# wwPDB EM Validation Summary Report (i)

Feb 24, 2022 – 01:14 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 7PUA |
| EMDB ID | : | EMD-13660 |
| Title | : | Middle 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 | : | 3.60 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

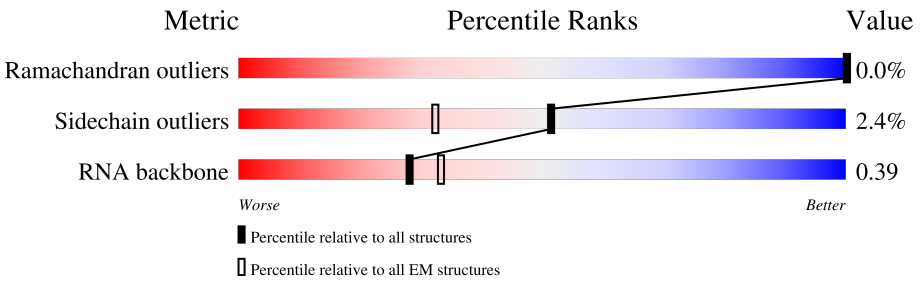
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.0.dev97 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.26 |

# 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 3.60 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 | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | 22% 49% 31% 19% |
| 2 | CB | 3 | 33% 67% |
| 3 | CC | 74 | 22% 100% |
| 4 | CE | 435 | 9% 84% • 14% |
| 5 | CF | 160 | 13% 92% 5% • |
| 6 | CH | 282 | • 77% • 22% |
| 7 | CI | 443 | 7% 94% • 5% |
| 8 | CJ | 817 | 6% 93% • • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | CK | 326 | 5% 53% 46% |
| 10 | CL | 87 | 10% 90% 6% 5% |
| 11 | CN | 166 | 95% 5% |
| 12 | CO | 429 | 6% 83% 16% |
| 13 | CP | 188 | 95% |
| 14 | CQ | 307 | 78% 20% |
| 15 | CR | 320 | 16% 37% 61% |
| 16 | CS | 244 | 5% 40% 59% |
| 17 | CU | 193 | 16% 17% 82% |
| 18 | Ca | 602 | 8% 82% 17% |
| 19 | Cb | 325 | 13% 44% 54% |
| 20 | Cd | 440 | 5% 45% 53% |
| 21 | Cg | 498 | 96% |
| 22 | Ci | 181 | 8% 88% 9% |
| 23 | Cj | 257 | 86% 12% |
| 24 | Ck | 874 | 6% 75% 23% |
| 25 | Cm | 215 | 14% 14% 86% |
| 26 | Cn | 250 | 8% 19% 80% |
| 27 | Cp | 187 | 89% 10% |
| 28 | DB | 1181 | 91% 6% |
| 29 | DC | 1165 | 11% 92% 6% |
| 30 | DD | 812 | 93% 6% |
| 31 | DE | 747 | 8% 82% 16% |
| 32 | DF | 666 | 88% 11% |
| 33 | DG | 631 | 86% 12% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | DH | 581 | 10% 95% |
| 35 | DI | 407 | 94% |
| 36 | DJ | 396 | 14% 88% 10% |
| 37 | DK | 324 | 10% 80% 19% |
| 38 | DL | 307 | 17% 74% 24% |
| 39 | DO | 282 | 7% 68% 31% |
| 40 | DP | 274 | 76% 23% |
| 41 | DR | 270 | 92% 7% |
| 42 | DT | 247 | 8% 94% |
| 43 | DU | 228 | 12% 94% 5% |
| 44 | DV | 183 | 5% 85% 13% |
| 45 | DW | 179 | 7% 74% 24% |
| 46 | DX | 169 | 75% 24% |
| 47 | DY | 163 | 7% 93% 6% |
| 48 | DZ | 94 | 5% 30% 70% |
| 49 | Da | 64 | 55% 44% |
| 50 | F2 | 1024 | 86% 13% |
| 51 | F3 | 966 | 10% 93% 6% |
| 52 | F5 | 754 | 18% 80% 18% |
| 53 | F6 | 676 | 34% 75% 23% |
| 54 | F7 | 679 | 5% 95% |
| 55 | F9 | 607 | 12% 87% 11% |
| 56 | FM | 370 | 5% 86% 12% |
| 56 | FN | 370 | 11% 85% 14% |
| 57 | FO | 334 | 96% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 58 | FP | 349 | 9% 99% |
| 59 | FW | 263 | 90% 10% |
| 60 | FX | 239 | 92% 8% |
| 61 | FZ | 178 | 40% 86% 10% |
| 62 | Fb | 151 | 81% 17% |
| 63 | Fc | 148 | 7% 54% 44% |
| 64 | Fd | 143 | 59% 64% 35% |
| 65 | Ff | 848 | 72% 27% |
| 66 | Fg | 550 | 93% 5% |
| 67 | Fh | 318 | 52% 73% 25% |
| 68 | Fi | 629 | 10% 74% 24% |
| 69 | IA | 787 | 86% 11% |
| 70 | IB | 803 | 13% 60% 39% |
| 71 | U8 | 30 | 67% 100% |
| 72 | UC | 9 | 100% |
| 73 | UD | 13 | 15% 100% |
| 74 | UF | 36 | 31% 100% |
| 75 | UG | 15 | 7% 100% |
| 76 | UI | 6 | 17% 100% |
| 77 | UK | 24 | 96% 100% |
| 78 | UM | 8 | 100% |
| 78 | UN | 8 | 25% 100% |
| 78 | UQ | 8 | 25% 100% |
| 79 | UP | 32 | 41% 100% |
| 80 | Ua | 10 | 10% 100% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 81 | Ug | 271 | 35% 88% 12% |

