



## wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 07:30 am GMT

PDB ID : 7PUB  
EMDB ID : EMD-13661  
Title : Late assembly intermediate of the Trypanosoma brucei mitoribosomal small subunit  
Authors : Lenarcic, T.; Leibundgut, M.; Saurer, M.; Ramrath, D.J.F.; Fluegel, T.; Boehringer, D.; Ban, N.  
Deposited on : 2021-09-29  
Resolution : 3.70 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:

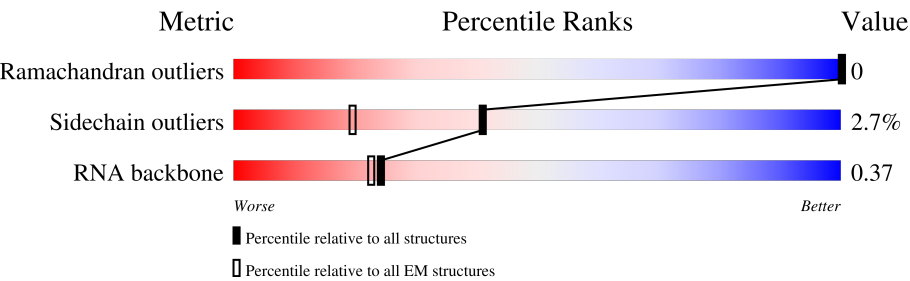
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 Å.

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



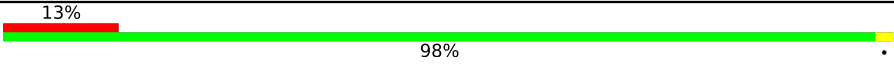
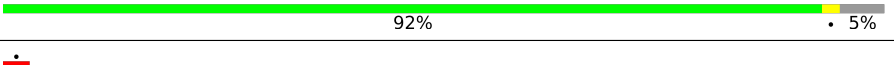
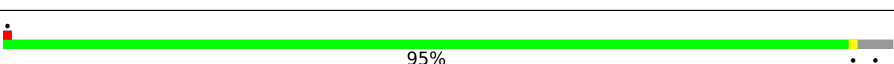
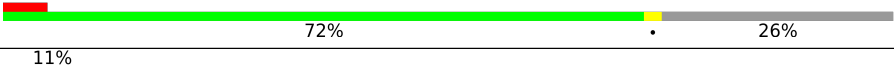
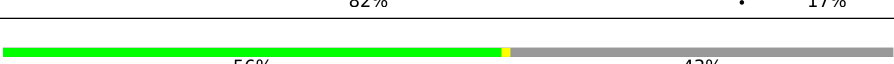
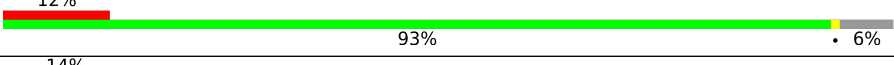
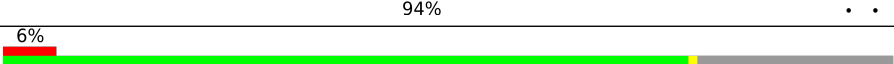
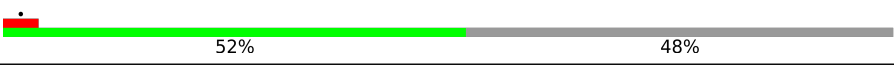
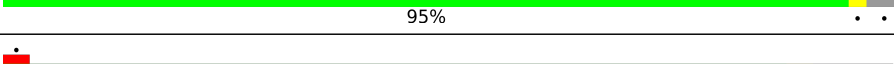
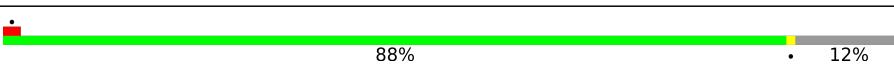


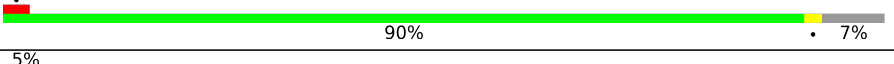
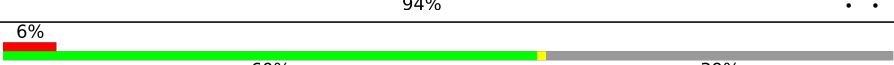


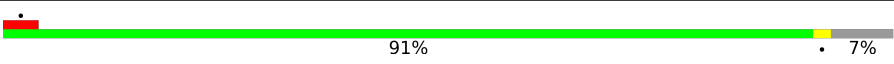
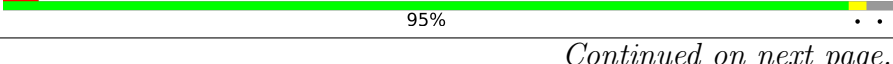


| Metric                | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Ramachandran outliers | 207382                   | 16835                    |
| Sidechain outliers    | 206894                   | 16415  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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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   | CA    | 621    | <div><div>13%</div><div>59%</div><div>41%</div></div> |
| 2   | CC    | 74     | <div><div>11%</div><div>95%</div><div>5%</div></div>  |
| 3   | CE    | 435    | <div><div>9%</div><div>95%</div><div>• •</div></div>  |
| 4   | CF    | 160    | <div><div>•</div><div>91%</div><div>• 7%</div></div>  |
| 5   | CH    | 282    | <div><div>8%</div><div>96%</div><div>• •</div></div>  |
| 6   | CI    | 443    | <div><div>7%</div><div>94%</div><div>• •</div></div>  |
| 7   | CJ    | 817    | <div><div>•</div><div>96%</div><div>• •</div></div>   |
| 8   | CK    | 326    | <div><div>7%</div><div>90%</div><div>• 9%</div></div> |




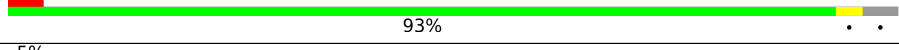
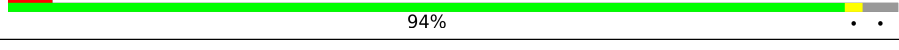

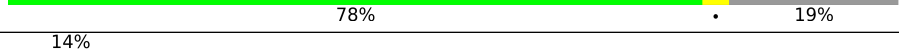
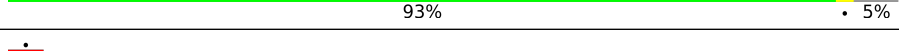
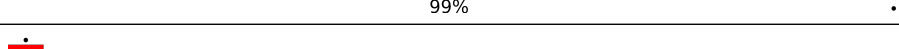
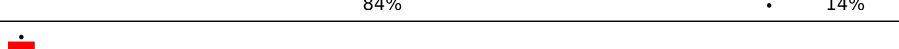
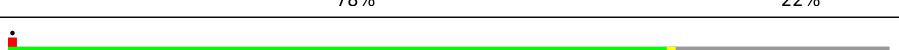

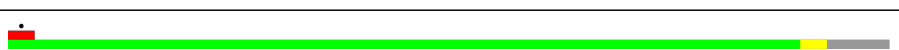
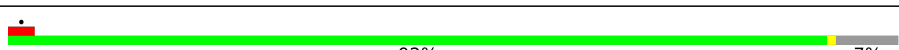
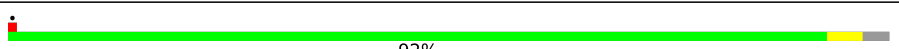




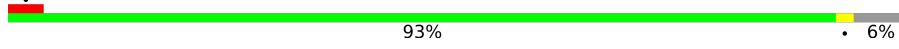
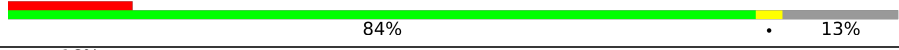
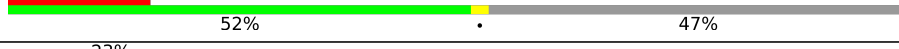



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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 9   | CL    | 87     |    |
| 10  | CN    | 166    |    |
| 11  | CO    | 429    |    |
| 12  | CP    | 188    |    |
| 13  | CQ    | 307    |    |
| 14  | CR    | 320    |    |
| 15  | CS    | 244    |    |
| 16  | CU    | 193    |    |
| 17  | Ca    | 602    |   |
| 18  | Cb    | 325    |  |
| 19  | Cd    | 440    |  |
| 20  | Cg    | 498    |  |
| 21  | Ci    | 181    |  |
| 22  | Cj    | 257    |  |
| 23  | Ck    | 874    |  |
| 24  | Cm    | 215    |  |
| 25  | Cn    | 250    |  |
| 26  | Cp    | 187    |  |
| 27  | Cq    | 263    |  |
| 28  | Cr    | 439    |  |
| 29  | Cv    | 1211   |  |
| 30  | DA    | 1788   |  |
| 31  | DB    | 1181   |  |
| 32  | DC    | 1165   |  |
| 33  | DD    | 812    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 34  | DE    | 747    |    |
| 35  | DF    | 666    |    |
| 36  | DG    | 631    |    |
| 37  | DH    | 581    |    |
| 38  | DI    | 407    |    |
| 39  | DJ    | 396    |    |
| 40  | DK    | 324    |    |
| 41  | DL    | 307    |    |
| 42  | DM    | 294    |    |
| 43  | DN    | 293    |    |
| 44  | DO    | 282    |    |
| 45  | DP    | 274    |  |
| 46  | DQ    | 268    |  |
| 47  | DR    | 270    |  |
| 48  | DS    | 261    |  |
| 49  | DT    | 247    |  |
| 50  | DU    | 228    |  |
| 51  | DV    | 183    |  |
| 52  | DW    | 179    |  |
| 53  | DX    | 169    |  |
| 54  | DY    | 163    |  |
| 55  | DZ    | 94     |  |
| 56  | Da    | 64     |  |
| 57  | F3    | 966    |  |
| 58  | F6    | 676    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 59  | F7    | 679    |                  |
| 60  | F9    | 608    |                  |
| 61  | FO    | 334    |                  |
| 62  | Ff    | 848    |                  |
| 63  | Fg    | 550    |                  |
| 64  | Fh    | 318    |                  |
| 65  | Fi    | 629    |                  |
| 66  | IA    | 787    |                  |
| 67  | IB    | 803    |                  |
| 68  | U6    | 21     |                  |
| 68  | UJ    | 21     |                  |
| 69  | U7    | 40     |                  |
| 70  | UE    | 53     |                  |
| 71  | UF    | 39     |                  |
| 72  | UG    | 13     |                  |
| 73  | UI    | 10     |                  |
| 74  | UK    | 3      |                  |
| 75  | UL    | 20     |                  |

## 2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 212864 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 9S rRNA.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 1   | CA    | 621      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 12330 | 5513 | 1927 | 4269 | 621 |         |       |

- Molecule 2 is a protein called uS3m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | CC    | 74       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 646   | 451 | 96 | 98 | 1 |         |       |

- Molecule 3 is a protein called Ribosomal\_S5\_C domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | CE    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3459  | 2188 | 642 | 613 | 16 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| CE    | 341     | ARG      | LYS    | variant | UNP Q38AX6 |

- Molecule 4 is a protein called bS6m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | CF    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1240  | 791 | 217 | 226 | 6 |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S8, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | CH    | 273      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1387 | 432 | 398 | 11 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| CH    | 74      | ASN      | SER    | variant | UNP Q388R7 |

- Molecule 6 is a protein called uS9m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | CI    | 427      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3410  | 2148 | 615 | 630 | 17 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| CI    | 370     | ALA      | VAL    | variant | UNP Q57W62 |

- Molecule 7 is a protein called LysM domain-containing protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 7   | CJ    | 803      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6535  | 4133 | 1152 | 1221 | 29 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| CJ    | 311     | LEU      | TYR    | variant | UNP Q57Z45 |
| CJ    | 484     | HIS      | ARG    | variant | UNP Q57Z45 |
| CJ    | 488     | SER      | ASN    | variant | UNP Q57Z45 |
| CJ    | 629     | ARG      | LYS    | variant | UNP Q57Z45 |

- Molecule 8 is a protein called uS11m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | CK    | 298      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2447  | 1520 | 465 | 445 | 17 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CK    | 3       | ARG      | GLN    | variant  | UNP Q389T7 |
| CK    | 138     | UNK      | ILE    | conflict | UNP Q389T7 |

- Molecule 9 is a protein called uS12m.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | CL    | 87       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 733   | 503 | 113 | 107 | 10 |         |       |

- Molecule 10 is a protein called uS14m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | CN    | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1322  | 843 | 251 | 220 | 8 |         |       |

- Molecule 11 is a protein called uS15m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | CO    | 308      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2552  | 1615 | 476 | 448 | 13 |         |       |

- Molecule 12 is a protein called bS16m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | CP    | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1489  | 956 | 274 | 250 | 9 |         |       |

- Molecule 13 is a protein called 30S Ribosomal protein S17, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | CQ    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1866  | 1186 | 355 | 317 | 8 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| CQ    | 138     | ALA      | VAL    | variant | UNP Q38DP8 |

- Molecule 14 is a protein called bS18m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | CR    | 267      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2210  | 1398 | 405 | 402 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| CR    | 8       | ILE      | VAL    | variant | UNP Q38AS2 |



- Molecule 15 is a protein called uS19m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | CS    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1149  | 743 | 205 | 195 | 6 |         |       |

- Molecule 16 is a protein called bS21m.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 16  | CU    | 181      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1522  | 957 | 303 | 250 | 12 |         |       |

- Molecule 17 is a protein called mS22.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | Ca    | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4911  | 3146 | 875 | 867 | 23 |         |       |

- Molecule 18 is a protein called mS23.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | Cb    | 252      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2056  | 1300 | 368 | 380 | 8 |         |       |

- Molecule 19 is a protein called mS26.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | Cd    | 230      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1961  | 1242 | 358 | 350 | 11 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Cd    | 299     | UNK      | GLY    | conflict | UNP Q38DK6 |
| Cd    | 364     | UNK      | GLY    | conflict | UNP Q38DK6 |

- Molecule 20 is a protein called mS29.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | Cg    | 480      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2494 | 682 | 699 | 20 |         |       |

- Molecule 21 is a protein called mS33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | Ci    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1343  | 845 | 246 | 243 | 9 |         |       |

- Molecule 22 is a protein called mS34.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | Cj    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1799  | 1142 | 311 | 342 | 4 |         |       |

- Molecule 23 is a protein called mS35.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 23  | Ck    | 682      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5442  | 3411 | 990 | 1016 | 25 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| Ck    | 107     | SER      | LEU    | variant | UNP Q387C7 |
| Ck    | 144     | PHE      | LEU    | variant | UNP Q387C7 |
| Ck    | 253     | TYR      | PHE    | variant | UNP Q387C7 |
| Ck    | 339     | GLU      | VAL    | variant | UNP Q387C7 |
| Ck    | 815     | GLY      | ARG    | variant | UNP Q387C7 |
| Ck    | 871     | GLY      | GLU    | variant | UNP Q387C7 |

- Molecule 24 is a protein called mS37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Cm    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1184  | 735 | 230 | 210 | 9 |         |       |

- Molecule 25 is a protein called mS38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 25  | Cn    | 62       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 528   | 345 | 105 | 75 | 3 |         |       |

- Molecule 26 is a protein called Protein FYV4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | Cp    | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1466  | 928 | 265 | 268 | 5 |         |       |

- Molecule 27 is a protein called Superoxide dismutase, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | Cq    | 252      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2005  | 1285 | 342 | 369 | 9 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| Cq    | 48      | THR      | ALA    | variant | UNP Q586A1 |
| Cq    | 167     | MET      | VAL    | variant | UNP Q586A1 |

- Molecule 28 is a protein called Sod\_Fe\_C domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 28  | Cr    | 267      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2083  | 1317 | 382 | 369 | 15 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| Cr    | 351     | LYS      | GLU    | variant | UNP Q585I1 |

- Molecule 29 is a protein called ECH\_2 domain-containing protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 29  | Cv    | 1040     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8404  | 5291 | 1508 | 1568 | 37 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| Cv    | 1179    | GLU      | GLY    | variant | UNP Q383R4 |

- Molecule 30 is a protein called mS48.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 30  | DA    | 1552     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 12448 | 7861 | 2220 | 2329 | 38 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DA    | 1181    | THR      | ILE    | variant | UNP Q57UJ2 |
| DA    | 1333    | ALA      | VAL    | variant | UNP Q57UJ2 |
| DA    | 1700    | ARG      | HIS    | variant | UNP Q57UJ2 |
| DA    | 1761    | LYS      | ARG    | variant | UNP Q57UJ2 |

- Molecule 31 is a protein called mS49.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 31  | DB    | 1111     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9148  | 5691 | 1717 | 1711 | 29 |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DB    | 23      | VAL      | ALA    | variant | UNP Q586P5 |
| DB    | 359     | ILE      | THR    | variant | UNP Q586P5 |
| DB    | 384     | GLN      | HIS    | variant | UNP Q586P5 |
| DB    | 402     | THR      | ILE    | variant | UNP Q586P5 |
| DB    | 423     | THR      | ALA    | variant | UNP Q586P5 |
| DB    | 586     | ARG      | HIS    | variant | UNP Q586P5 |
| DB    | 593     | ARG      | LYS    | variant | UNP Q586P5 |
| DB    | 647     | SER      | GLY    | variant | UNP Q586P5 |

- Molecule 32 is a protein called mS50.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 32  | DC    | 1089     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8709  | 5498 | 1538 | 1642 | 31 |         |       |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DC    | 53      | ALA      | THR    | variant | UNP Q57YB5 |
| DC    | 365     | LYS      | GLU    | variant | UNP Q57YB5 |
| DC    | 385     | THR      | ALA    | variant | UNP Q57YB5 |
| DC    | 405     | ILE      | VAL    | variant | UNP Q57YB5 |
| DC    | 641     | SER      | PRO    | variant | UNP Q57YB5 |
| DC    | 651     | LYS      | GLU    | variant | UNP Q57YB5 |
| DC    | 731     | GLU      | ASP    | variant | UNP Q57YB5 |
| DC    | 814     | GLN      | HIS    | variant | UNP Q57YB5 |
| DC    | 1097    | ALA      | VAL    | variant | UNP Q57YB5 |
| DC    | 1113    | THR      | ILE    | variant | UNP Q57YB5 |

- Molecule 33 is a protein called mS51.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 33  | DD    | 790      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6513  | 4121 | 1181 | 1170 | 41 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DD    | 371     | PRO      | SER    | variant | UNP Q385L8 |
| DD    | 599     | ALA      | VAL    | variant | UNP Q385L8 |

- Molecule 34 is a protein called mS52.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 34  | DE    | 588      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4798  | 3052 | 868 | 859 | 19 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DE    | 378     | UNK      | LYS    | variant | UNP Q386Q7 |
| DE    | 384     | UNK      | THR    | variant | UNP Q386Q7 |

- Molecule 35 is a protein called mS53.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 35  | DF    | 589      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4738  | 2974 | 895 | 844 | 25 |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DF    | 18      | THR      | ALA    | variant  | UNP Q38ET1 |
| DF    | 258     | ASP      | ASN    | variant  | UNP Q38ET1 |
| DF    | 372     | ASN      | ASP    | variant  | UNP Q38ET1 |
| DF    | 406     | ASN      | SER    | variant  | UNP Q38ET1 |
| DF    | 510     | ASP      | GLY    | variant  | UNP Q38ET1 |
| DF    | 577     | ALA      | VAL    | variant  | UNP Q38ET1 |
| DF    | 636     | UNK      | GLY    | conflict | UNP Q38ET1 |
| DF    | 638     | LYS      | ARG    | variant  | UNP Q38ET1 |

- Molecule 36 is a protein called mS54.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36  | DG    | 552      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4482  | 2820 | 818 | 813 | 31 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DG    | 428     | ASN      | SER    | variant | UNP Q57ZP8 |
| DG    | 429     | GLY      | SER    | variant | UNP Q57ZP8 |

- Molecule 37 is a protein called mS55.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37  | DH    | 559      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4541  | 2849 | 843 | 828 | 21 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DH    | 191     | HIS      | GLN    | variant | UNP Q580V1 |
| DH    | 194     | PRO      | ARG    | variant | UNP Q580V1 |
| DH    | 488     | GLY      | SER    | variant | UNP Q580V1 |

- Molecule 38 is a protein called mS56.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 38  | DI    | 390      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3182  | 2020 | 554 | 594 | 14 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DI    | 92      | GLU      | GLY    | variant | UNP Q587C2 |
| DI    | 116     | ASP      | GLU    | variant | UNP Q587C2 |

- Molecule 39 is a protein called mS57.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 39  | DJ    | 357      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2914  | 1858 | 512 | 530 | 14 |         |       |

- Molecule 40 is a protein called mS58.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40  | DK    | 263      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2083  | 1312 | 374 | 392 | 5 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DK    | 61      | SER      | PRO    | variant | UNP Q38BP1 |
| DK    | 257     | GLY      | SER    | variant | UNP Q38BP1 |

- Molecule 41 is a protein called mS59.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 41  | DL    | 291      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2360  | 1495 | 441 | 412 | 12 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DL    | 274     | THR      | ALA    | variant | UNP Q38BS2 |

