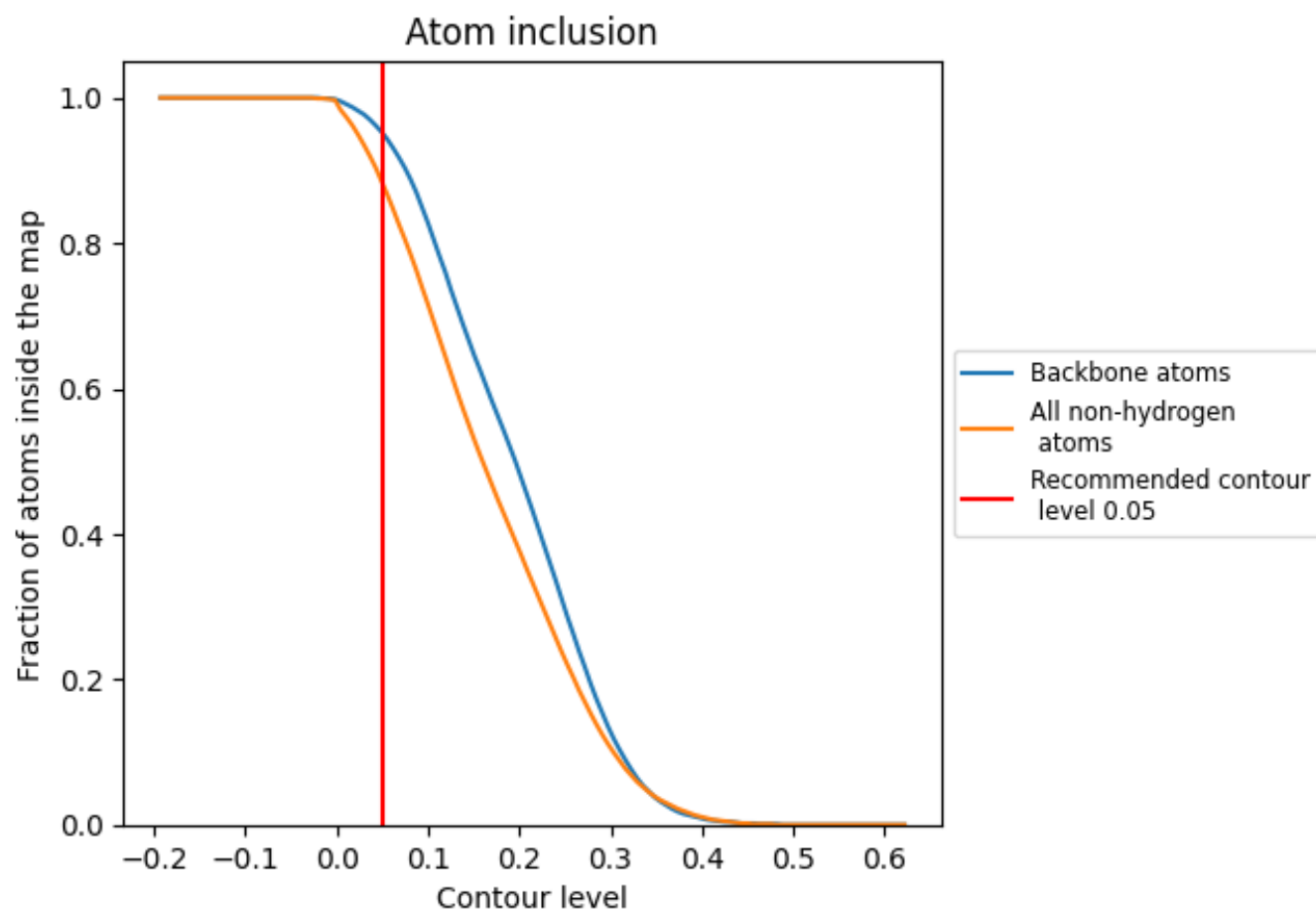
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8830   |  0.4190   |
| 0     |  0.9250   |  0.5300   |
| 1     |  0.9250   |  0.4850   |
| 2     |  0.9860   |  0.5770   |
| 3     |  0.9780   |  0.5780   |
| 4     |  0.9450   |  0.5540   |
| 5     |  0.9240   |  0.5160   |
| 6     |  0.8930   |  0.4710   |
| 7     |  0.8920   |  0.4670   |
| 8     |  0.6860   |  0.2340   |
| 9     |  0.9180   |  0.5120   |
| A     |  0.9750   |  0.4950   |
| A0    |  0.8290   |  0.2950   |
| A1    |  0.8030   |  0.3120   |
| A2    |  0.8030  |  0.3440  |
| A3    |  0.8740 |  0.4040 |
| A4    |  0.7250 |  0.2000 |
| AA    |  0.9860 |  0.4130 |
| AB    |  0.8660 |  0.3870 |
| AC    |  0.8600 |  0.4110 |
| AD    |  0.8540 |  0.3920 |
| AE    |  0.8500 |  0.3670 |
| AF    |  0.8340 |  0.3430 |
| AG    |  0.8230 |  0.3470 |
| AH    |  0.8350 |  0.3760 |
| AI    |  0.8660 |  0.3760 |
| AJ    |  0.8420 |  0.3990 |
| AK    |  0.8900 |  0.3860 |
| AL    |  0.8380 |  0.3560 |
| AM    |  0.8370 |  0.3410 |
| AN    |  0.8590 |  0.4040 |
| AO    |  0.8880 |  0.3580 |
| AP    |  0.8590 |  0.3790 |
| AQ    |  0.8700 |  0.3830 |
| AR    |  0.8350 |  0.3220 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| AS    |  0.8450   |  0.3470   |
| AT    |  0.8520   |  0.3780   |
| AU    |  0.8260   |  0.3050   |
| AV    |  0.7720   |  0.2060   |
| AW    |  0.8390   |  0.3760   |
| AX    |  0.8030   |  0.2660   |
| AY    |  0.8120   |  0.3130   |
| AZ    |  0.8310   |  0.3290   |
| Aw    |  0.8350   |  0.2130   |
| Ax    |  0.8990   |  0.2390   |