# 2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 205280 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 |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | CA | 501 | 9866 | 4403 | 1529 | 3433 | 501 | 0 | 0 |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| CA | 614 | U | - | expression tag | GB 13740 |
| CA | 615 | U | - | expression tag | GB 13740 |
| CA | 616 | U | - | expression tag | GB 13740 |
| CA | 617 | U | - | expression tag | GB 13740 |
| CA | 618 | U | - | expression tag | GB 13740 |
| CA | 619 | U | - | expression tag | GB 13740 |
| CA | 620 | U | - | expression tag | GB 13740 |
| CA | 621 | U | - | expression tag | GB 13740 |

- Molecule 2 is a RNA chain called 9S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | CB | 3 | 64 | 29 | 12 | 20 | 3 | 0 | 0 |

- Molecule 3 is a protein called uS3m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | CC | 74 | 646 | 451 | 96 | 98 | 1 | 0 | 0 |

- Molecule 4 is a protein called Ribosomal_S5_C domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | CE | 373 | 3024 | 1915 | 556 | 538 | 15 | 0 | 0 |

- Molecule 5 is a protein called bS6m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | CF | 155 | 1279 | 810 | 226 | 237 | 6 | 0 | 0 |

- Molecule 6 is a protein called 30S ribosomal protein S8, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | CH | 219 | 1799 | 1130 | 343 | 317 | 9 | 0 | 0 |

- Molecule 7 is a protein called uS9m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | CI | 421 | 3352 | 2111 | 598 | 627 | 16 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called LysM domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | CJ | 782 | 6376 | 4034 | 1122 | 1191 | 29 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| CJ | 488 | SER | ASN | conflict | UNP C9ZPU0 |

- Molecule 9 is a protein called uS11m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | CK | 177 | 1440 | 895 | 273 | 264 | 8 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 10 is a protein called uS12m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | CL | 83 | 701 | 480 | 109 | 102 | 10 | 0 | 0 |

- Molecule 11 is a protein called uS14m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | CN | 157 | 1322 | 843 | 251 | 220 | 8 | 0 | 0 |