- Molecule 42 is a protein called mS60.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 42  | DM    | 294      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2430  | 1533 | 459 | 426 | 12 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DM    | 69      | PHE      | TYR    | variant | UNP Q57XL2 |
| DM    | 97      | ASN      | SER    | variant | UNP Q57XL2 |
| DM    | 138     | SER      | PRO    | variant | UNP Q57XL2 |
| DM    | 173     | ALA      | THR    | variant | UNP Q57XL2 |
| DM    | 206     | ALA      | THR    | variant | UNP Q57XL2 |

- Molecule 43 is a protein called mS61.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43  | DN    | 253      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2062  | 1313 | 374 | 365 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DN    | 51      | GLY      | SER    | variant | UNP Q38D60 |

- Molecule 44 is a protein called mS62.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44  | DO    | 221      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1796  | 1123 | 325 | 338 | 10 |         |       |

- Molecule 45 is a protein called mS63.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45  | DP    | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1760  | 1132 | 312 | 307 | 9 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DP    | 3       | HIS      | ARG    | variant | UNP Q38F25 |

- Molecule 46 is a protein called AKAP7\_NLS domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | DQ    | 255      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2055  | 1290 | 388 | 368 | 9 |         |       |

- Molecule 47 is a protein called mS65.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 47  | DR    | 250      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2019  | 1301 | 368 | 340 | 10 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DR    | 65      | GLY      | SER    | variant | UNP Q57UA2 |
| DR    | 94      | GLY      | GLU    | variant | UNP Q57UA2 |
| DR    | 128     | PRO      | SER    | variant | UNP Q57UA2 |
| DR    | 229     | ARG      | GLN    | variant | UNP Q57UA2 |

- Molecule 48 is a protein called mS66.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48  | DS    | 243      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1950  | 1216 | 364 | 356 | 14 |         |       |

- Molecule 49 is a protein called Rhodanese domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 49  | DT    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2058  | 1321 | 364 | 362 | 11 |         |       |

- Molecule 50 is a protein called Ubiquitin-like domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | DU    | 213      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1754  | 1103 | 310 | 335 | 6 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DU    | 119     | ILE      | LEU    | variant | UNP Q582T9 |
| DU    | 152     | ILE      | VAL    | variant | UNP Q582T9 |

- Molecule 51 is a protein called mS69.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | DV    | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1346  | 855 | 252 | 235 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DV    | 163     | ALA      | THR    | variant | UNP Q57UZ6 |

- Molecule 52 is a protein called mS70.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | DW    | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1359  | 866 | 260 | 228 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DW    | 74      | THR      | MET    | variant | UNP Q383N9 |

- Molecule 53 is a protein called mS71.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | DX    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1174  | 747 | 223 | 197 | 7 |         |       |

- Molecule 54 is a protein called mS72.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | DY    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1295  | 829 | 247 | 214 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| DY    | 34      | HIS      | ASP    | variant | UNP Q57YD4 |

- Molecule 55 is a protein called mS73.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | DZ    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 697   | 457 | 113 | 123 | 4 |         |       |

- Molecule 56 is a protein called mS74.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 56  | Da    | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 305   | 193 | 67 | 43 | 2 |         |       |

- Molecule 57 is a protein called mt-SAF3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 57  | F3    | 252      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2003  | 1259 | 354 | 378 | 12 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| F3    | 44      | THR      | ALA    | variant | UNP Q38E61 |
| F3    | 190     | VAL      | ILE    | variant | UNP Q38E61 |
| F3    | 303     | ALA      | SER    | variant | UNP Q38E61 |
| F3    | 418     | ASP      | ASN    | variant | UNP Q38E61 |

- Molecule 58 is a protein called mt-SAF6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58  | F6    | 416      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3358  | 2124 | 580 | 636 | 18 |         |       |

- Molecule 59 is a protein called mt-SAF7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 59  | F7    | 576      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4584  | 2922 | 792 | 837 | 33 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| F7    | 36      | ILE      | THR    | variant | UNP Q57UW6 |
| F7    | 470     | GLU      | LYS    | variant | UNP Q57UW6 |
| F7    | 474     | VAL      | ALA    | variant | UNP Q57UW6 |

- Molecule 60 is a protein called mt-SAF9.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 60  | F9    | 342      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2815  | 1736 | 530 | 539 | 10 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| F9    | 117     | ALA      | SER    | variant | UNP Q57YC0 |
| F9    | 145     | TYR      | HIS    | variant | UNP Q57YC0 |
| F9    | 316     | LYS      | GLU    | variant | UNP Q57YC0 |
| F9    | 412     | GLY      | VAL    | variant | UNP Q57YC0 |
| F9    | 449     | VAL      | ALA    | variant | UNP Q57YC0 |
| F9    | 537     | GLY      | SER    | variant | UNP Q57YC0 |

- Molecule 61 is a protein called mt-SAF22.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 61  | FO    | 267      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2236  | 1407 | 432 | 385 | 12 |         |       |

- Molecule 62 is a protein called DNA photolyase, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 62  | Ff    | 614      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4941  | 3135 | 885 | 898 | 23 |         |       |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Ff    | 109     | ALA      | VAL    | variant  | UNP Q382U6 |
| Ff    | 127     | UNK      | TYR    | conflict | UNP Q382U6 |
| Ff    | 138     | GLN      | ARG    | variant  | UNP Q382U6 |
| Ff    | 200     | CYS      | SER    | variant  | UNP Q382U6 |
| Ff    | 319     | ALA      | THR    | variant  | UNP Q382U6 |
| Ff    | 334     | ASN      | THR    | variant  | UNP Q382U6 |
| Ff    | 350     | ILE      | THR    | variant  | UNP Q382U6 |
| Ff    | 362     | ALA      | VAL    | variant  | UNP Q382U6 |
| Ff    | 844     | THR      | SER    | variant  | UNP Q382U6 |

- Molecule 63 is a protein called Acyl transferase-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 63  | Fg    | 513      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3994  | 2512 | 698 | 754 | 30 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Fg    | 90      | LYS      | ARG    | variant  | UNP Q38DK4 |
| Fg    | 152     | VAL      | LEU    | variant  | UNP Q38DK4 |
| Fg    | 159     | ILE      | VAL    | variant  | UNP Q38DK4 |
| Fg    | 363     | MET      | ARG    | variant  | UNP Q38DK4 |
| Fg    | 399     | UNK      | GLU    | conflict | UNP Q38DK4 |
| Fg    | 525     | LYS      | ARG    | variant  | UNP Q38DK4 |

- Molecule 64 is a protein called mt-SAF37.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 64  | Fh    | 274      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2230  | 1384 | 420 | 411 | 15 |         |       |

- Molecule 65 is a protein called mt-SAF38.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 65  | Fi    | 469      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3734  | 2363 | 683 | 665 | 23 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| Fi    | 35      | THR      | SER    | variant | UNP Q57ZP1 |
| Fi    | 69      | GLY      | SER    | variant | UNP Q57ZP1 |
| Fi    | 185     | PRO      | HIS    | variant | UNP Q57ZP1 |

- Molecule 66 is a protein called Translation initiation factor IF-2, putative.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 66  | IA    | 693      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5414  | 3397 | 972 | 1018 | 27 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| IA    | 373     | LYS      | GLU    | variant | UNP Q57WE3 |
| IA    | 451     | ILE      | VAL    | variant | UNP Q57WE3 |
| IA    | 584     | ASN      | SER    | variant | UNP Q57WE3 |
| IA    | 679     | ASP      | VAL    | variant | UNP Q57WE3 |

- Molecule 67 is a protein called mt-SAF39.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 67  | IB    | 511      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4103  | 2561 | 764 | 760 | 18 |         |       |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| IB    | 136     | LYS      | GLU    | variant | UNP Q387Q6 |
| IB    | 226     | ASP      | ASN    | variant | UNP Q387Q6 |
| IB    | 237     | CYS      | SER    | variant | UNP Q387Q6 |
| IB    | 259     | THR      | ARG    | variant | UNP Q387Q6 |
| IB    | 268     | GLU      | LYS    | variant | UNP Q387Q6 |
| IB    | 275     | CYS      | TYR    | variant | UNP Q387Q6 |
| IB    | 312     | THR      | SER    | variant | UNP Q387Q6 |
| IB    | 459     | ASP      | ALA    | variant | UNP Q387Q6 |
| IB    | 572     | HIS      | ARG    | variant | UNP Q387Q6 |

- Molecule 68 is a protein called Unk.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 68  | U6    | 21       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 105   | 63 | 21 | 21 |         |       |
| 68  | UJ    | 21       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 105   | 63 | 21 | 21 |         |       |

- Molecule 69 is a protein called Unk7.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 69  | U7    | 40       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 200   | 120 | 40 | 40 |         |       |

- Molecule 70 is a protein called UnkE.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 70  | UE    | 53       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 265   | 159 | 53 | 53 |         |       |

- Molecule 71 is a protein called UnkF.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 71  | UF    | 39       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 195   | 117 | 39 | 39 |         |       |

- Molecule 72 is a protein called UnkG.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 72  | UG    | 13       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 65    | 39 | 13 | 13 |         |       |

- Molecule 73 is a protein called UnkI.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 73  | UI    | 10       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 50    | 30 | 10 | 10 |         |       |

- Molecule 74 is a protein called UnkK.

| Mol | Chain | Residues | Atoms |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---------|-------|
| 74  | UK    | 3        | Total | C | N | O | 0       | 0     |
|     |       |          | 15    | 9 | 3 | 3 |         |       |

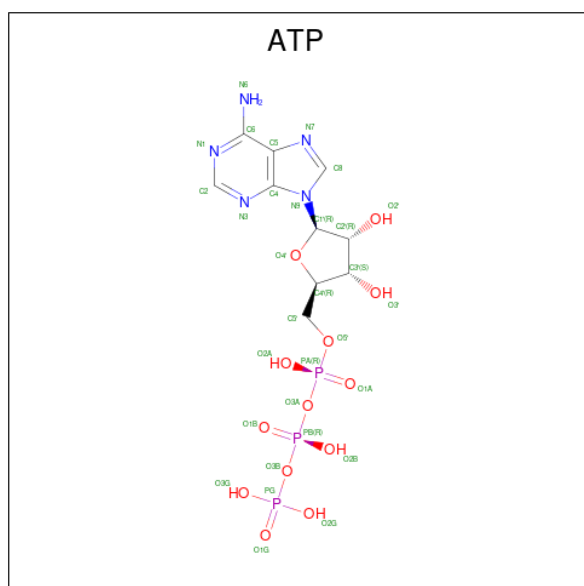
- Molecule 75 is a protein called UnkL.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 75  | UL    | 20       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 100   | 60 | 20 | 20 |         |       |

- Molecule 76 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 76  | CA    | 3        | Total | Mg | 0       |
|     |       |          | 3     | 3  |         |
| 76  | CQ    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 76  | Cg    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 76  | IA    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 77 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

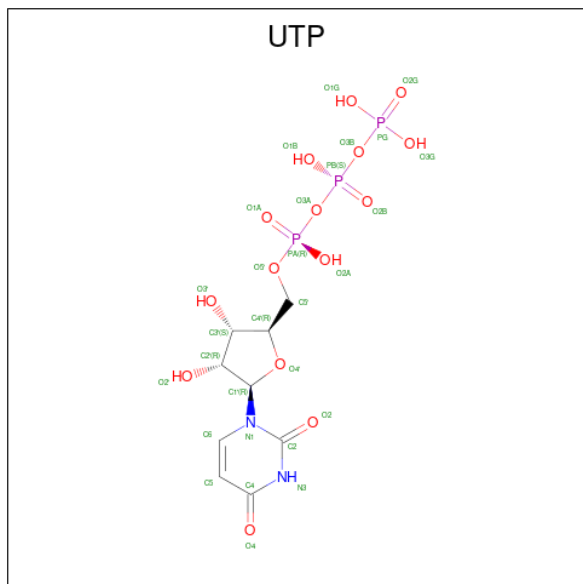


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 77  | Cg    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 78 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 78  | Cr    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 78  | DA    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 78  | DS    | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |

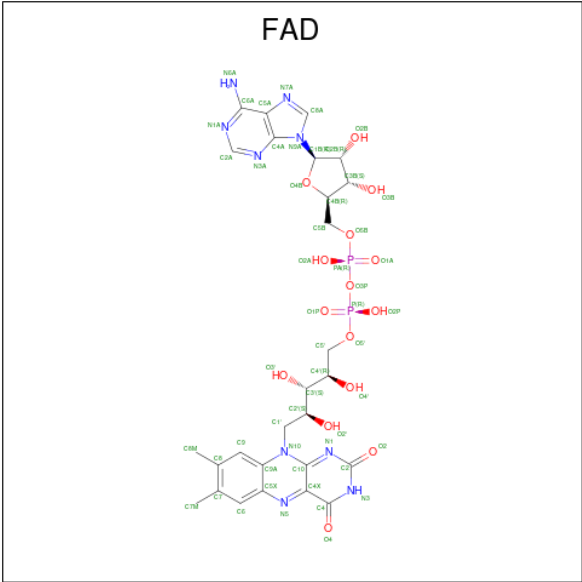
- Molecule 79 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula:  $C_9H_{15}N_2O_{15}P_3$ ).



| Mol | Chain | Residues | Atoms |   |   |    |   | AltConf |
|-----|-------|----------|-------|---|---|----|---|---------|
| 79  | DJ    | 1        | Total | C | N | O  | P | 0       |
|     |       |          | 29    | 9 | 2 | 15 | 3 |         |

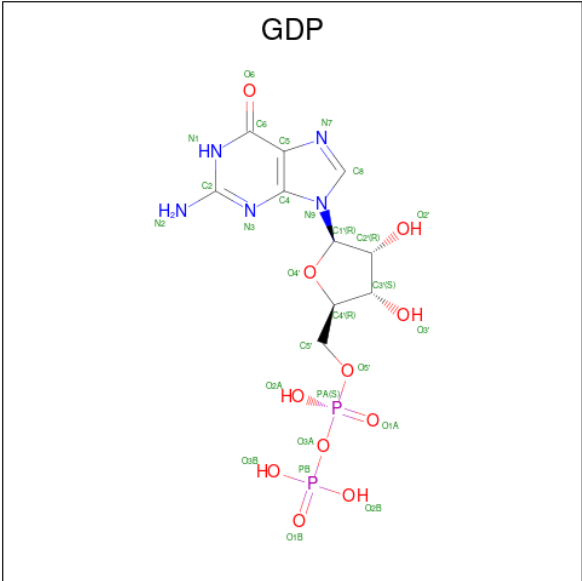
- Molecule 80 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).





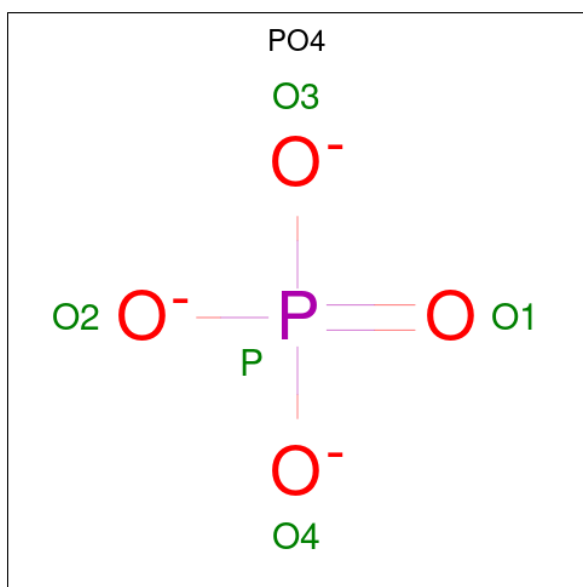
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 80  | Ff    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |

- Molecule 81 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 81  | IA    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

- Molecule 82 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 82  | IA    | 1        | Total | O | P | 0       |
|     |       |          | 5     | 4 | 1 |         |

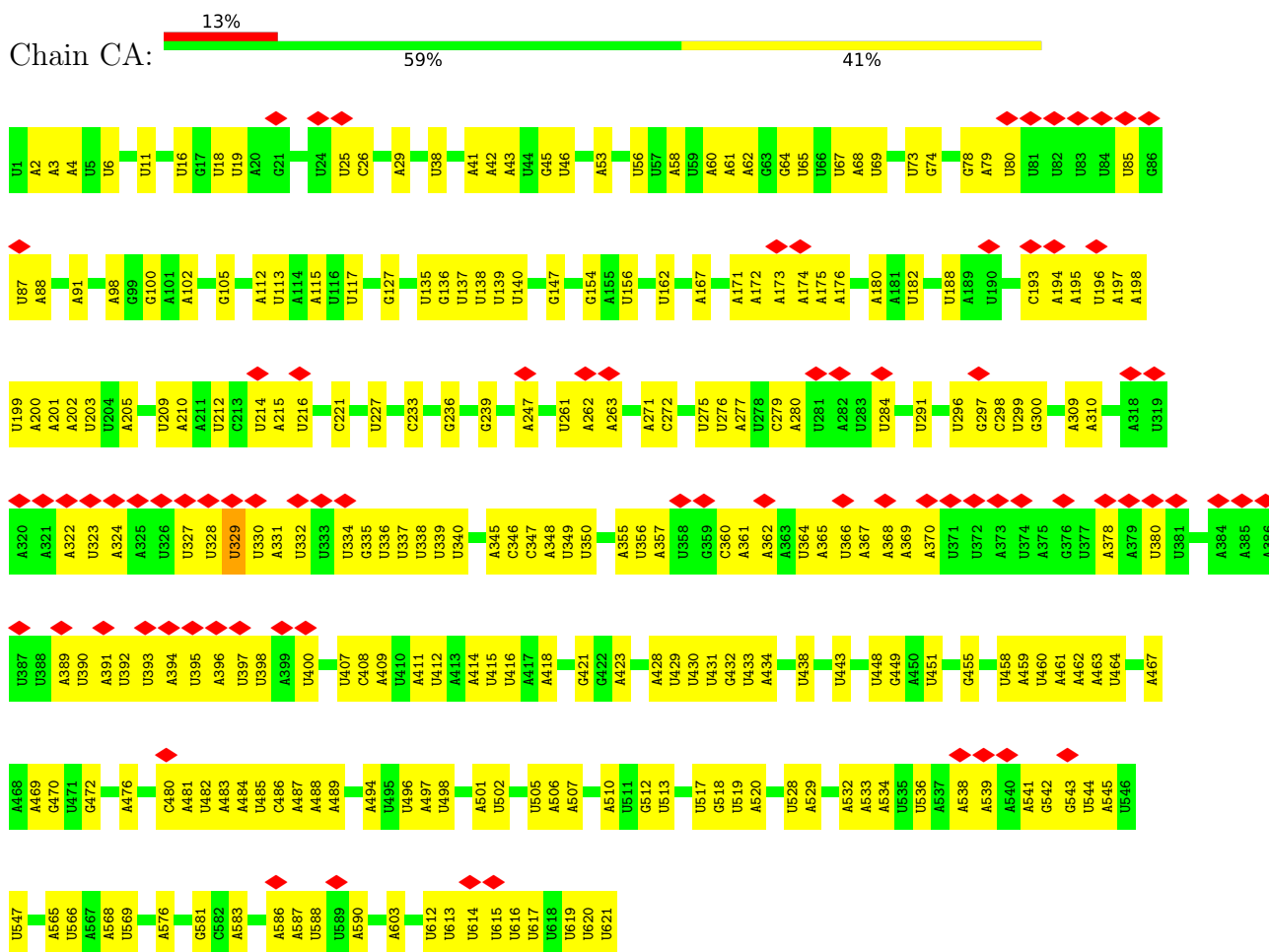
- Molecule 83 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 83  | Cg    | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |
| 83  | IA    | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |

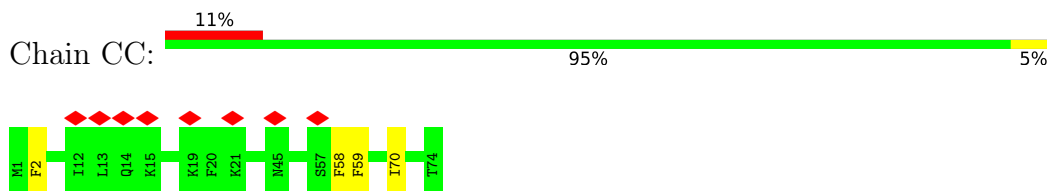
### 3 Residue-property plots

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

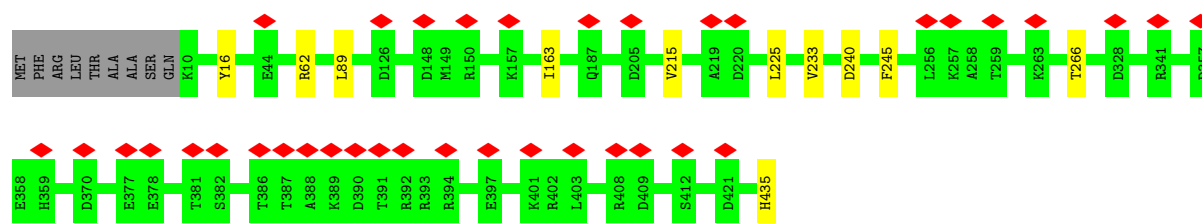
#### • Molecule 1: 9S rRNA



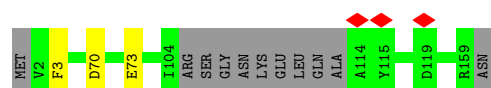
#### • Molecule 2: uS3m



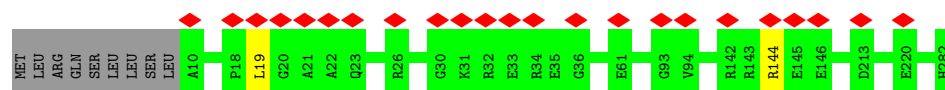
#### • Molecule 3: Ribosomal\_S5\_C domain-containing protein