| Az    |  0.8330   |  0.2450   |
| B     |  0.8600   |  0.2520   |
| C     |  0.4210   |  0.2230   |
| D     |  0.9520   |  0.5180   |
| E     |  0.9440   |  0.5380   |
| F     |  0.9600   |  0.5550   |
| G     |  0.2660   |  0.1440   |
| H     |  0.5640   |  0.2670   |
| I     |  0.8120   |  0.4010   |
| J     |  0.7630  |  0.3010  |
| K     |  0.9580 |  0.5570 |
| L     |  0.9600 |  0.5090 |
| M     |  0.9490 |  0.5510 |
| N     |  0.9480 |  0.5270 |
| O     |  0.9500 |  0.5470 |
| OX    |  0.5590 |  0.3070 |
| P     |  0.9130 |  0.5020 |
| Q     |  0.9250 |  0.5020 |
| R     |  0.9550 |  0.5530 |
| S     |  0.9410 |  0.5470 |
| T     |  0.9540 |  0.5630 |
| U     |  0.8460 |  0.4930 |
| V     |  0.8990 |  0.4970 |
| W     |  0.9260 |  0.5370 |
| X     |  0.9150 |  0.5200 |
| Y     |  0.9330 |  0.5390 |
| Z     |  0.9430 |  0.5460 |
| a     |  0.8230 |  0.4550 |
| b     |  0.9490 |  0.5430 |
| c     |  0.9040 |  0.5050 |
| d     |  0.7960 |  0.4310 |
| e     |  0.7080 |  0.2090 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| f     |  0.7610 |  0.3010 |
| g     |  0.9350 |  0.5360 |
| h     |  0.9070 |  0.4840 |
| i     |  0.9660 |  0.5670 |
| j     |  0.8890 |  0.4870 |
| k     |  0.8300 |  0.4330 |
| l     |  0.8190 |  0.3780 |
| m     |  0.8010 |  0.2580 |
| n     |  0.7210 |  0.3600 |
| o     |  0.9610 |  0.5620 |
| p     |  0.8270 |  0.4470 |
| q     |  0.8010 |  0.3690 |
| r     |  0.9420 |  0.5390 |
| s     |  0.9310 |  0.5280 |
| t     |  0.5550 |  0.2160 |
| u     |  0.4220 |  0.1710 |
| z     |  0.2950 |  0.0970 |