- Molecule 12 is a protein called uS15m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | CO | 360 | 2989 | 1899 | 557 | 517 | 16 | 0 | 0 |

- Molecule 13 is a protein called bS16m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | CP | 180 | 1489 | 956 | 274 | 250 | 9 | 0 | 0 |

- Molecule 14 is a protein called 30S Ribosomal protein S17, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | CQ | 247 | 2015 | 1279 | 379 | 348 | 9 | 0 | 0 |

- Molecule 15 is a protein called bS18m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | CR | 124 | 1051 | 680 | 196 | 173 | 2 | 0 | 0 |

- Molecule 16 is a protein called uS19m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | CS | 99 | 822 | 534 | 144 | 140 | 4 | 0 | 0 |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| CS | -11 | ILE | ASN | conflict | UNP A0A3L6L621 |
| CS | -10 | VAL | CYS | conflict | UNP A0A3L6L621 |
| CS | -9 | TYR | LEU | conflict | UNP A0A3L6L621 |
| CS | -8 | PHE | LEU | conflict | UNP A0A3L6L621 |
| CS | -7 | HIS | PRO | conflict | UNP A0A3L6L621 |
| CS | -6 | CYS | LEU | conflict | UNP A0A3L6L621 |
| CS | -5 | CYS | LEU | conflict | UNP A0A3L6L621 |
| CS | -4 | THR | TYR | conflict | UNP A0A3L6L621 |
| CS | -3 | ARG | GLU | conflict | UNP A0A3L6L621 |
| CS | -2 | LYS | GLU | conflict | UNP A0A3L6L621 |
| CS | ? | - | VAL | deletion | UNP A0A3L6L621 |
| CS | ? | - | ARG | deletion | UNP A0A3L6L621 |

- Molecule 17 is a protein called bS21m.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | CU | 35 | 288 | 182 | 57 | 47 | 2 | 0 | 0 |

- Molecule 18 is a protein called mS22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | Ca | 501 | 4247 | 2720 | 753 | 753 | 21 | 0 | 0 |

- Molecule 19 is a protein called mS23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | Cb | 149 | 1242 | 801 | 226 | 209 | 6 | 0 | 0 |

There are 15 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Cb | 302 | GLY | ARG | conflict | UNP C9ZNU0 |
| Cb | 312 | UNK | - | expression tag | UNP C9ZNU0 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Cb | 313 | CYS | - | expression tag | UNP C9ZNU0 |
| Cb | 314 | SER | - | expression tag | UNP C9ZNU0 |
| Cb | 315 | ARG | - | expression tag | UNP C9ZNU0 |
| Cb | 316 | ASP | - | expression tag | UNP C9ZNU0 |
| Cb | 317 | GLY | - | expression tag | UNP C9ZNU0 |
| Cb | 318 | PHE | - | expression tag | UNP C9ZNU0 |
| Cb | 319 | ALA | - | expression tag | UNP C9ZNU0 |
| Cb | 320 | LEU | - | expression tag | UNP C9ZNU0 |
| Cb | 321 | MET | - | expression tag | UNP C9ZNU0 |
| Cb | 322 | LYS | - | expression tag | UNP C9ZNU0 |
| Cb | 323 | ALA | - | expression tag | UNP C9ZNU0 |
| Cb | 324 | ASN | - | expression tag | UNP C9ZNU0 |
| Cb | 325 | LYS | - | expression tag | UNP C9ZNU0 |

- Molecule 20 is a protein called mS26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | Cd | 205 | 1768 | 1124 | 323 | 312 | 9 | 0 | 0 |

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 21 is a protein called mS29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | Cg | 487 | 3943 | 2524 | 691 | 708 | 20 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Cg | 181 | VAL | ALA | conflict | UNP Q585C2 |
| Cg | 498 | ARG | - | expression tag | UNP Q585C2 |

- Molecule 22 is a protein called mS33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | Ci | 165 | 1348 | 848 | 247 | 244 | 9 | 0 | 0 |