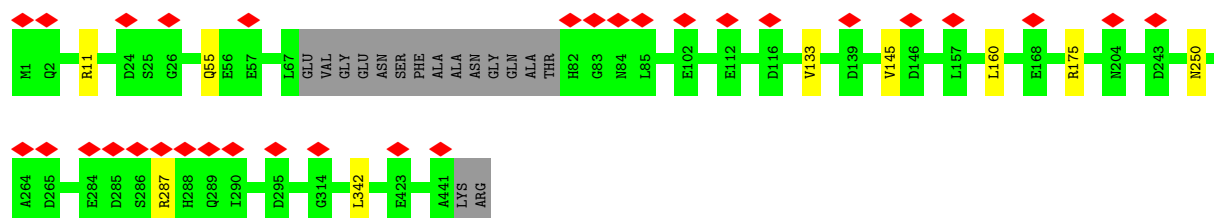
- Molecule 4: bS6m



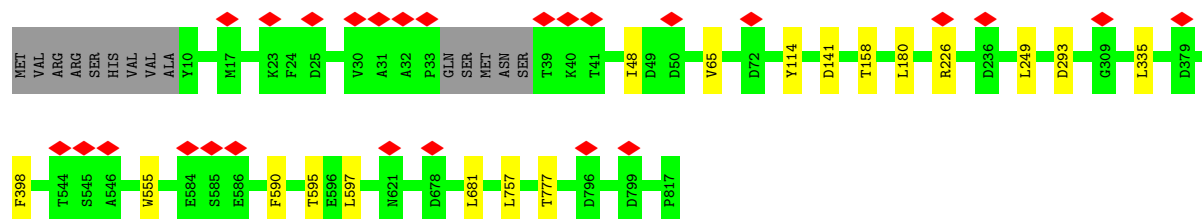
- Molecule 5: 30S ribosomal protein S8, putative



- Molecule 6: uS9m

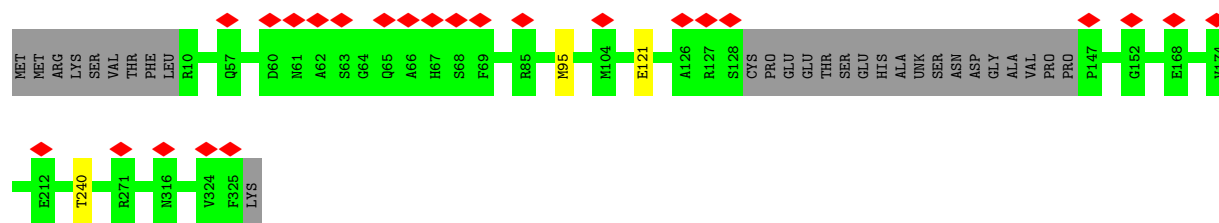


- Molecule 7: LysM domain-containing protein



- Molecule 8: uS11m

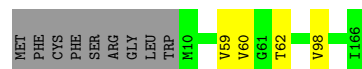




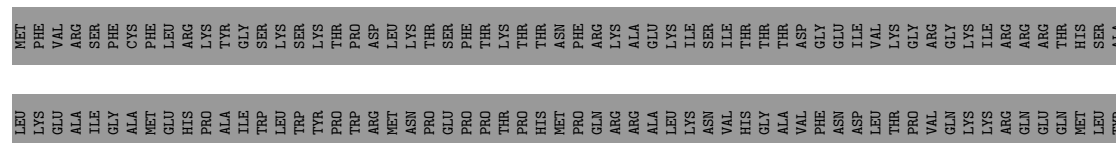
• Molecule 9: uS12m



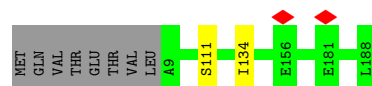
• Molecule 10: uS14m



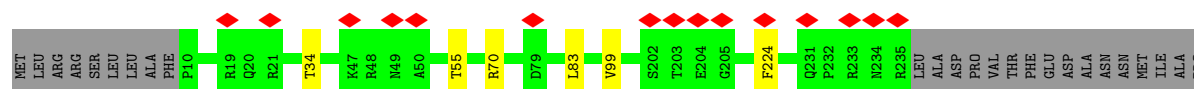
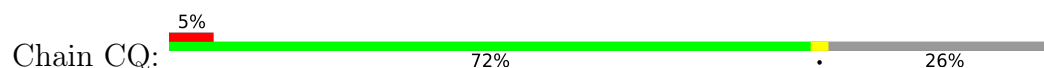
• Molecule 11: uS15m



• Molecule 12: bS16m



• Molecule 13: 30S Ribosomal protein S17, putative



ASN  
ALA  
PRO  
ALA  
ALA  
ALA  
LEU  
ASP  
ALA  
SER  
SER  
ASP  
PRO  
PRO  
LEU  
LEU  
ASP  
ARG  
GLY  
GLY  
TYR  
THR  
GLU  
VAL  
GLU  
GLN  
ASP  
THR  
ARG  
ASN  
LYS  
GLY  
ASP  
ASP  
TYR  
TRP  
MET  
ASN  
LEU  
GLN  
PRO  
LYS  
GLU  
LYS  
TYR  
ASP  
PHE  
LYS  
SER  
PHE  
LYS  
SER  
PRO

• Molecule 14: bS18m

Chain CR: 11% 82% 17%

MET ASN ARG THR GLY SER T8 Y9 A10 H11 Q15 F16 A17 V18 T36 E41 E44 L80 D91 F103 D104 K108 Q111 N128 D146 A189 Y190 Q191 R219 R223 E226 S231 G232 S233 A234 S235 A236 R237 G238 S239 G240 G241 G242

T243 E257 S262 L263 H264 W266 M271 E272 D273 V274 GLY ARG SER VAL LYS ASN PRO THR VAL PRO GLY LEU MET THR SER THR LYS MET GLY LYS LYS PHE HIS ASN LEU TYR SER SER THR THR LYS ARG MET GLY PHE SER ASN PRO THR LEU GLY ILE LYS VAL

• Molecule 15: uS19m

Chain CS: 56% 43%

MET ALA PHE ARG ASN THR PHE THR PRO GLY LYS PHE SER THR VAL SER LYS ASN TLE VAL VAL LEU LEU ILE TRP ARG VAL LYS PHE LEU ARG ALA GLY PHE ALA HIS SER LEU MET VAL LEU PRO VAL SER LEU TYR SER LYS ILE LEU LEU CYS ASP VAL LYS LYS

TLE VAL TYR PHE HIS CYS THR ARG LYS SER MET LEU ARG CYS PRO CYS VAL TRP PRO LEU PRO THR LYS SER VAL VAL TLE GLY THR ALA PHE LEU GLN LYS ARG PHE LEU LYS I106 V177 L228 F243 LYS

• Molecule 16: bS21m

Chain CU: 12% 93% 6%

MET LEU HIS THR THR ARG LEU TRP THR GLY Y12 N51 I54 K82 K118 E121 D122 R125 T146 D147 N148 V149 A150 R151 E152 R153 R160 Q161 V162 R163 A164 P166 M167 N169 Y188 R189 W190 R191 V192 ASN

• Molecule 17: mS22

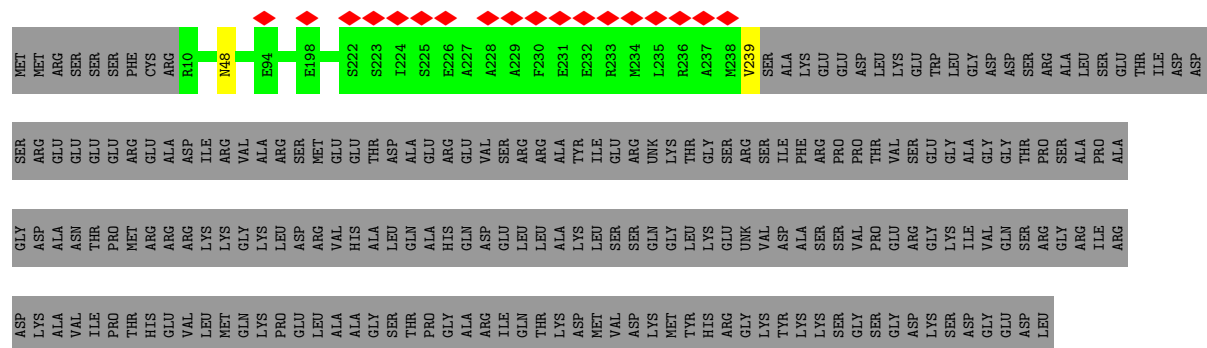
Chain Ca: 14% 94%

MET LEU ARG ARG ALA TYR ILE GLN ARG TYR PRO PHE ASN LYS ARG GLY PRO GLU H21 H26 H27 E31 P32 P33 LYS PRO LEU GLN TRP ARG D40 P41 K42 V43 V44 T45 R46 D47 L48 S49 V50 M51 K52 S53 F54 D55 A56 D72 E73 K86 L112 K116 R132 A135 S136 G137 K138 D139 N140 T141 D145 D146 E154 N165 A166 G167 D187 E218 A219 L220 Q222 Q223 S224 P225 H226 N227 K228 E229 Q230 L231 Q232 R233 K234 L235 A236 F237 Q238 T239 S240 L241 G242 T243 P244 E245 F247 D248 D260 L267 F272 D312 K346 D358 G412 L480 E496 Q519 Y520 A530 R536 K544 L563 R566 E573 V579 A582 Q587 A593 Y594 E601 LEU

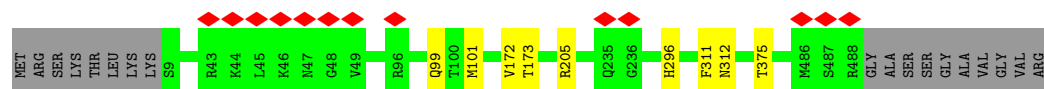
• Molecule 18: mS23

Chain Cb: 6% 77% 22%

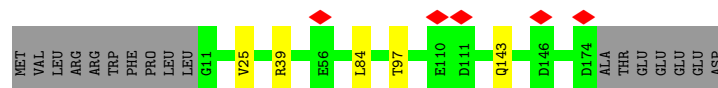
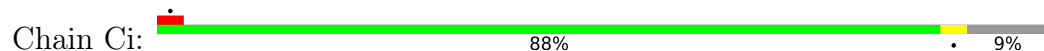
- Molecule 19: mS26



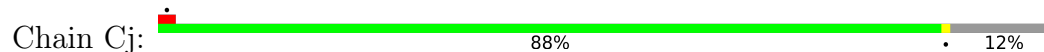
- Molecule 20: mS29



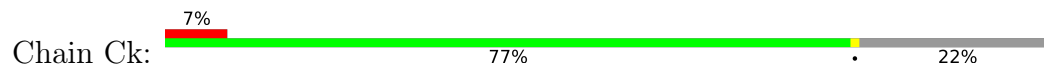
- Molecule 21: mS33



- Molecule 22: mS34

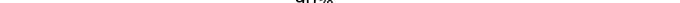


- Molecule 23: mS35

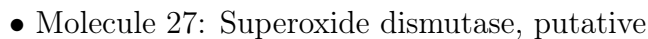








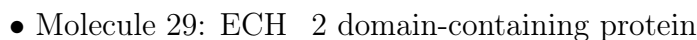
90% 7%



| Response       | Percentage |
|----------------|------------|
| Not a good job | 5%         |
| A good job     | 94%        |

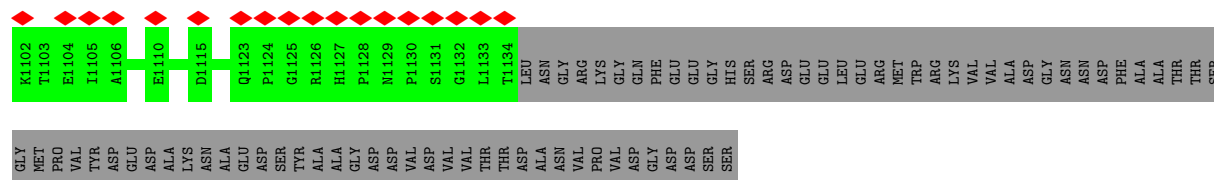


| Frequency | Percentage |
|-----------|------------|
| Often     | 6%         |
| Sometimes | 60%        |
| Never     | 39%        |

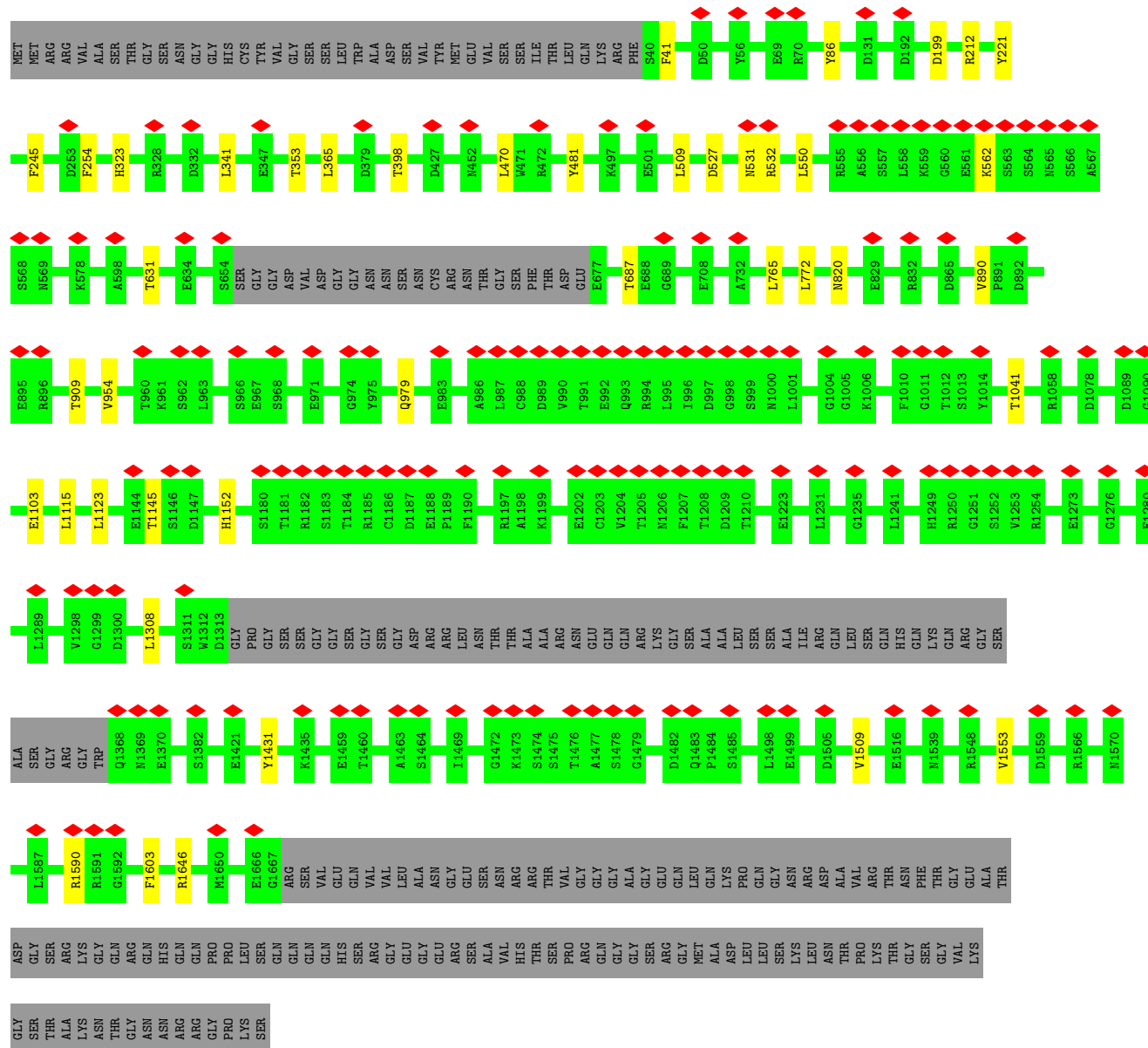
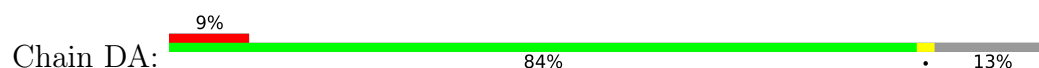


| Frequency | Percentage |
|-----------|------------|
| Often     | 6%         |
| Sometimes | 84%        |
| Never     | 14%        |



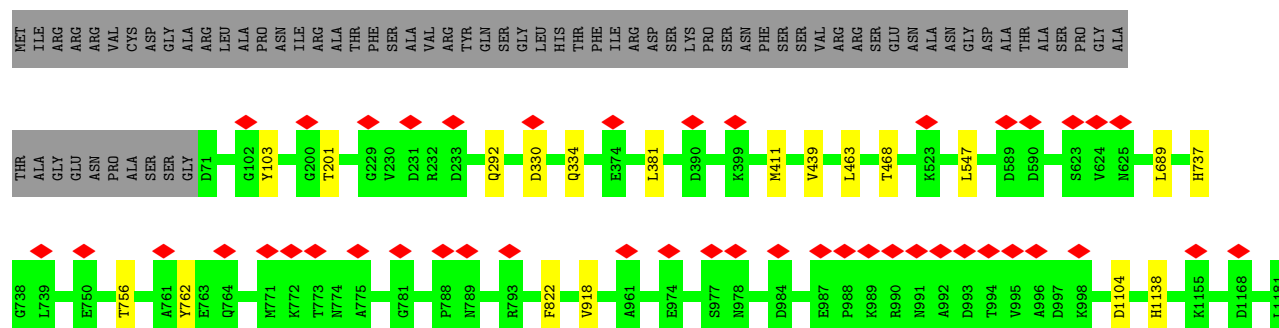


• Molecule 30: mS48



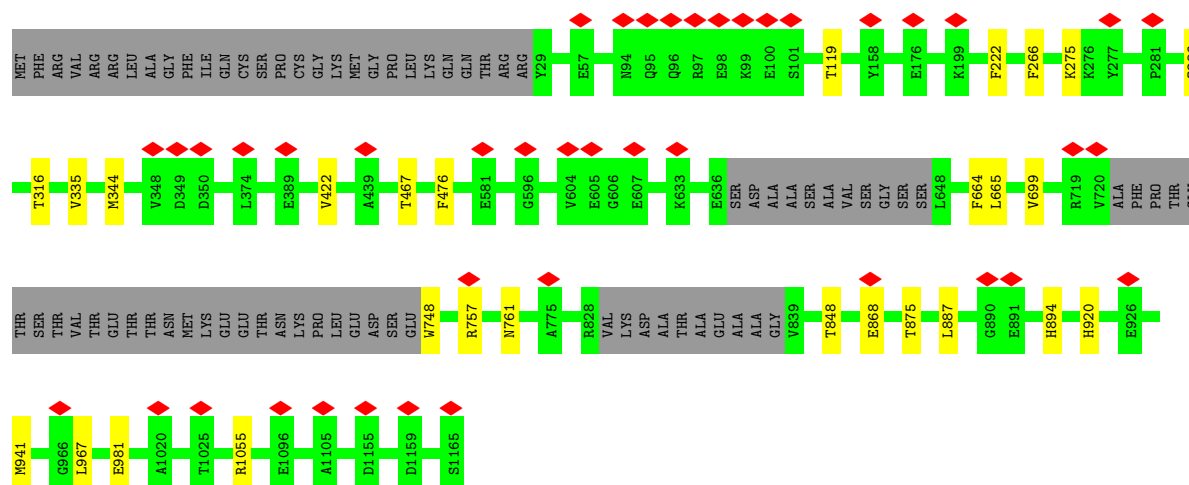
• Molecule 31: mS49





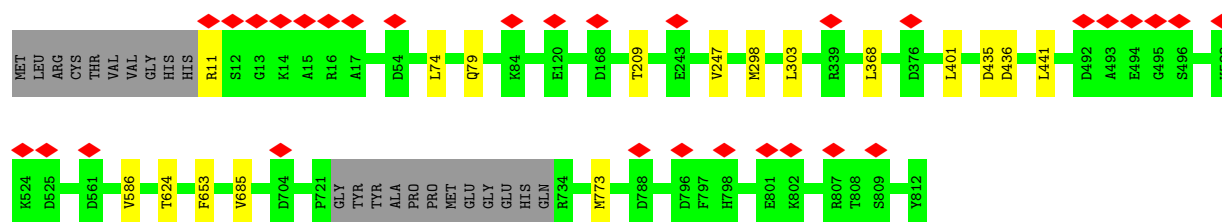
• Molecule 32: mS50

Chain DC: 91% 7%



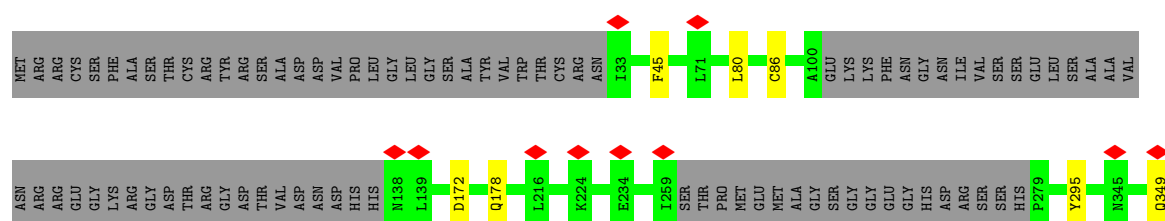
• Molecule 33: mS51

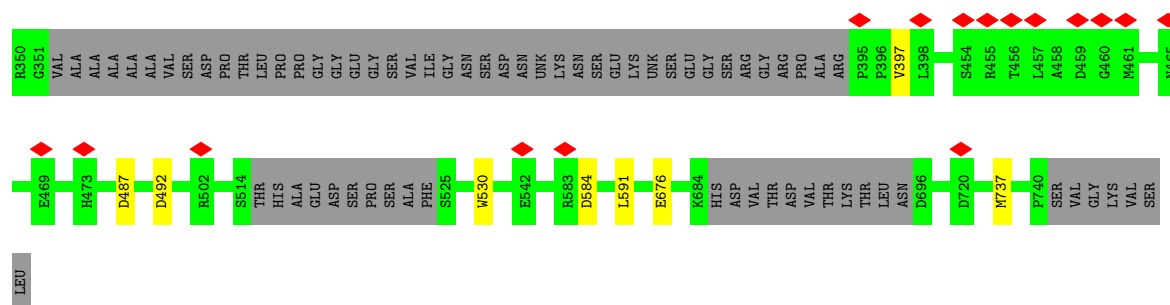
Chain DD: 95%



• Molecule 34: mS52

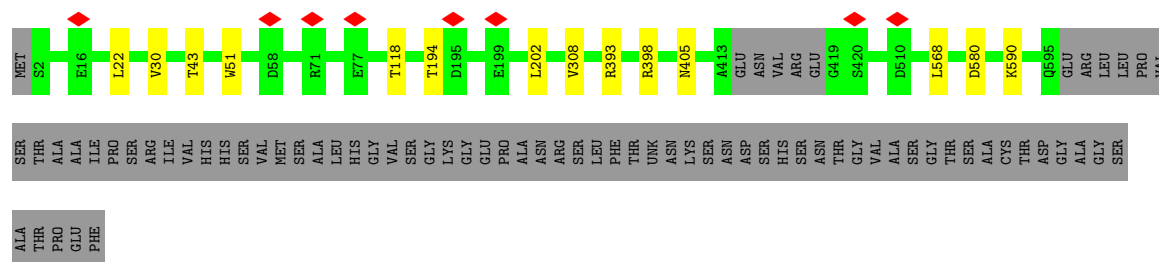
Chain DE: 77% 21%





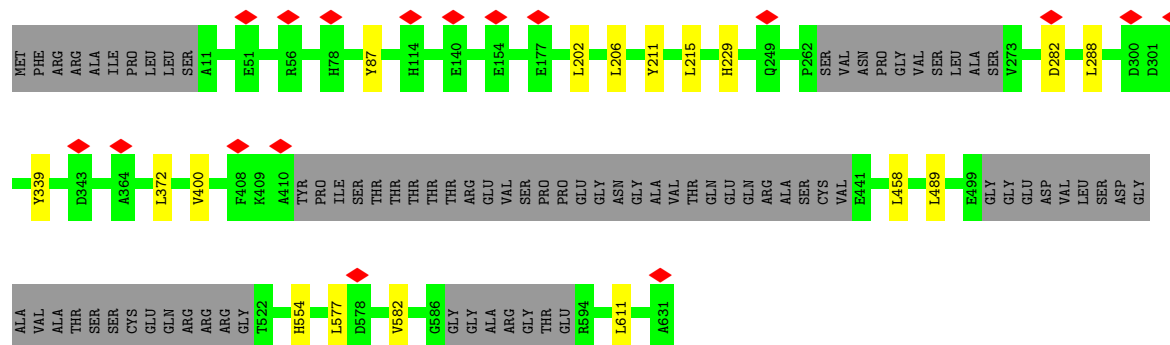
• Molecule 35: mS53

Chain DF: 86% 12%



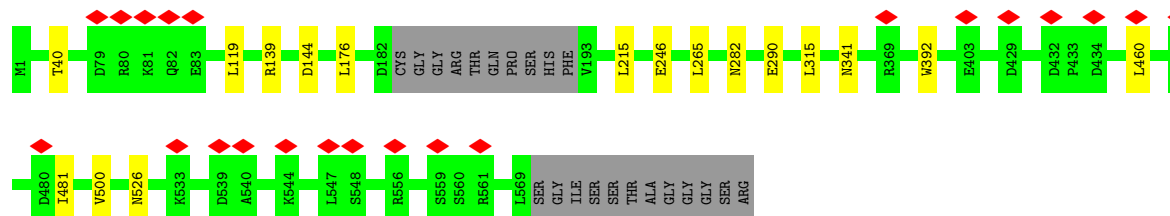
• Molecule 36: mS54

Chain DG: 85% 13%

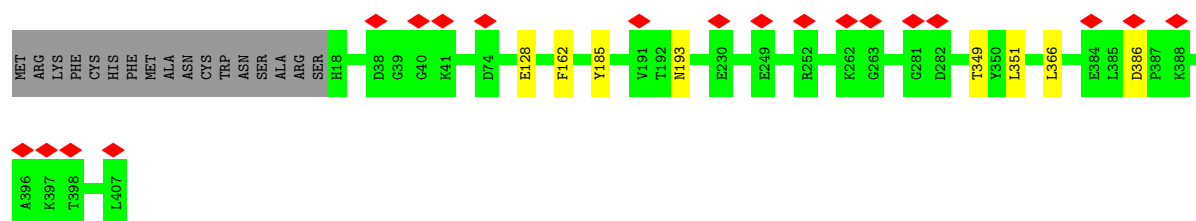


• Molecule 37: mS55

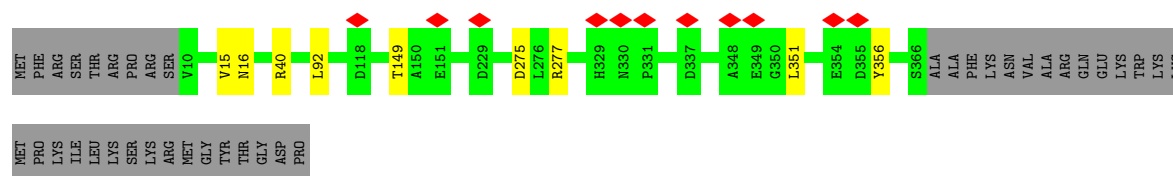
Chain DH: 93%



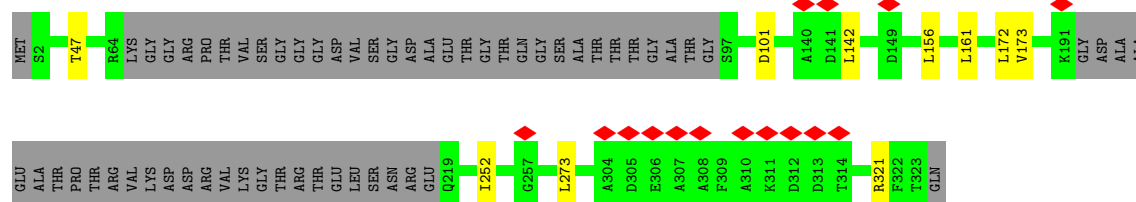
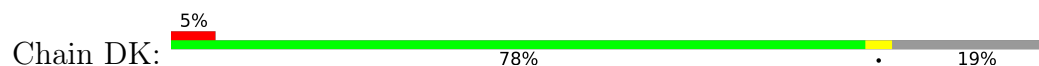
• Molecule 38: mS56



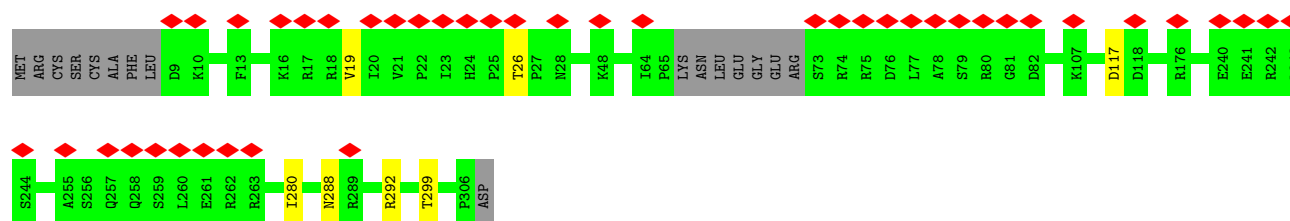
- Molecule 39: mS57



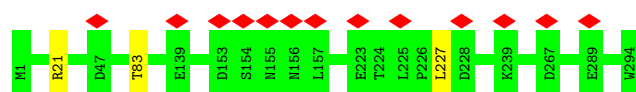
- Molecule 40: mS58




- Molecule 41: mS59

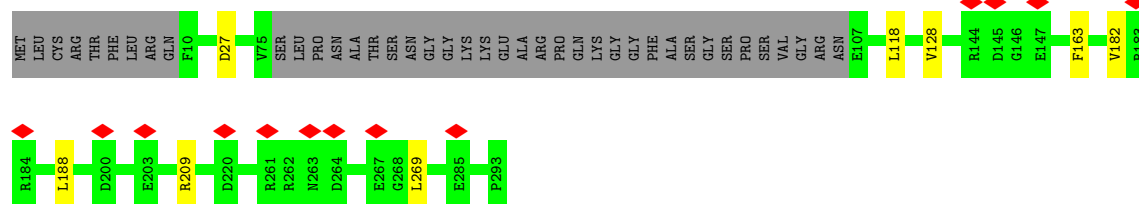


- Molecule 42: mS60




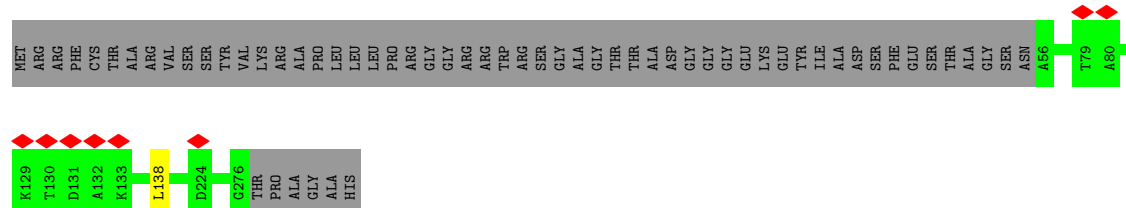
- Molecule 43: mS61

Chain DN:  84% 14%




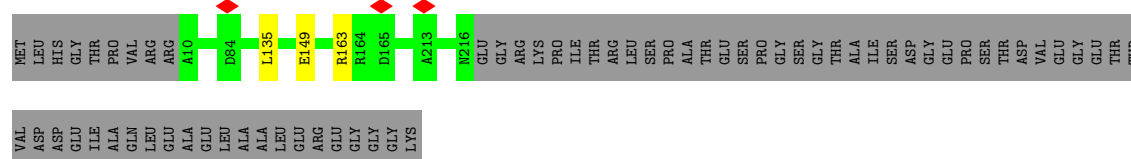
- Molecule 44: mS62

Chain DO:  78% 22%



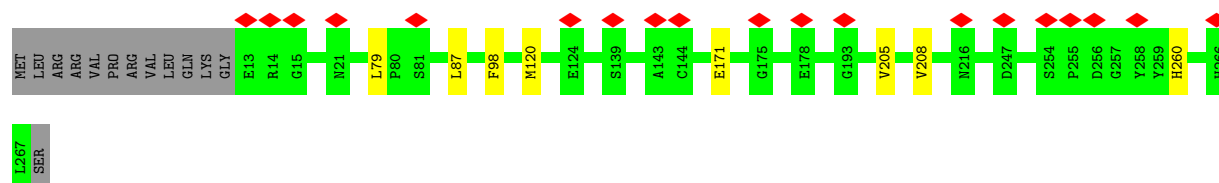
- Molecule 45: mS63

Chain DP:  74% 24%



- Molecule 46: AKAP7\_NLS domain-containing protein

Chain DQ:  92% 5%



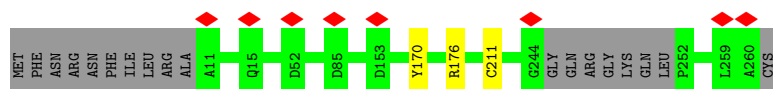
- Molecule 47: mS65

Chain DR:  89% 7%



- Molecule 48: mS66

Chain DS:  92% 7%



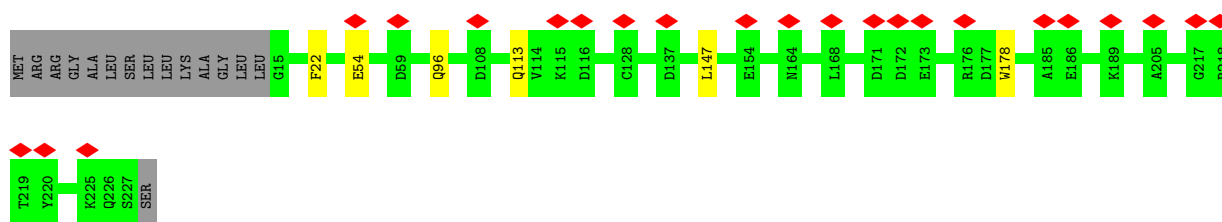
- Molecule 49: Rhodanese domain-containing protein

Chain DT:  92% 7%




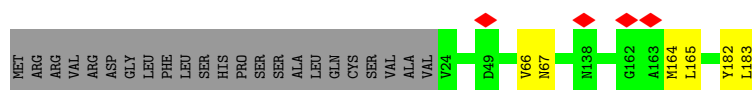
- Molecule 50: Ubiquitin-like domain-containing protein

Chain DU:  10% 91% 7%



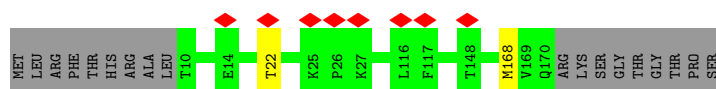
- Molecule 51: mS69

Chain DV:  84% 13%




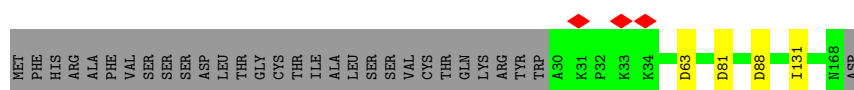
- Molecule 52: mS70

Chain DW:  89% 10%



- Molecule 53: mS71


Chain DX:  80% 18%

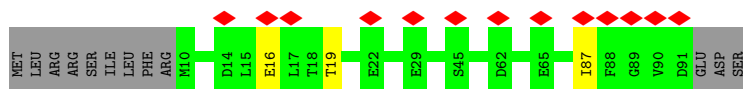


- Molecule 54: mS72

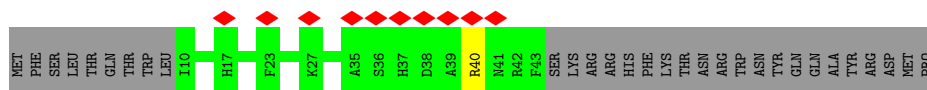
Chain DY:  93% 6%



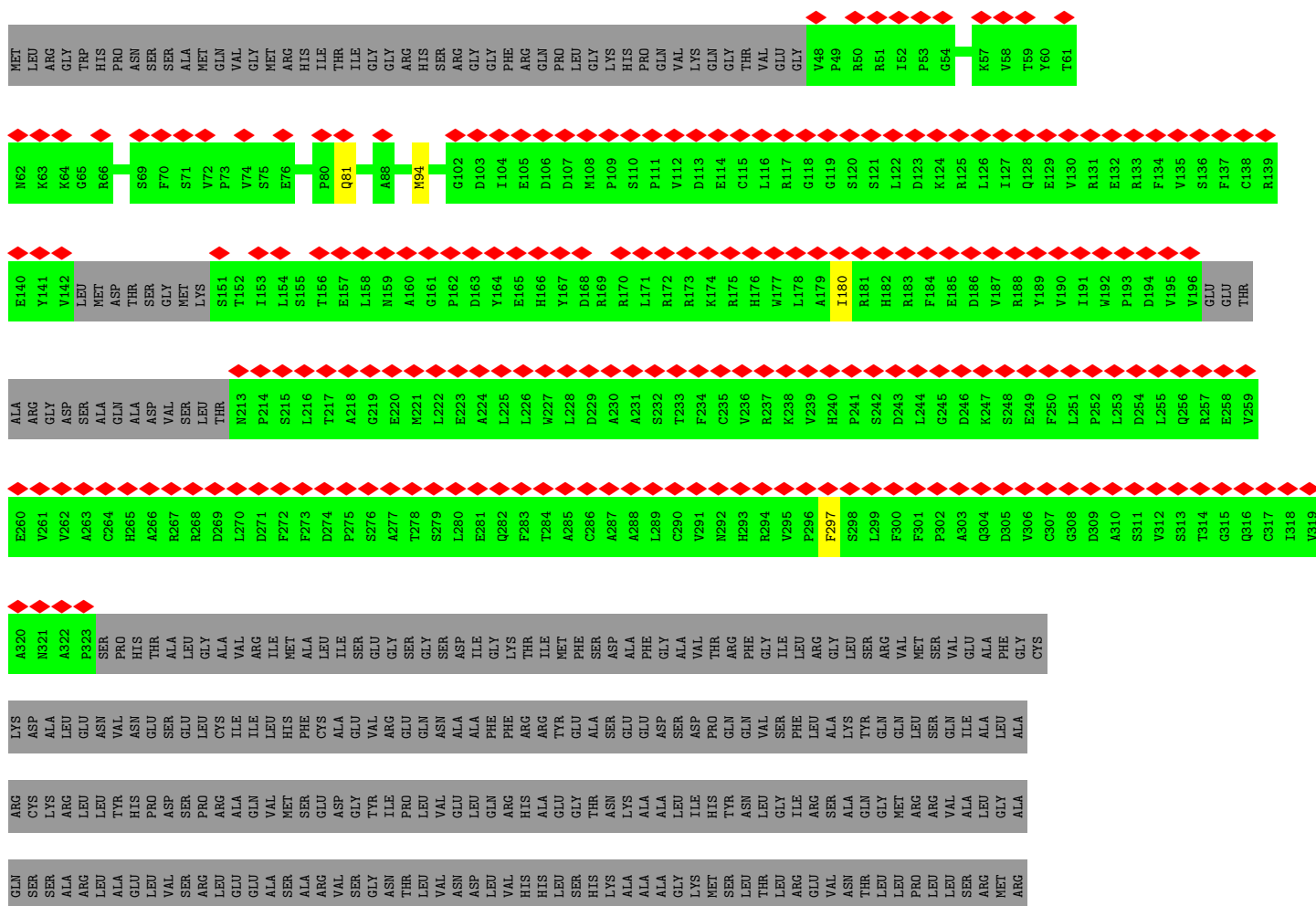
Chain DZ: 



Chain Da: 



Chain F3:  23% 26% 74%





|     |     |     |     |     |     |     |     |     |     |     |       |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-----|-----|
| GLN | VAL | ARG | ASN | VAL | ALA | ALA | ASN | VAL | VAL | ALA | ASP   | ILE | ARG |
| VAL | ARG | GLY | VAL | PHE | PHE | GLY | GLY | GLY | GLY | PHE | GLY   | ARG | GLY |
| PRO | HIS | THR | HIS | LEU | ALA | LEU | THR | LEU | LEU | ALA | VAL   | VAL | PRO |
| HIS | ALA | ALA | ALA | GLY | LYS | GLY | GLY | GLY | GLY | LYS | ASN   | MET | GLY |
| SER | SER | PRO | PRO | TYR | TYR | TYR | TYR | TYR | TYR | LYS | HIS   | HIS | ALA |
| PHE | GLY | GLY | GLY | GLY | HIS | HIS | HIS | HIS | HIS | LEU | LEU   | GLY | LEU |
| ASP | ASP | VAL | VAL | SER | ASP | ASP | ASP | ASP | ASP | GLY | GLY   | CYS | ASP |
| VAL | VAL | GLY | ILE | ALA | LYS | GLY | THR | ALA | GLY | LYS | CYS   | SER | ALA |
| ALA | ALA | ILE | PRO | SER | ALA | ALA | TRP | ALA | ASP | GLN | MET   | PHE | ARG |
| LEU | LEU | ASP | ASP | LEU | TRP | GLY | LEU | GLY | VAL | LEU | HIS   | ASP | ASP |
| ALA | ALA | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | LEU   | ARG | VAL |
| SER | SER | LEU | THR | LEU | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | PHE |
| ASN | ASN | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
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| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
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| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
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| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
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| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
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| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
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| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
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| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
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| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
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| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
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| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
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| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR   | THR | THR |
| ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN | ASN   | ASN | ASN |
| VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL | VAL   | VAL | VAL |
| GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY   | GLY | GLY |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR</ |     |     |

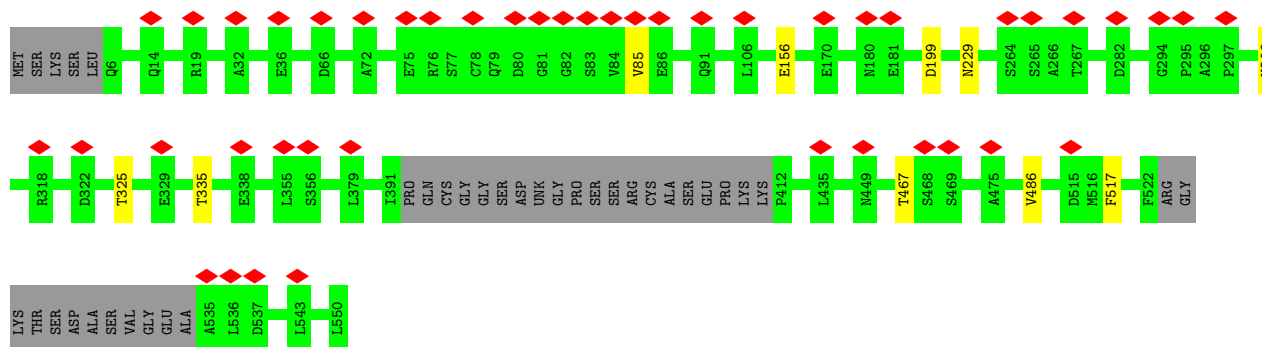
- Molecule 58: mt-SAF6



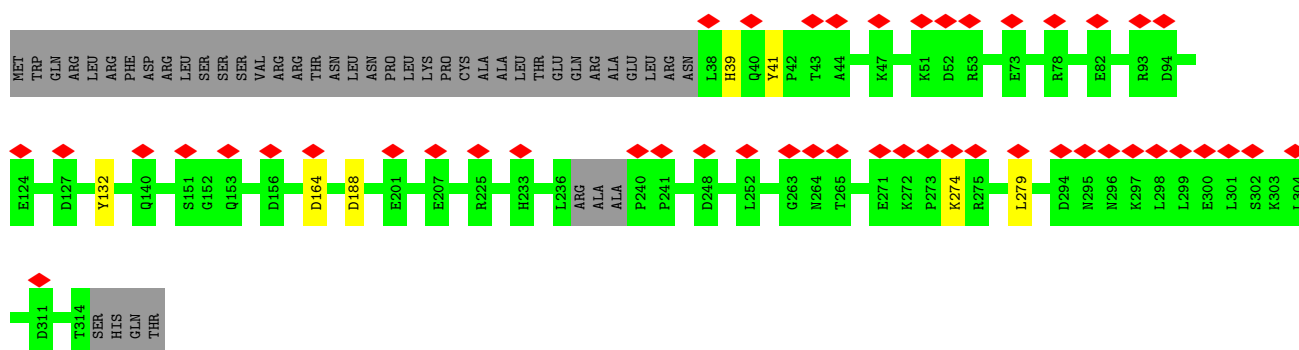
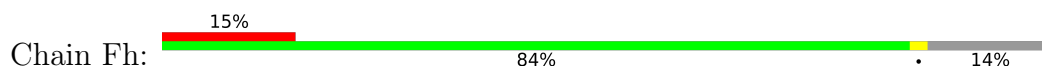
|      |      |      |      |      |      |      |     |     |     |
|------|------|------|------|------|------|------|-----|-----|-----|
| GLU  | GLU  | S447 | L384 | C317 | W241 | SER  | THR | THR | MET |
| GLU  | ARG  | E448 | R387 | S318 | E242 | LEU  | VAL | PHE | TYR |
| ARG  | M449 | ARG  |      | H319 | ASP  | E243 | LEU | GLU | TYR |
| ARG  | T450 | ARG  | L388 | Q320 | M244 | GLU  | ARG | ALA | LYS |
| LYS  | F451 | LYS  | Y389 | D321 | P245 | ALA  | VAL | PRO | LEU |
| GLN  | F452 | GLN  | E390 | A322 | V246 | VAL  | ASN | ASP | HIS |
| GLN  | L453 | GLN  | L391 | L323 | G450 | GLU  | LYS | ASP | SER |
| HIS  | S392 | HIS  | S392 | L323 | V248 | SER  | PHE | ASN | PHE |
| ASP  | S454 | ASP  | R324 | R324 | N249 | MET  | LEU | MET | THR |
| GLU  | P455 | GLU  | L325 | L325 | N250 | THR  | ARG | GLY | GLY |
| GLU  | D456 | GLU  | Y394 | M326 | N250 | THR  | ASP | ASN | LYS |
| LEU  | D457 | LEU  | K395 | E327 | Q251 | GLN  | LEU | GLY | VAL |
| MET  | L396 | MET  | L396 | E327 | F252 | TRP  | LEU | GLU | HIS |
| VAL  | D458 | VAL  | L397 | L328 | S253 | SER  | ARG | THR | PRO |
| GLU  | L459 | GLU  | S398 | L329 | F253 | LEU  | ARG | ARG | ASP |
| CYS  | L460 | CYS  | T399 | H330 | G255 | THR  | ALA | ALA | PHE |
| GLN  | D461 | GLN  | L400 | R331 | D256 | PRO  | ALA | GLY | PHE |
| GLU  | A462 | GLU  | W401 | N332 | L257 | ALA  | CYS | GLY | HIS |
| LYS  | N463 | LYS  | H402 | R333 | T258 | PRO  | ILE | SER | SER |
| GLY  | L464 | GLY  | L403 | E334 | G259 | ASN  | ASP | GLY | ASN |
| ARG  | L465 | ARG  | F406 | I337 | T260 | THR  | VAL | PRO | ARG |
| SER  | L466 | SER  |      |      |      | GLN  | THR | VAL | GLN |
| GLY  | L467 | GLY  | R407 | Q338 | I261 | E204 | GLU | SER | THR |
| ASP  | A467 | ASP  | T408 | Y339 | T262 | L206 | SER | SER | VAL |
| ASP  | L468 | ASP  | M409 | G340 | I263 | E207 | ILE | LEU | VAL |
| SER  | F469 | SER  | W410 | L341 | D266 | A208 | SER | VAL | ASN |
| PRO  | P470 | PRO  | F412 | S342 |      |      | ALA | ALA | ARG |
| THR  | Y470 | THR  | E411 | K343 | F267 | Q210 | ASP | MET | VAL |
| VAL  | M471 | VAL  | G413 | L344 | E270 | I211 | ALA | GLY | ALA |
| ALA  | F472 | ALA  | G414 | T345 | Q271 | L212 | THR | ASP | ARG |
| E539 | D473 | GLU  | W415 | L346 | F272 | F213 | ALA | GLY | LEU |
| H543 | G474 | GLU  | D416 | E347 | M276 | S214 | ALA | SER | GLU |
| L544 | D475 | GLU  | A417 | Y348 |      | R215 | ALA | SER | LEU |
| Y545 | A476 | GLU  | F418 | G349 | D216 | GLU  | PRO | LEU | SER |
| R546 | L477 | GLU  | S419 | N350 | L217 | ALA  | THR | SER | LEU |
| Q547 | V478 | GLU  | N420 | R351 | S218 | LYS  | ILE | TRP | TRP |
| D606 | V479 | GLU  | D421 | H352 | P219 | LEU  | ILE | ALA | LYS |
| K628 | V481 | GLU  | C422 | R355 | L220 | ARG  | GLN | LEU | LYS |
|      | E482 | GLU  | T423 | A356 | Q221 | ARG  | THR | THR | PHE |
| M629 | E483 | GLU  | Y424 | E288 | S222 | ARG  | PHE | SER | LYS |
| L630 | V484 | GLU  | A425 |      | A223 | PRO  | GLY | LEU | SER |
| D631 | Q485 | GLU  | E426 | V360 | ARG  | ARG  | GLY | LEU | GLY |
| R634 | GLU  | GLU  | E426 | I361 | A224 | GLY  | PRO | PRO | HIS |
|      | ALA  | ALA  | R427 | L362 | A225 | ASN  | ASN | GLN | LEU |
| THR  | LYS  | LYS  | W430 | N363 | L226 | HIS  | PHE | PRO | GLN |
| THR  | SER  | SER  | S431 | C364 | S227 | ARG  | ALA | ALA | PRO |
| GLY  | ARG  | ARG  | K432 | S365 | T228 | GLY  | PRO | PRO | PRO |
| LYS  | LYS  | LYS  | E433 | L366 | E298 | ALA  | SER | SER | SER |
| LYS  | ARG  | ARG  | L434 | T367 | Q299 | THR  | THR | ASN | SER |
| SER  | GLU  | GLU  | F435 | S368 | L300 | GLY  | GLY | ARG | PHE |
| R642 | LEU  | LEU  | R436 | E369 | E303 | R231 | THR | HIS | THR |
| R643 | LEU  | LEU  | L437 | Q370 | L304 | H232 | GLY | ARG | GLY |
| F644 | ALA  | ALA  | G438 | R371 | E309 | L236 | PRO | PRO | LYS |
| E645 | SER  | SER  | P439 | L372 | N237 | L236 | LEU | LEU | LEU |
| MET  | ALA  | ALA  | S440 | L372 | Y238 | N237 | LEU | LEU | LEU |
|      | GLN  | GLN  | L441 | K376 | S239 | Y238 | LEU | LEU | LEU |
| ARG  | ARG  | ARG  | A442 | D312 | S239 | A240 | LEU | LEU | LEU |
| GLU  | GLU  | GLU  | P443 | I378 | S239 |      |     |     |     |
| GLU  | GLU  | GLU  | W444 | S379 | I313 |      |     |     |     |
|      |      |      | P380 | L314 | S239 |      |     |     |     |
|      |      |      | D445 | V315 | S239 |      |     |     |     |
|      |      |      | W446 | S316 | A240 |      |     |     |     |



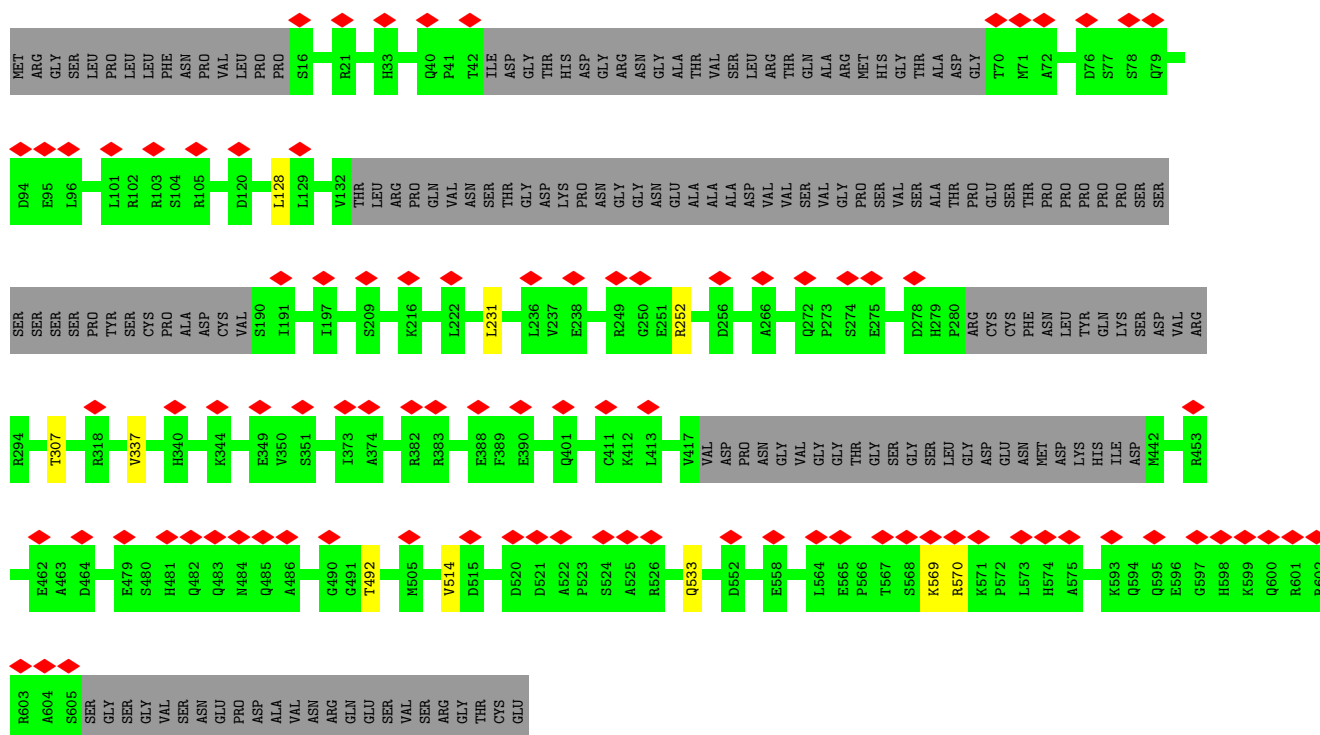
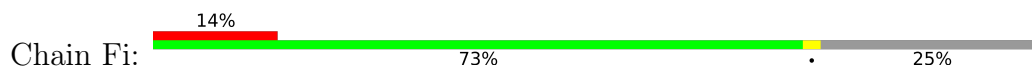




• Molecule 64: mt-SAF37



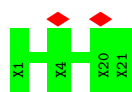
• Molecule 65: mt-SAF38



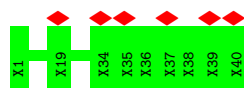
- Chain IA:  5% 86% 12%



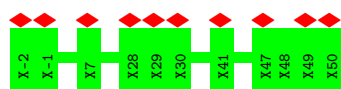
- 



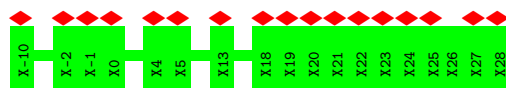
- Molecule 69: Unk7



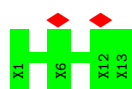
- Molecule 70: UnkE



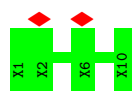
- Molecule 71: UnkF



- Molecule 72: UnkG



- Molecule 73: UnkI

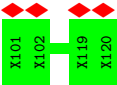


- Molecule 74: UnkK



There are no outlier residues recorded for this chain.

- Molecule 75: UnkL



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 17391                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.222                                   | Depositor |
| Minimum map value                    | -0.107                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.009                                   | Depositor |
| Recommended contour level            | 0.04                                    | Depositor |
| Map size (Å)                         | 500.4, 500.4, 500.4                     | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.39, 1.39, 1.39                        | Depositor |



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, UTP, GDP, PO4, MG, FAD, ZN

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$    |
| 1   | CA    | 0.17         | 0/13759     | 0.70        | 1/21382 (0.0%) |
| 2   | CC    | 0.26         | 0/666       | 0.43        | 0/900          |
| 3   | CE    | 0.25         | 0/3547      | 0.50        | 0/4798         |
| 4   | CF    | 0.25         | 0/1266      | 0.51        | 0/1708         |
| 5   | CH    | 0.25         | 0/2276      | 0.52        | 0/3071         |
| 6   | CI    | 0.25         | 0/3479      | 0.49        | 0/4693         |
| 7   | CJ    | 0.25         | 0/6725      | 0.48        | 0/9152         |
| 8   | CK    | 0.25         | 0/2502      | 0.51        | 0/3357         |
| 9   | CL    | 0.28         | 0/759       | 0.50        | 0/1026         |
| 10  | CN    | 0.25         | 0/1361      | 0.47        | 0/1840         |
| 11  | CO    | 0.26         | 0/2614      | 0.49        | 0/3520         |
| 12  | CP    | 0.24         | 0/1533      | 0.49        | 0/2074         |
| 13  | CQ    | 0.25         | 0/1919      | 0.50        | 0/2595         |
| 14  | CR    | 0.25         | 0/2276      | 0.48        | 0/3087         |
| 15  | CS    | 0.26         | 0/1183      | 0.48        | 0/1593         |
| 16  | CU    | 0.24         | 0/1560      | 0.51        | 0/2094         |
| 17  | Ca    | 0.25         | 0/5066      | 0.47        | 0/6852         |
| 18  | Cb    | 0.25         | 0/2105      | 0.48        | 0/2842         |
| 19  | Cd    | 0.25         | 0/2016      | 0.44        | 0/2715         |
| 20  | Cg    | 0.25         | 0/4016      | 0.46        | 0/5455         |
| 21  | Ci    | 0.25         | 0/1383      | 0.49        | 0/1871         |
| 22  | Cj    | 0.25         | 0/1849      | 0.48        | 0/2521         |
| 23  | Ck    | 0.24         | 0/5540      | 0.49        | 0/7490         |
| 24  | Cm    | 0.25         | 0/1215      | 0.49        | 0/1630         |
| 25  | Cn    | 0.25         | 0/543       | 0.52        | 0/725          |
| 26  | Cp    | 0.25         | 0/1511      | 0.48        | 0/2049         |
| 27  | Cq    | 0.25         | 0/2066      | 0.44        | 0/2815         |
| 28  | Cr    | 0.24         | 0/2131      | 0.48        | 0/2895         |
| 29  | Cv    | 0.24         | 0/8625      | 0.48        | 0/11690        |
| 30  | DA    | 0.24         | 0/12744     | 0.48        | 0/17248        |
| 31  | DB    | 0.24         | 0/9369      | 0.50        | 0/12692        |
| 32  | DC    | 0.25         | 0/8913      | 0.49        | 0/12092        |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 33  | DD    | 0.25         | 0/6699   | 0.49        | 0/9072          |
| 34  | DE    | 0.25         | 0/4920   | 0.49        | 0/6666          |
| 35  | DF    | 0.25         | 0/4847   | 0.51        | 0/6569          |
| 36  | DG    | 0.24         | 0/4578   | 0.50        | 0/6202          |
| 37  | DH    | 0.25         | 0/4645   | 0.50        | 0/6295          |
| 38  | DI    | 0.25         | 0/3248   | 0.48        | 0/4401          |
| 39  | DJ    | 0.25         | 0/2999   | 0.46        | 0/4071          |
| 40  | DK    | 0.24         | 0/2123   | 0.47        | 0/2865          |
| 41  | DL    | 0.25         | 0/2420   | 0.51        | 0/3262          |
| 42  | DM    | 0.24         | 0/2488   | 0.49        | 0/3362          |
| 43  | DN    | 0.24         | 0/2118   | 0.52        | 0/2874          |
| 44  | DO    | 0.25         | 0/1832   | 0.50        | 0/2471          |
| 45  | DP    | 0.24         | 0/1813   | 0.47        | 0/2457          |
| 46  | DQ    | 0.24         | 0/2105   | 0.52        | 0/2855          |
| 47  | DR    | 0.25         | 0/2084   | 0.51        | 1/2841 (0.0%)   |
| 48  | DS    | 0.24         | 0/1997   | 0.50        | 0/2694          |
| 49  | DT    | 0.25         | 0/2133   | 0.47        | 0/2889          |
| 50  | DU    | 0.24         | 0/1799   | 0.50        | 0/2438          |
| 51  | DV    | 0.25         | 0/1382   | 0.51        | 0/1871          |
| 52  | DW    | 0.24         | 0/1407   | 0.49        | 0/1916          |
| 53  | DX    | 0.25         | 0/1207   | 0.50        | 0/1620          |
| 54  | DY    | 0.26         | 0/1337   | 0.51        | 0/1814          |
| 55  | DZ    | 0.25         | 0/725    | 0.43        | 0/984           |
| 56  | Da    | 0.26         | 0/317    | 0.54        | 0/422           |
| 57  | F3    | 0.24         | 0/2049   | 0.48        | 0/2782          |
| 58  | F6    | 0.24         | 0/3434   | 0.47        | 0/4661          |
| 59  | F7    | 0.24         | 0/4684   | 0.47        | 0/6341          |
| 60  | F9    | 0.24         | 0/2863   | 0.50        | 0/3835          |
| 61  | FO    | 0.24         | 0/2292   | 0.52        | 0/3096          |
| 62  | Ff    | 0.25         | 0/5082   | 0.48        | 0/6918          |
| 63  | Fg    | 0.24         | 0/4074   | 0.48        | 0/5522          |
| 64  | Fh    | 0.24         | 0/2278   | 0.50        | 0/3073          |
| 65  | Fi    | 0.24         | 0/3833   | 0.50        | 0/5202          |
| 66  | IA    | 0.25         | 0/5512   | 0.49        | 0/7462          |
| 67  | IB    | 0.25         | 0/4193   | 0.51        | 0/5672          |
| All | All   | 0.24         | 0/218034 | 0.51        | 2/297947 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 47  | DR    | 190 | LEU  | CA-CB-CG | 5.49 | 127.92      | 115.30   |

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| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1   | CA    | 329 | U    | OP2-P-O3' | 5.33 | 116.94      | 105.20   |

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | CC    | 72/74 (97%)   | 66 (92%)  | 6 (8%)  | 0        | 100         | 100 |
| 3   | CE    | 424/435 (98%) | 406 (96%) | 18 (4%) | 0        | 100         | 100 |
| 4   | CF    | 145/160 (91%) | 139 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 5   | CH    | 271/282 (96%) | 263 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 6   | CI    | 423/443 (96%) | 411 (97%) | 12 (3%) | 0        | 100         | 100 |
| 7   | CJ    | 799/817 (98%) | 771 (96%) | 28 (4%) | 0        | 100         | 100 |
| 8   | CK    | 294/326 (90%) | 284 (97%) | 10 (3%) | 0        | 100         | 100 |
| 9   | CL    | 85/87 (98%)   | 81 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 10  | CN    | 155/166 (93%) | 149 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 11  | CO    | 306/429 (71%) | 292 (95%) | 14 (5%) | 0        | 100         | 100 |
| 12  | CP    | 178/188 (95%) | 171 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 13  | CQ    | 224/307 (73%) | 219 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 14  | CR    | 265/320 (83%) | 258 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 15  | CS    | 137/244 (56%) | 132 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 16  | CU    | 179/193 (93%) | 175 (98%) | 4 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 17  | Ca    | 571/602 (95%)   | 549 (96%)  | 22 (4%) | 0        | 100         | 100 |
| 18  | Cb    | 248/325 (76%)   | 236 (95%)  | 12 (5%) | 0        | 100         | 100 |
| 19  | Cd    | 228/440 (52%)   | 223 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 20  | Cg    | 478/498 (96%)   | 473 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 21  | Ci    | 162/181 (90%)   | 156 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 22  | Cj    | 225/257 (88%)   | 220 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 23  | Ck    | 676/874 (77%)   | 666 (98%)  | 10 (2%) | 0        | 100         | 100 |
| 24  | Cm    | 143/215 (66%)   | 138 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 25  | Cn    | 60/250 (24%)    | 59 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 26  | Cp    | 171/187 (91%)   | 167 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 27  | Cq    | 250/263 (95%)   | 241 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 28  | Cr    | 263/439 (60%)   | 258 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 29  | Cv    | 1032/1211 (85%) | 994 (96%)  | 38 (4%) | 0        | 100         | 100 |
| 30  | DA    | 1546/1788 (86%) | 1513 (98%) | 33 (2%) | 0        | 100         | 100 |
| 31  | DB    | 1109/1181 (94%) | 1076 (97%) | 33 (3%) | 0        | 100         | 100 |
| 32  | DC    | 1081/1165 (93%) | 1023 (95%) | 58 (5%) | 0        | 100         | 100 |
| 33  | DD    | 786/812 (97%)   | 758 (96%)  | 28 (4%) | 0        | 100         | 100 |
| 34  | DE    | 576/747 (77%)   | 549 (95%)  | 27 (5%) | 0        | 100         | 100 |
| 35  | DF    | 585/666 (88%)   | 559 (96%)  | 26 (4%) | 0        | 100         | 100 |
| 36  | DG    | 542/631 (86%)   | 529 (98%)  | 13 (2%) | 0        | 100         | 100 |
| 37  | DH    | 555/581 (96%)   | 530 (96%)  | 25 (4%) | 0        | 100         | 100 |
| 38  | DI    | 388/407 (95%)   | 372 (96%)  | 16 (4%) | 0        | 100         | 100 |
| 39  | DJ    | 355/396 (90%)   | 351 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 40  | DK    | 257/324 (79%)   | 249 (97%)  | 8 (3%)  | 0        | 100         | 100 |
| 41  | DL    | 287/307 (94%)   | 283 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 42  | DM    | 292/294 (99%)   | 277 (95%)  | 15 (5%) | 0        | 100         | 100 |
| 43  | DN    | 249/293 (85%)   | 243 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 44  | DO    | 219/282 (78%)   | 207 (94%)  | 12 (6%) | 0        | 100         | 100 |
| 45  | DP    | 205/274 (75%)   | 198 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 46  | DQ    | 253/268 (94%)   | 249 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 47  | DR    | 246/270 (91%)   | 240 (98%)  | 6 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 48  | DS    | 239/261 (92%)     | 238 (100%)  | 1 (0%)   | 0        | 100         | 100 |
| 49  | DT    | 237/247 (96%)     | 223 (94%)   | 14 (6%)  | 0        | 100         | 100 |
| 50  | DU    | 211/228 (92%)     | 204 (97%)   | 7 (3%)   | 0        | 100         | 100 |
| 51  | DV    | 158/183 (86%)     | 144 (91%)   | 14 (9%)  | 0        | 100         | 100 |
| 52  | DW    | 159/179 (89%)     | 152 (96%)   | 7 (4%)   | 0        | 100         | 100 |
| 53  | DX    | 137/169 (81%)     | 129 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 54  | DY    | 152/163 (93%)     | 145 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 55  | DZ    | 80/94 (85%)       | 78 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 56  | Da    | 32/64 (50%)       | 31 (97%)    | 1 (3%)   | 0        | 100         | 100 |
| 57  | F3    | 246/966 (26%)     | 243 (99%)   | 3 (1%)   | 0        | 100         | 100 |
| 58  | F6    | 410/676 (61%)     | 402 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 59  | F7    | 566/679 (83%)     | 544 (96%)   | 22 (4%)  | 0        | 100         | 100 |
| 60  | F9    | 338/608 (56%)     | 329 (97%)   | 9 (3%)   | 0        | 100         | 100 |
| 61  | FO    | 263/334 (79%)     | 255 (97%)   | 8 (3%)   | 0        | 100         | 100 |
| 62  | Ff    | 610/848 (72%)     | 593 (97%)   | 17 (3%)  | 0        | 100         | 100 |
| 63  | Fg    | 507/550 (92%)     | 487 (96%)   | 20 (4%)  | 0        | 100         | 100 |
| 64  | Fh    | 270/318 (85%)     | 259 (96%)   | 11 (4%)  | 0        | 100         | 100 |
| 65  | Fi    | 459/629 (73%)     | 438 (95%)   | 21 (5%)  | 0        | 100         | 100 |
| 66  | IA    | 687/787 (87%)     | 668 (97%)   | 19 (3%)  | 0        | 100         | 100 |
| 67  | IB    | 507/803 (63%)     | 491 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| All | All   | 24263/29685 (82%) | 23456 (97%) | 807 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |    |
|-----|-------|--------------|-----------|----------|-------------|----|
| 2   | CC    | 73/73 (100%) | 69 (94%)  | 4 (6%)   | 18          | 45 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 3   | CE    | 365/372 (98%)   | 354 (97%)  | 11 (3%)  | 36          | 58 |
| 4   | CF    | 135/144 (94%)   | 132 (98%)  | 3 (2%)   | 47          | 65 |
| 5   | CH    | 237/246 (96%)   | 235 (99%)  | 2 (1%)   | 79          | 85 |
| 6   | CI    | 360/371 (97%)   | 351 (98%)  | 9 (2%)   | 42          | 62 |
| 7   | CJ    | 710/723 (98%)   | 692 (98%)  | 18 (2%)  | 42          | 62 |
| 8   | CK    | 259/283 (92%)   | 256 (99%)  | 3 (1%)   | 67          | 79 |
| 9   | CL    | 79/79 (100%)    | 77 (98%)   | 2 (2%)   | 42          | 62 |
| 10  | CN    | 142/150 (95%)   | 138 (97%)  | 4 (3%)   | 38          | 60 |
| 11  | CO    | 270/377 (72%)   | 263 (97%)  | 7 (3%)   | 41          | 61 |
| 12  | CP    | 160/168 (95%)   | 158 (99%)  | 2 (1%)   | 65          | 77 |
| 13  | CQ    | 201/270 (74%)   | 195 (97%)  | 6 (3%)   | 36          | 58 |
| 14  | CR    | 233/279 (84%)   | 228 (98%)  | 5 (2%)   | 48          | 67 |
| 15  | CS    | 123/220 (56%)   | 121 (98%)  | 2 (2%)   | 58          | 74 |
| 16  | CU    | 159/169 (94%)   | 158 (99%)  | 1 (1%)   | 84          | 90 |
| 17  | Ca    | 518/543 (95%)   | 507 (98%)  | 11 (2%)  | 48          | 67 |
| 18  | Cb    | 219/277 (79%)   | 216 (99%)  | 3 (1%)   | 62          | 76 |
| 19  | Cd    | 207/381 (54%)   | 205 (99%)  | 2 (1%)   | 73          | 82 |
| 20  | Cg    | 424/437 (97%)   | 415 (98%)  | 9 (2%)   | 48          | 67 |
| 21  | Ci    | 144/160 (90%)   | 139 (96%)  | 5 (4%)   | 31          | 56 |
| 22  | Cj    | 194/219 (89%)   | 192 (99%)  | 2 (1%)   | 73          | 82 |
| 23  | Ck    | 589/746 (79%)   | 579 (98%)  | 10 (2%)  | 56          | 73 |
| 24  | Cm    | 124/184 (67%)   | 120 (97%)  | 4 (3%)   | 34          | 57 |
| 25  | Cn    | 54/210 (26%)    | 51 (94%)   | 3 (6%)   | 17          | 45 |
| 26  | Cp    | 161/175 (92%)   | 157 (98%)  | 4 (2%)   | 42          | 62 |
| 27  | Cq    | 210/221 (95%)   | 205 (98%)  | 5 (2%)   | 44          | 63 |
| 28  | Cr    | 223/369 (60%)   | 218 (98%)  | 5 (2%)   | 47          | 65 |
| 29  | Cv    | 894/1033 (86%)  | 870 (97%)  | 24 (3%)  | 40          | 61 |
| 30  | DA    | 1319/1514 (87%) | 1277 (97%) | 42 (3%)  | 34          | 57 |
| 31  | DB    | 976/1030 (95%)  | 957 (98%)  | 19 (2%)  | 52          | 70 |
| 32  | DC    | 923/985 (94%)   | 896 (97%)  | 27 (3%)  | 37          | 59 |
| 33  | DD    | 693/711 (98%)   | 676 (98%)  | 17 (2%)  | 42          | 62 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |    |
|-----|-------|----------------|------------|----------|-------------|----|
| 34  | DE    | 514/642 (80%)  | 499 (97%)  | 15 (3%)  | 37          | 59 |
| 35  | DF    | 499/560 (89%)  | 485 (97%)  | 14 (3%)  | 38          | 60 |
| 36  | DG    | 481/543 (89%)  | 464 (96%)  | 17 (4%)  | 31          | 56 |
| 37  | DH    | 489/504 (97%)  | 472 (96%)  | 17 (4%)  | 31          | 56 |
| 38  | DI    | 350/365 (96%)  | 342 (98%)  | 8 (2%)   | 45          | 64 |
| 39  | DJ    | 313/347 (90%)  | 304 (97%)  | 9 (3%)   | 37          | 59 |
| 40  | DK    | 218/261 (84%)  | 208 (95%)  | 10 (5%)  | 23          | 49 |
| 41  | DL    | 249/263 (95%)  | 242 (97%)  | 7 (3%)   | 38          | 60 |
| 42  | DM    | 252/252 (100%) | 249 (99%)  | 3 (1%)   | 67          | 79 |
| 43  | DN    | 225/256 (88%)  | 217 (96%)  | 8 (4%)   | 30          | 55 |
| 44  | DO    | 185/229 (81%)  | 184 (100%) | 1 (0%)   | 86          | 92 |
| 45  | DP    | 187/239 (78%)  | 184 (98%)  | 3 (2%)   | 58          | 74 |
| 46  | DQ    | 227/239 (95%)  | 219 (96%)  | 8 (4%)   | 31          | 56 |
| 47  | DR    | 219/235 (93%)  | 209 (95%)  | 10 (5%)  | 23          | 49 |
| 48  | DS    | 213/228 (93%)  | 210 (99%)  | 3 (1%)   | 62          | 76 |
| 49  | DT    | 220/228 (96%)  | 209 (95%)  | 11 (5%)  | 20          | 47 |
| 50  | DU    | 190/201 (94%)  | 184 (97%)  | 6 (3%)   | 34          | 57 |
| 51  | DV    | 145/165 (88%)  | 139 (96%)  | 6 (4%)   | 26          | 52 |
| 52  | DW    | 148/163 (91%)  | 146 (99%)  | 2 (1%)   | 62          | 76 |
| 53  | DX    | 122/149 (82%)  | 118 (97%)  | 4 (3%)   | 33          | 57 |
| 54  | DY    | 137/146 (94%)  | 134 (98%)  | 3 (2%)   | 47          | 65 |
| 55  | DZ    | 72/84 (86%)    | 69 (96%)   | 3 (4%)   | 25          | 51 |
| 56  | Da    | 30/59 (51%)    | 29 (97%)   | 1 (3%)   | 33          | 57 |
| 57  | F3    | 223/809 (28%)  | 219 (98%)  | 4 (2%)   | 54          | 71 |
| 58  | F6    | 368/590 (62%)  | 350 (95%)  | 18 (5%)  | 21          | 47 |
| 59  | F7    | 493/577 (85%)  | 475 (96%)  | 18 (4%)  | 29          | 54 |
| 60  | F9    | 288/504 (57%)  | 283 (98%)  | 5 (2%)   | 56          | 73 |
| 61  | FO    | 234/290 (81%)  | 224 (96%)  | 10 (4%)  | 25          | 50 |
| 62  | Ff    | 519/715 (73%)  | 502 (97%)  | 17 (3%)  | 33          | 57 |
| 63  | Fg    | 441/469 (94%)  | 431 (98%)  | 10 (2%)  | 45          | 64 |
| 64  | Fh    | 242/281 (86%)  | 235 (97%)  | 7 (3%)   | 37          | 59 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 65  | Fi    | 404/536 (75%)     | 394 (98%)   | 10 (2%)  | 42          | 62 |
| 66  | IA    | 586/661 (89%)     | 571 (97%)   | 15 (3%)  | 41          | 61 |
| 67  | IB    | 435/675 (64%)     | 421 (97%)   | 14 (3%)  | 34          | 57 |
| All | All   | 21296/25584 (83%) | 20728 (97%) | 568 (3%) | 41          | 61 |

5 of 568 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | F7    | 75  | LEU  |
| 59  | F7    | 517 | PHE  |
| 59  | F7    | 67  | TYR  |
| 63  | Fg    | 486 | VAL  |
| 30  | DA    | 979 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 321 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | DO    | 88  | GLN  |
| 62  | Ff    | 317 | GLN  |
| 46  | DQ    | 73  | HIS  |
| 54  | DY    | 106 | GLN  |
| 65  | Fi    | 401 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 1   | CA    | 620/621 (99%) | 252 (40%)         | 2 (0%)          |

5 of 252 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 2   | A    |
| 1   | CA    | 3   | A    |
| 1   | CA    | 4   | A    |
| 1   | CA    | 6   | U    |
| 1   | CA    | 11  | U    |

All (2) RNA pucker outliers are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 299 | U    |
| 1   | CA    | 512 | G    |

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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 |
| 81  | GDP  | IA    | 1000 | 76   | 24,30,30     | 0.94 | 1 (4%)   | 30,47,47    | 1.32 | 4 (13%)  |
| 80  | FAD  | Ff    | 901  | -    | 53,58,58     | 0.47 | 0        | 68,89,89    | 0.52 | 2 (2%)   |
| 82  | PO4  | IA    | 1001 | 76   | 4,4,4        | 0.91 | 0        | 6,6,6       | 0.44 | 0        |
| 79  | UTP  | DJ    | 401  | -    | 22,30,30     | 0.98 | 1 (4%)   | 27,47,47    | 1.09 | 1 (3%)   |
| 77  | ATP  | Cg    | 1000 | 76   | 26,33,33     | 0.61 | 0        | 31,52,52    | 0.75 | 1 (3%)   |

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   |
|-----|------|-------|------|------|---------|-------------|---------|
| 80  | FAD  | Ff    | 901  | -    | -       | 11/30/50/50 | 0/6/6/6 |
| 79  | UTP  | DJ    | 401  | -    | -       | 2/20/38/38  | 0/2/2/2 |
| 77  | ATP  | Cg    | 1000 | 76   | -       | 2/18/38/38  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 81  | GDP  | IA    | 1000 | 76   | -       | 3/12/32/32 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 79  | DJ    | 401  | UTP  | C4-N3 | 3.17  | 1.38        | 1.33     |
| 81  | IA    | 1000 | GDP  | C6-N1 | -2.38 | 1.34        | 1.37     |

The worst 5 of 8 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | DJ    | 401  | UTP  | C5-C4-N3    | -3.94 | 114.64      | 123.31   |
| 81  | IA    | 1000 | GDP  | PA-O3A-PB   | -3.34 | 121.36      | 132.83   |
| 81  | IA    | 1000 | GDP  | C3'-C2'-C1' | 3.23  | 105.84      | 100.98   |
| 80  | Ff    | 901  | FAD  | P-O3P-PA    | -2.56 | 124.04      | 132.83   |
| 81  | IA    | 1000 | GDP  | C5-C6-N1    | 2.32  | 118.04      | 113.95   |

There are no chirality outliers.

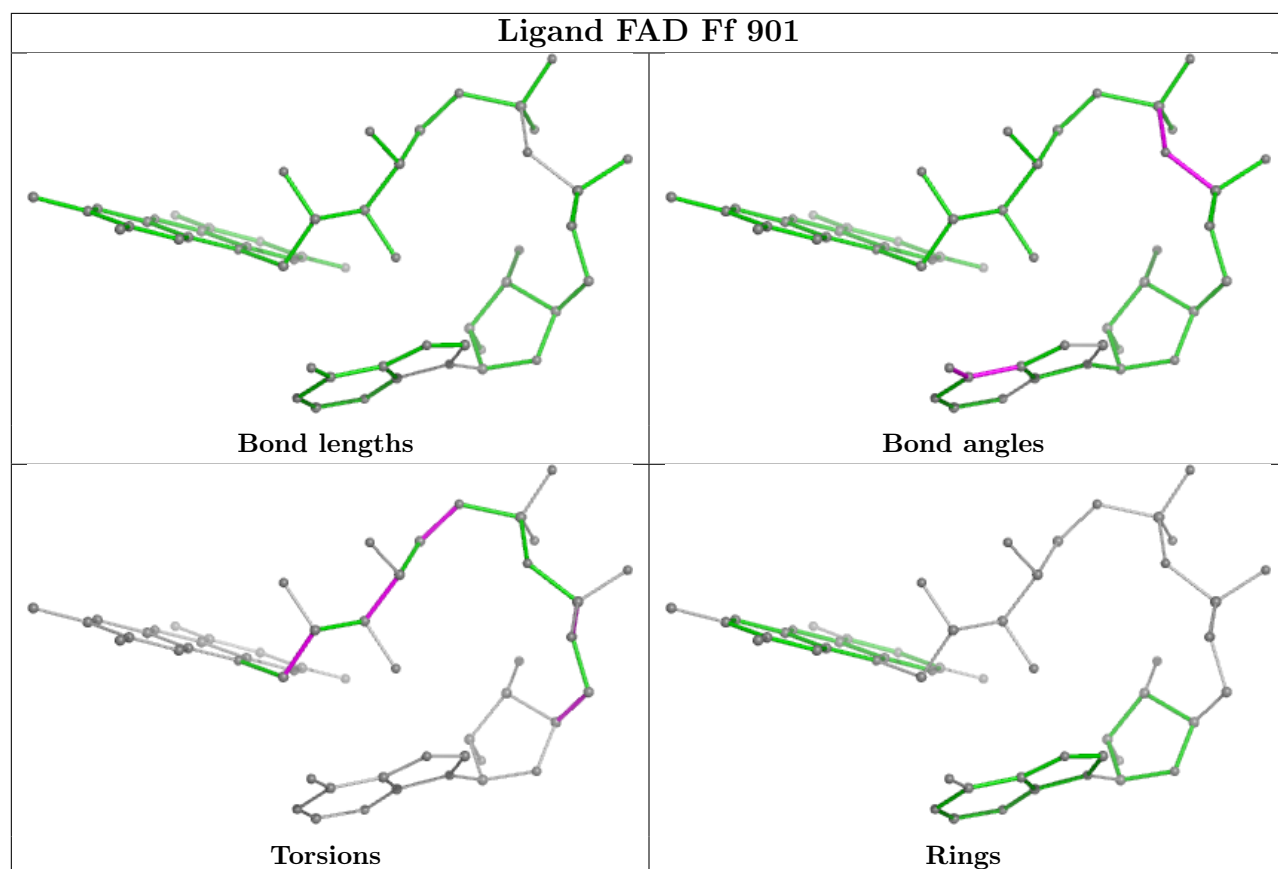
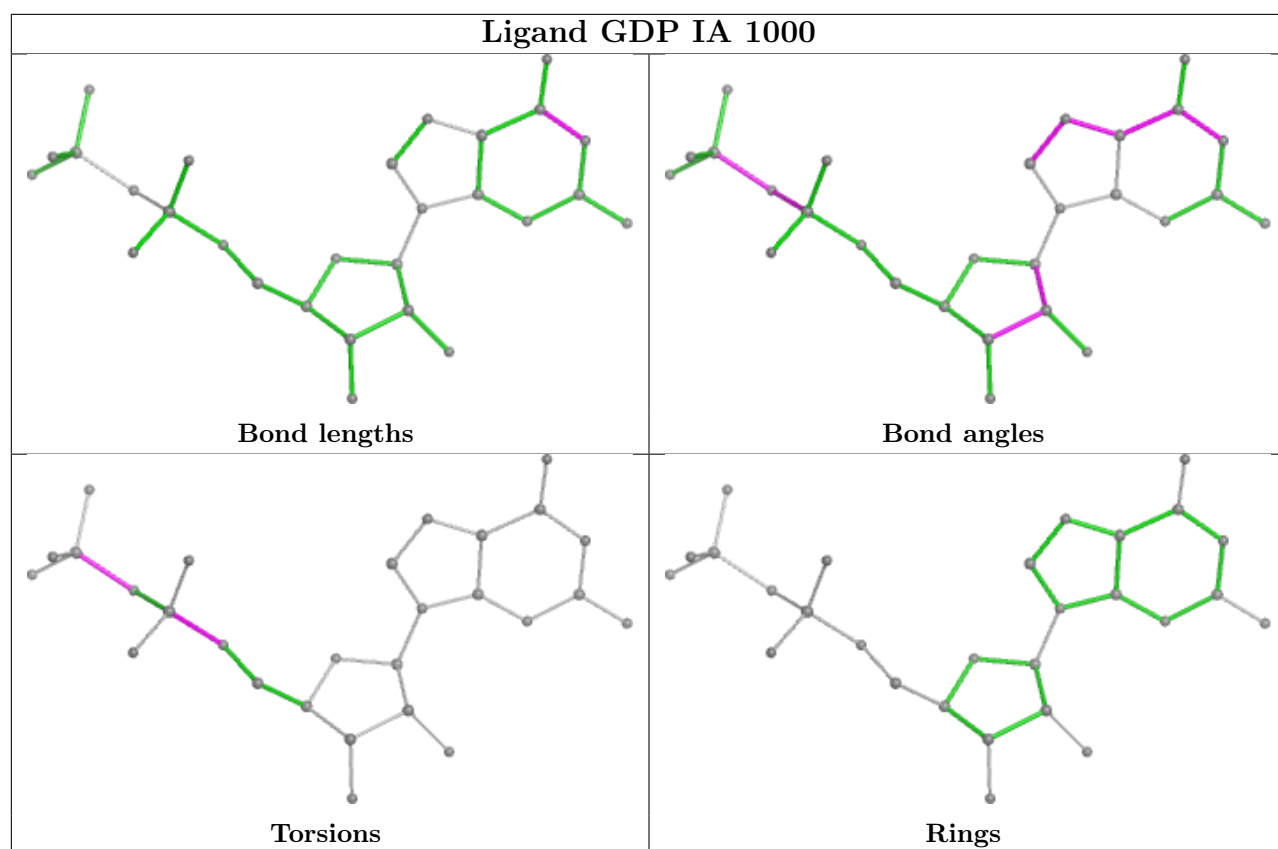
5 of 18 torsion outliers are listed below:

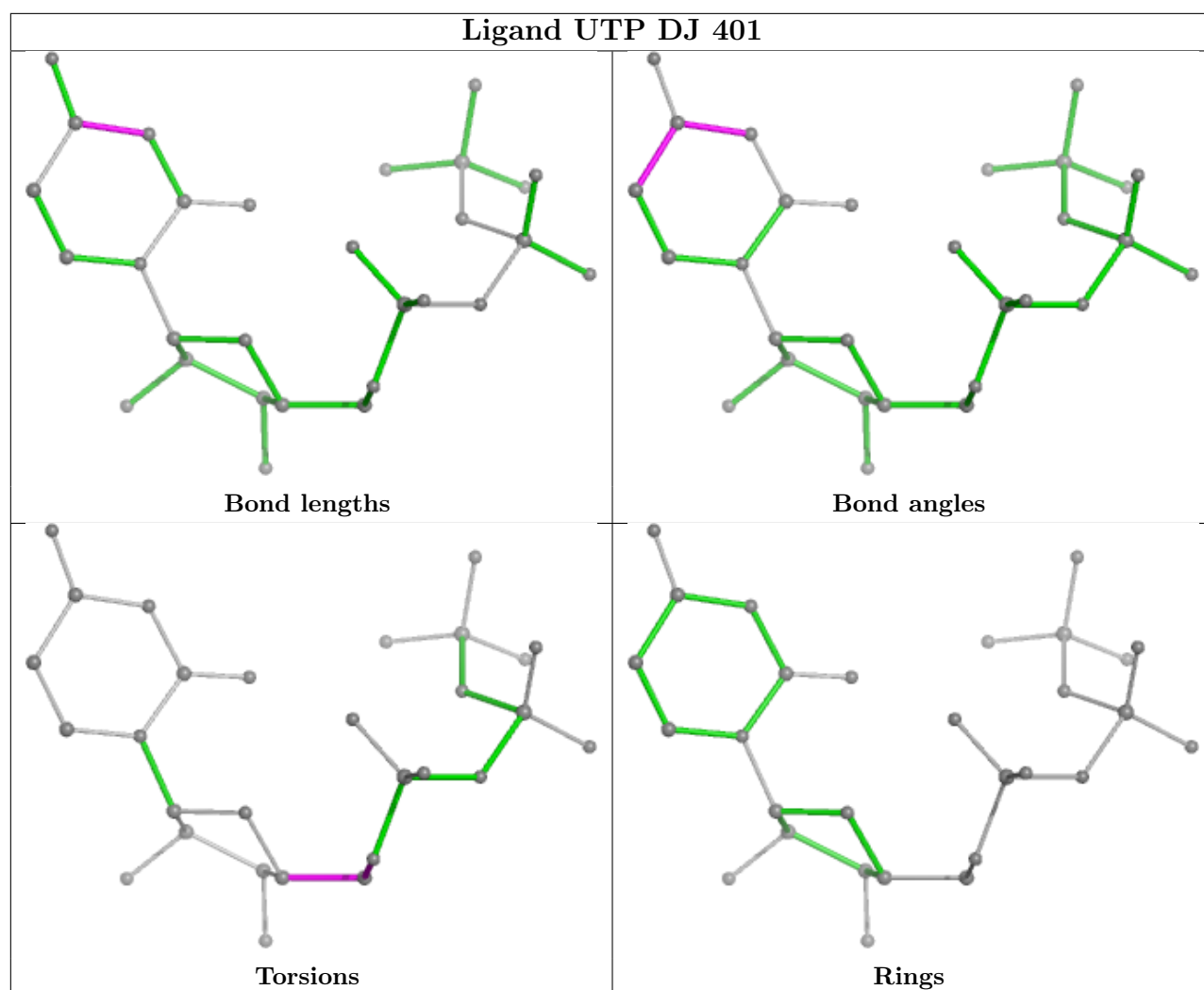
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 80  | Ff    | 901 | FAD  | C5B-O5B-PA-O3P  |
| 80  | Ff    | 901 | FAD  | N10-C1'-C2'-O2' |
| 80  | Ff    | 901 | FAD  | N10-C1'-C2'-C3' |
| 80  | Ff    | 901 | FAD  | C2'-C3'-C4'-O4' |
| 80  | Ff    | 901 | FAD  | C2'-C3'-C4'-C5' |

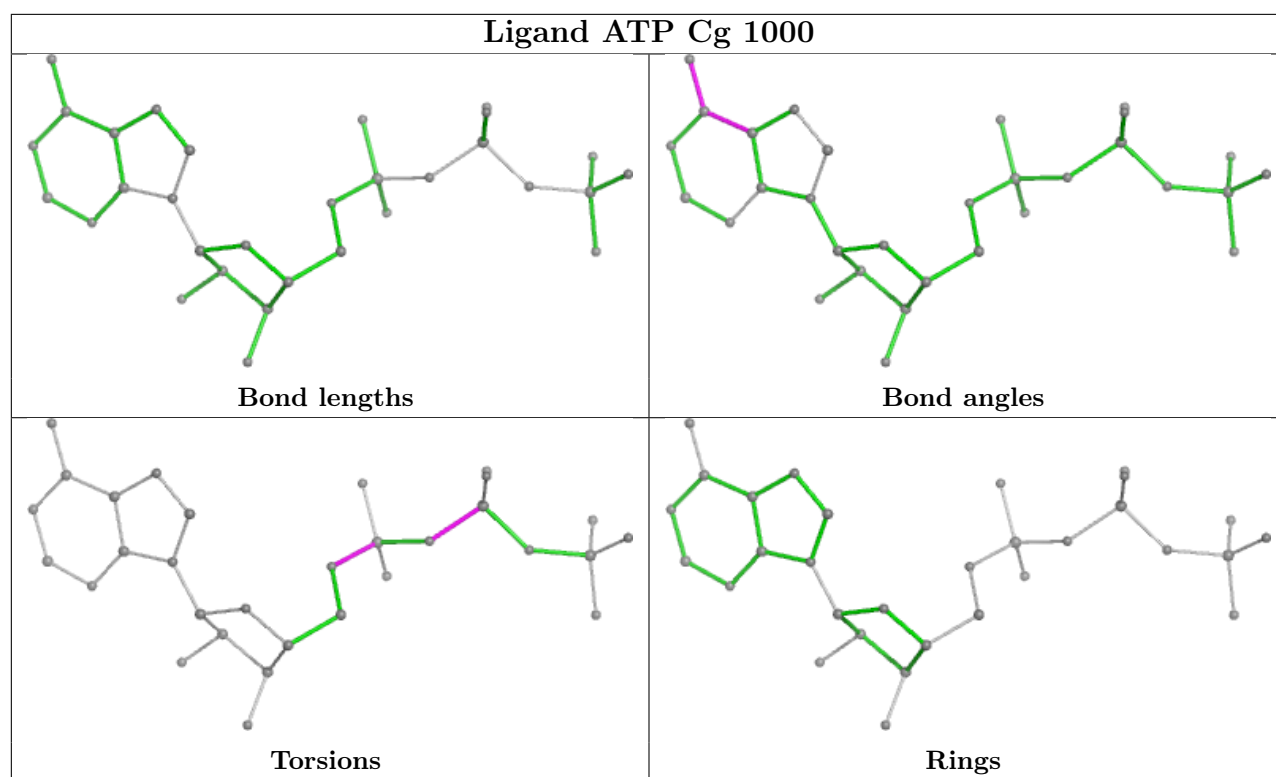
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

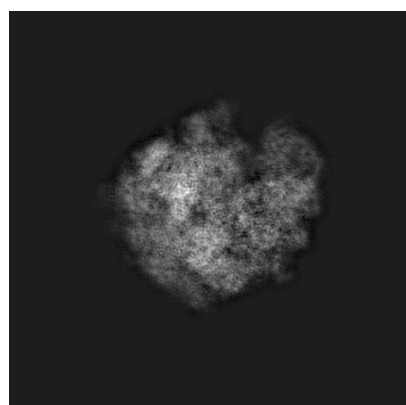
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13661. These allow visual inspection of the internal detail of the map and identification of artifacts.

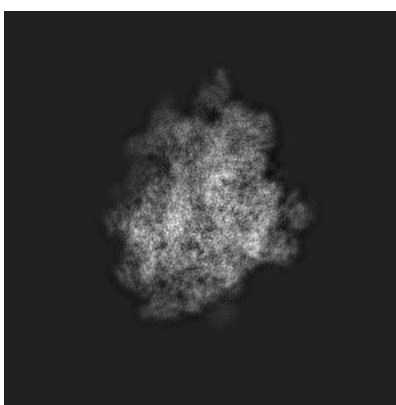
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

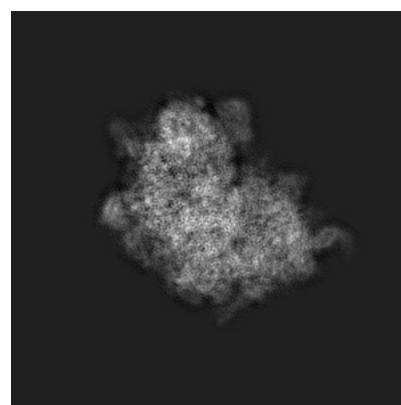
#### 6.1.1 Primary map



X



Y

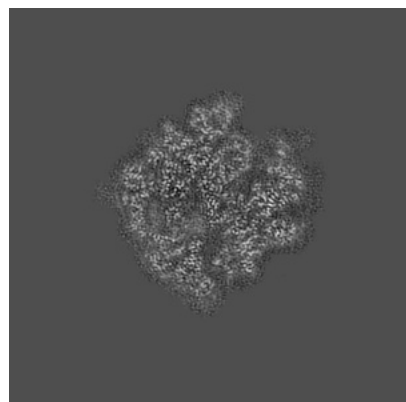


Z

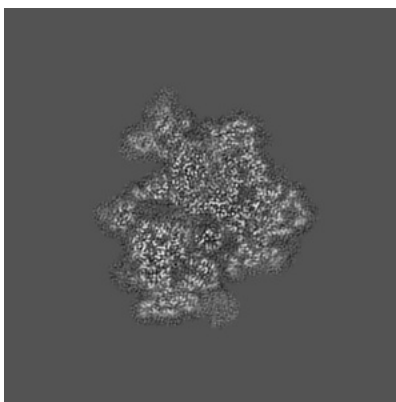
The images above show the map projected in three orthogonal directions.

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

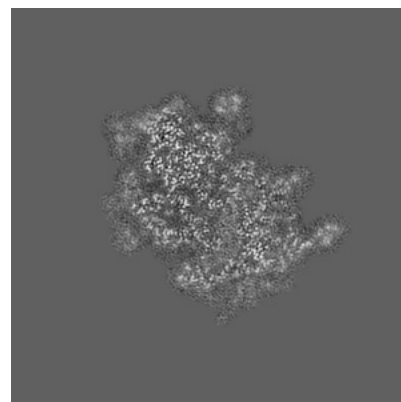
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

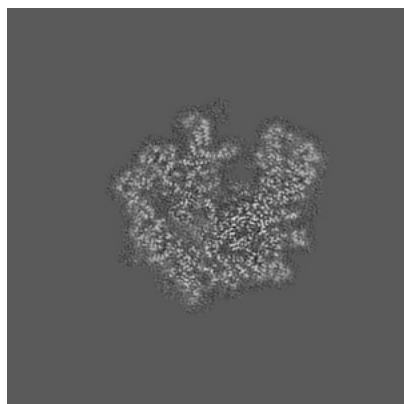


Z Index: 180

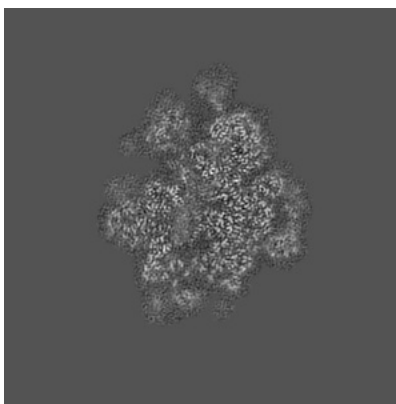
The images above show central slices of the map in three orthogonal directions.

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

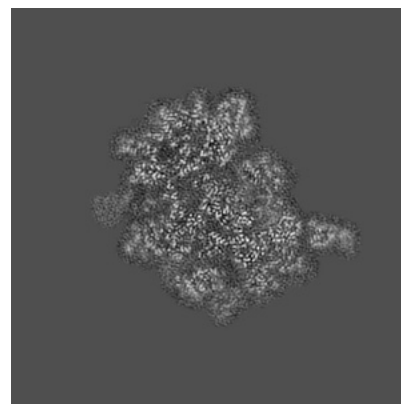
### 6.3.1 Primary map



X Index: 158



Y Index: 165

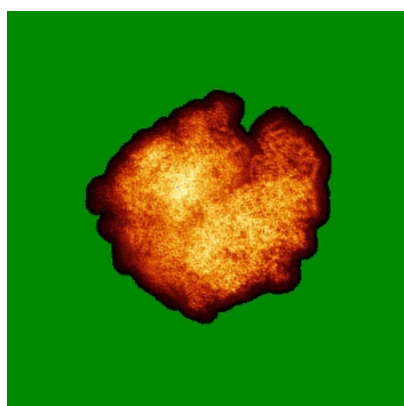


Z Index: 192

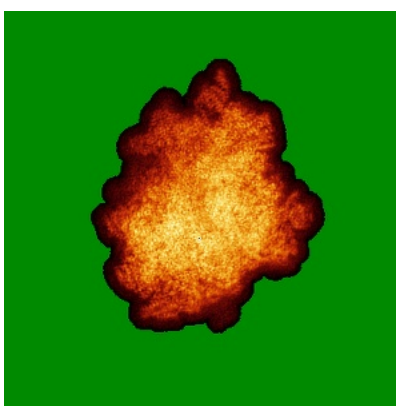
The images above show the largest variance slices of the map in three orthogonal directions.

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

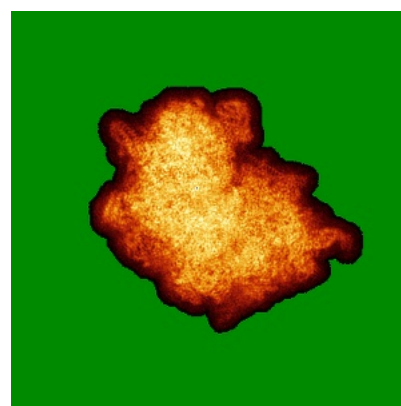
### 6.4.1 Primary map



X



Y

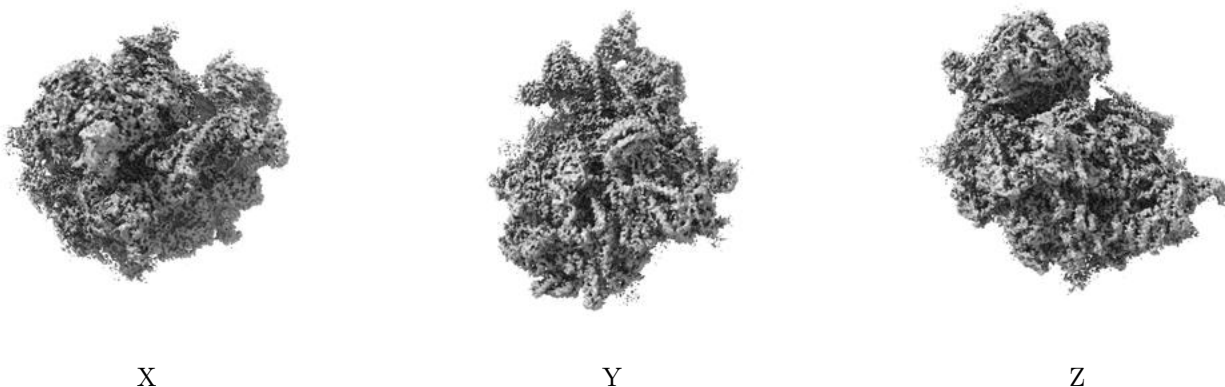


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

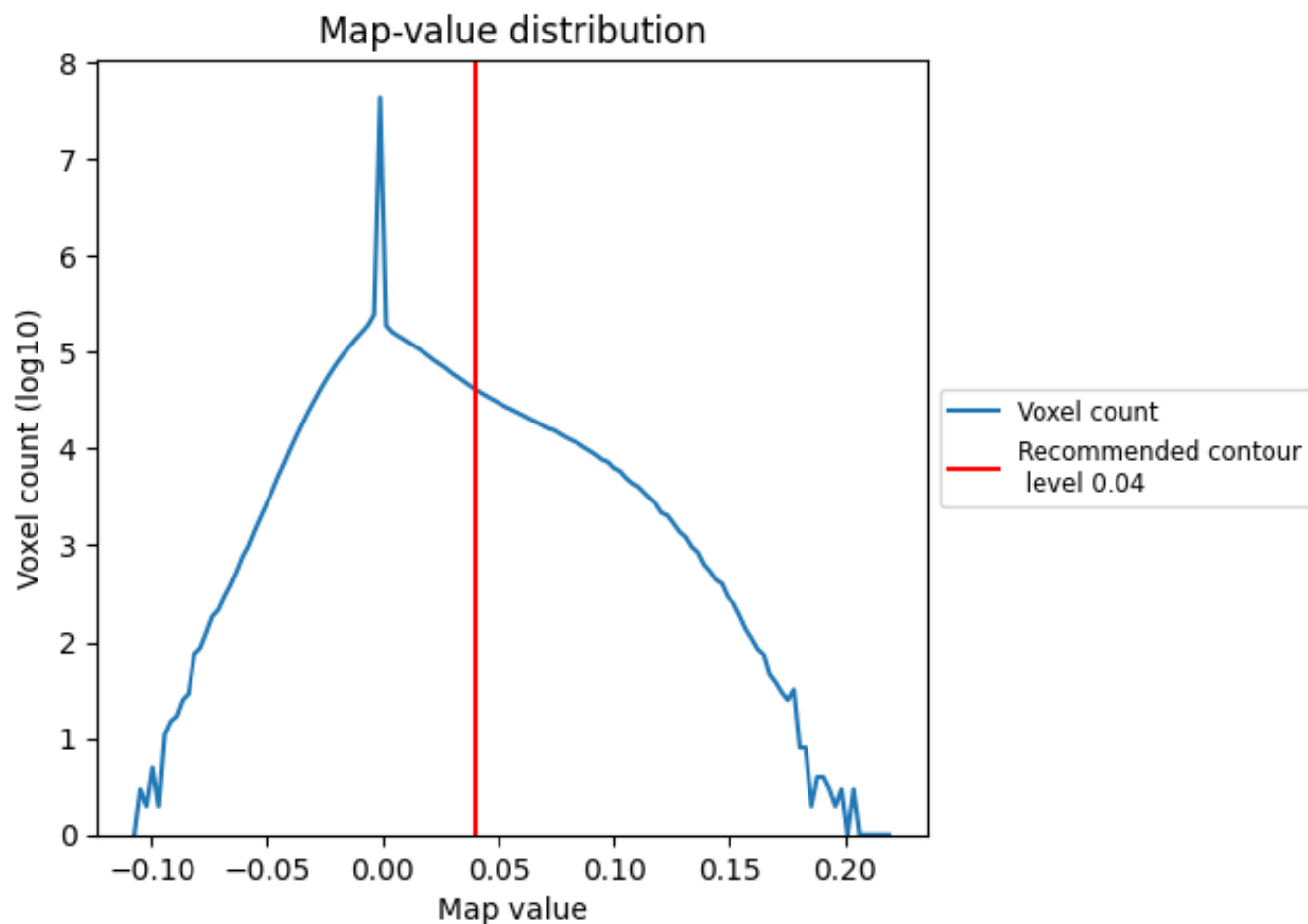
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

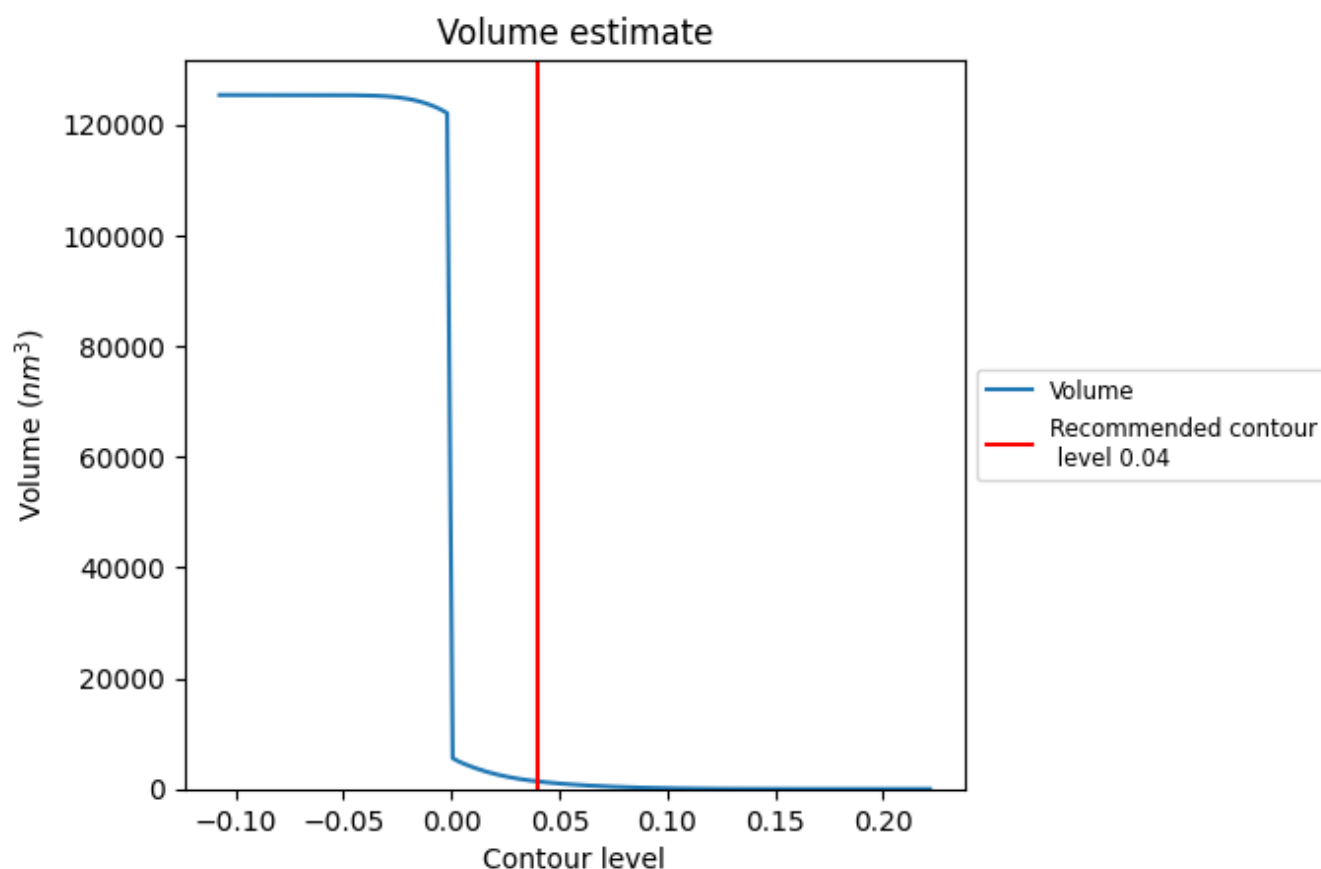
This section contains the results of statistical analysis of the map.

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



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

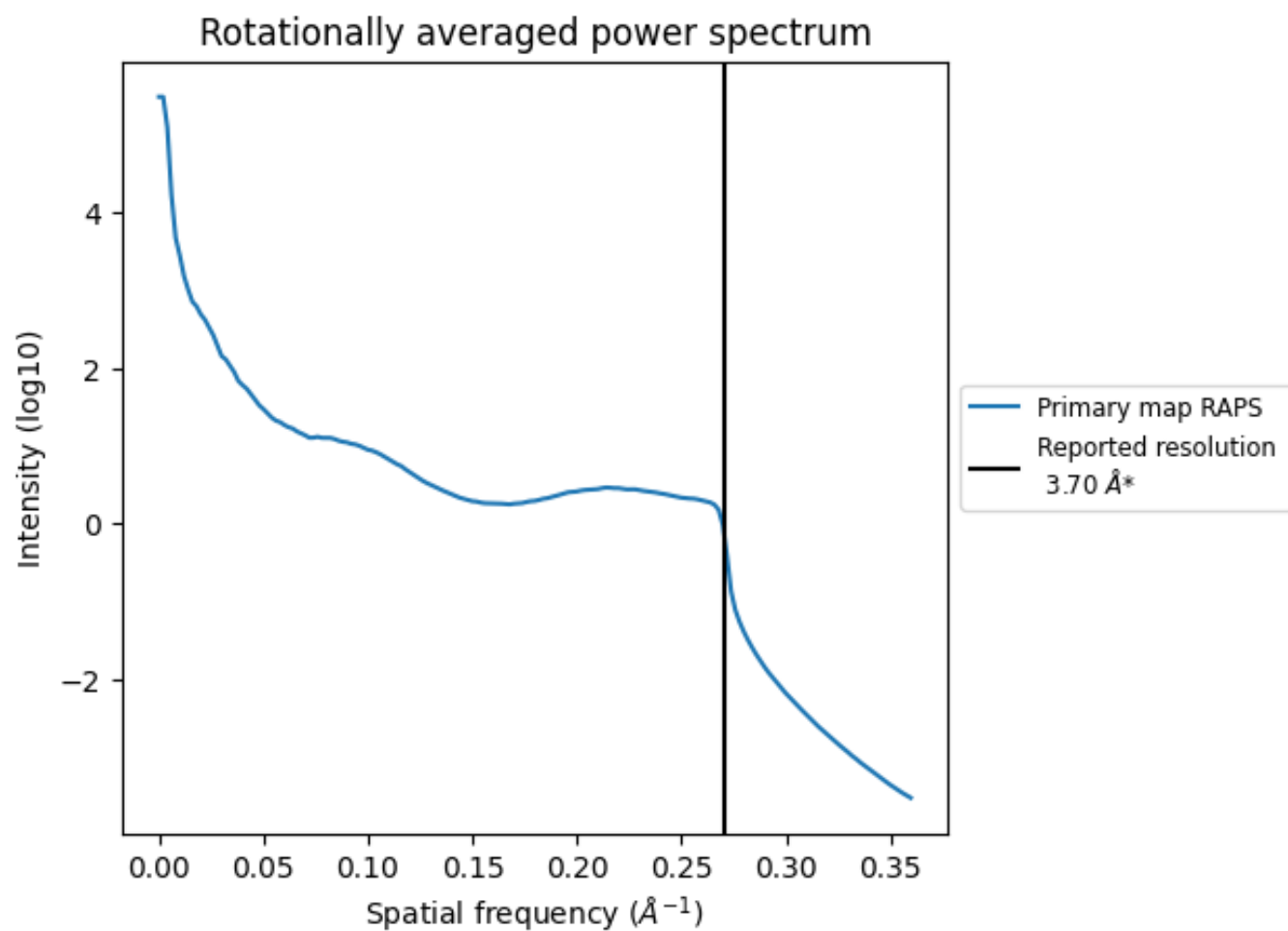
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1367 nm<sup>3</sup>; this corresponds to an approximate mass of 1235 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 0.270 Å<sup>-1</sup>

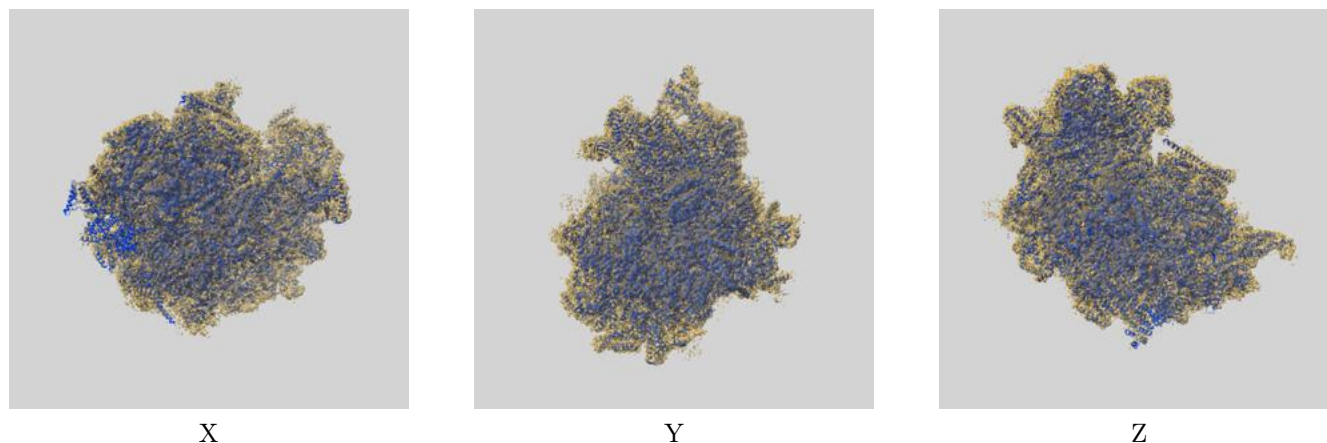
## 8 Fourier-Shell correlation

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

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

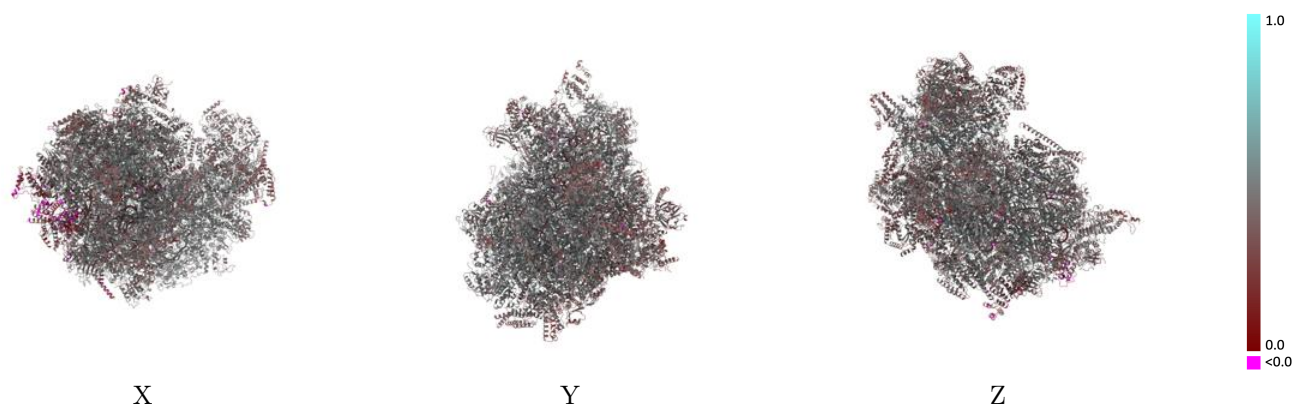
This section contains information regarding the fit between EMDB map EMD-13661 and PDB model 7PUB. Per-residue inclusion information can be found in section [3](#) on page [27](#).

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



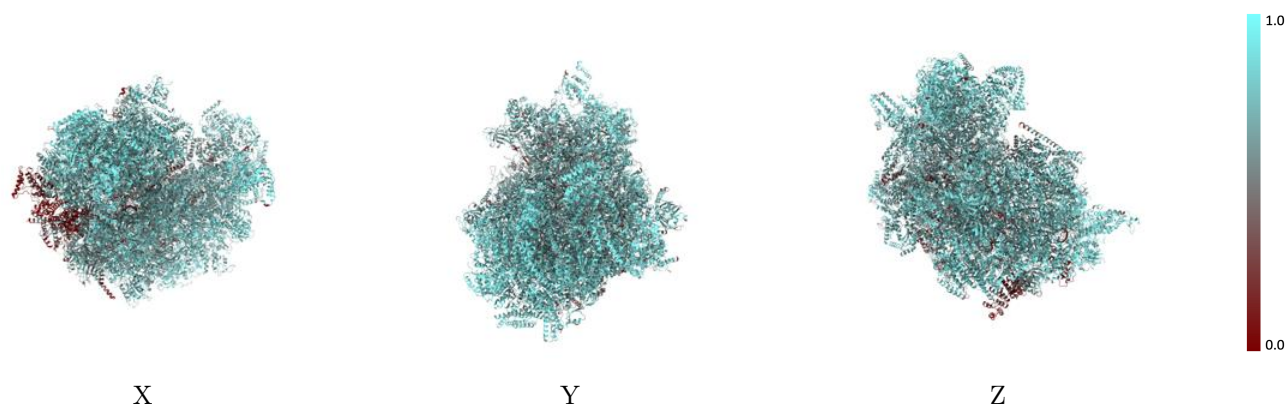
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



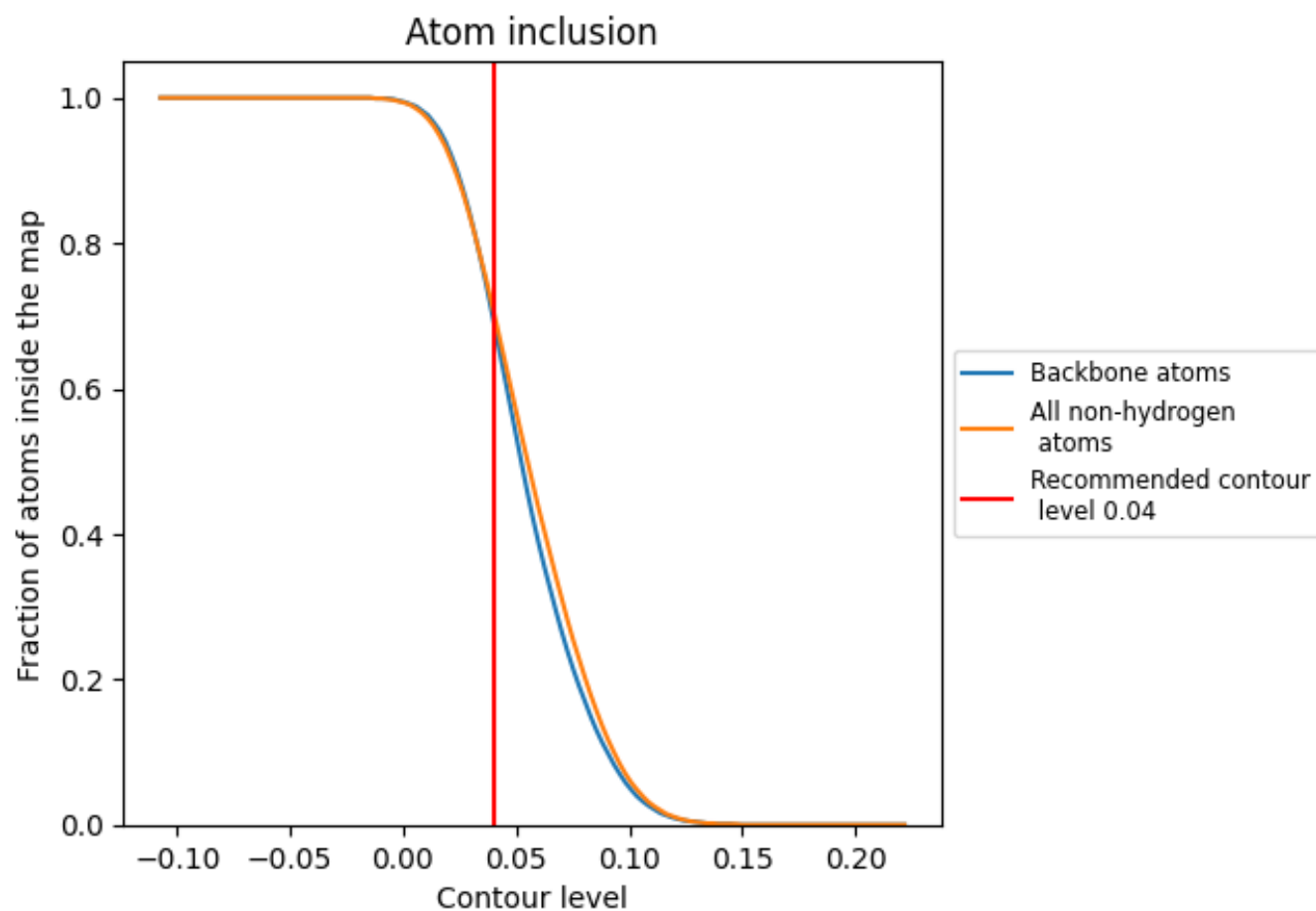
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 71% 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 (0.04) and Q-score for the entire model and for each chain.





















































































| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7070   |  0.4360   |
| CA    |  0.7550   |  0.4250   |
| CC    |  0.6620   |  0.4760   |
| CE    |  0.6950   |  0.4700   |
| CF    |  0.7820   |  0.4500   |
| CH    |  0.6990   |  0.4650   |
| CI    |  0.7100   |  0.4570   |
| CJ    |  0.7850   |  0.4760   |
| CK    |  0.7150   |  0.4410   |
| CL    |  0.6770   |  0.4740   |
| CN    |  0.8160   |  0.4970   |
| CO    |  0.7250   |  0.4420   |
| CP    |  0.7870   |  0.4760   |
| CQ    |  0.7380   |  0.4790   |
| CR    |  0.6760  |  0.4530  |
| CS    |  0.8250 |  0.4850 |
| CU    |  0.6630 |  0.4440 |
| Ca    |  0.6580 |  0.4460 |
| Cb    |  0.6930 |  0.4330 |
| Cd    |  0.7700 |  0.4470 |
| Cg    |  0.8260 |  0.4660 |
| Ci    |  0.8320 |  0.4950 |
| Cj    |  0.8230 |  0.4410 |
| Ck    |  0.7570 |  0.4360 |
| Cm    |  0.5120 |  0.3880 |
| Cn    |  0.5280 |  0.4310 |
| Cp    |  0.7630 |  0.4340 |
| Cq    |  0.7560 |  0.4430 |
| Cr    |  0.7010 |  0.3850 |
| Cv    |  0.7420 |  0.4560 |
| DA    |  0.7100 |  0.4140 |
| DB    |  0.7730 |  0.4580 |
| DC    |  0.7830 |  0.4050 |
| DD    |  0.7840 |  0.4530 |
| DE    |  0.7670 |  0.4120 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| DF    |  0.8280   |  0.4630   |
| DG    |  0.7700   |  0.4150   |
| DH    |  0.7720   |  0.4640   |
| DI    |  0.7820   |  0.4510   |
| DJ    |  0.7980   |  0.4640   |
| DK    |  0.7690   |  0.4550   |
| DL    |  0.6340   |  0.4630   |
| DM    |  0.7670   |  0.4590   |
| DN    |  0.7340   |  0.4620   |
| DO    |  0.7600   |  0.4290   |
| DP    |  0.8270   |  0.4090   |
| DQ    |  0.6800   |  0.4240   |
| DR    |  0.8150   |  0.4230   |
| DS    |  0.7940   |  0.4500   |
| DT    |  0.8160   |  0.4840   |
| DU    |  0.6730   |  0.4450   |
| DV    |  0.7860   |  0.4790   |
| DW    |  0.7890  |  0.4610  |
| DX    |  0.8370 |  0.4650 |
| DY    |  0.7970 |  0.4690 |
| DZ    |  0.6410 |  0.4590 |
| Da    |  0.6150 |  0.4420 |
| F3    |  0.1220 |  0.1800 |
| F6    |  0.4070 |  0.3160 |
| F7    |  0.3270 |  0.3290 |
| F9    |  0.6640 |  0.4400 |
| FO    |  0.7170 |  0.4510 |
| Ff    |  0.7490 |  0.4530 |
| Fg    |  0.6900 |  0.4100 |
| Fh    |  0.6030 |  0.4360 |
| Fi    |  0.5830 |  0.4190 |
| IA    |  0.6890 |  0.4450 |
| IB    |  0.6770 |  0.4480 |
| U6    |  0.4480 |  0.3440 |
| U7    |  0.6850 |  0.4160 |
| UE    |  0.6340 |  0.4640 |
| UF    |  0.5080 |  0.4100 |
| UG    |  0.6150 |  0.4680 |
| UI    |  0.7000 |  0.3140 |
| UJ    |  0.7240 |  0.3360 |
| UK    |  0.9330 |  0.4980 |
| UL    |  0.6500 |  0.4290 |