- Molecule 23 is a protein called mS34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | Cj | 226 | 1792 | 1138 | 310 | 340 | 4 | 0 | 0 |

- Molecule 24 is a protein called mS35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | Ck | 673 | 5371 | 3371 | 974 | 1002 | 24 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 25 is a protein called mS37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | Cm | 31 | 232 | 136 | 43 | 47 | 6 | 0 | 0 |

- Molecule 26 is a protein called mS38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | Cn | 49 | 425 | 278 | 88 | 56 | 3 | 0 | 0 |

- Molecule 27 is a protein called Protein FYV4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | Cp | 168 | 1428 | 904 | 259 | 260 | 5 | 0 | 0 |

- Molecule 28 is a protein called mS49.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 28 | DB | 1106 | 9112 | 5669 | 1712 | 1703 | 28 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| DB | 359 | ILE | THR | conflict | UNP C9ZJE4 |

- Molecule 29 is a protein called mS50.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | DC | 1099 | 8766 | 5528 | 1548 | 1659 | 31 | 0 | 0 |

- Molecule 30 is a protein called mS51.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | DD | 764 | 6308 | 3998 | 1131 | 1143 | 36 | 0 | 0 |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| DD | 1 | UNK | - | expression tag | UNP D0A752 |
| DD | 2 | UNK | - | expression tag | UNP D0A752 |
| DD | 3 | UNK | - | expression tag | UNP D0A752 |
| DD | 4 | UNK | - | expression tag | UNP D0A752 |
| DD | 5 | UNK | - | expression tag | UNP D0A752 |
| DD | 6 | UNK | - | expression tag | UNP D0A752 |
| DD | 7 | UNK | - | expression tag | UNP D0A752 |
| DD | 8 | UNK | - | expression tag | UNP D0A752 |
| DD | 9 | UNK | - | expression tag | UNP D0A752 |
| DD | 10 | UNK | - | expression tag | UNP D0A752 |
| DD | 11 | UNK | - | expression tag | UNP D0A752 |
| DD | 12 | UNK | - | expression tag | UNP D0A752 |
| DD | 13 | UNK | - | expression tag | UNP D0A752 |
| DD | 14 | UNK | - | expression tag | UNP D0A752 |
| DD | 15 | UNK | - | expression tag | UNP D0A752 |
| DD | 16 | UNK | - | expression tag | UNP D0A752 |
| DD | 17 | UNK | - | expression tag | UNP D0A752 |
| DD | 26 | UNK | ARG | conflict | UNP D0A752 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| DD | 27 | UNK | MET | conflict | UNP D0A752 |
| DD | 28 | UNK | MET | conflict | UNP D0A752 |
| DD | 29 | UNK | ARG | conflict | UNP D0A752 |
| DD | 30 | UNK | ALA | conflict | UNP D0A752 |
| DD | 31 | UNK | GLY | conflict | UNP D0A752 |
| DD | 32 | UNK | SER | conflict | UNP D0A752 |
| DD | 33 | UNK | GLY | conflict | UNP D0A752 |
| DD | 34 | UNK | TYR | conflict | UNP D0A752 |
| DD | 35 | UNK | GLN | conflict | UNP D0A752 |
| DD | 36 | UNK | GLN | conflict | UNP D0A752 |
| DD | 37 | UNK | LEU | conflict | UNP D0A752 |
| DD | 38 | UNK | ARG | conflict | UNP D0A752 |
| DD | 39 | UNK | ARG | conflict | UNP D0A752 |
| DD | 40 | UNK | MET | conflict | UNP D0A752 |
| DD | 41 | UNK | GLY | conflict | UNP D0A752 |
| DD | 42 | UNK | MET | conflict | UNP D0A752 |
| DD | 43 | UNK | PRO | conflict | UNP D0A752 |
| DD | 44 | UNK | MET | conflict | UNP D0A752 |
| DD | 45 | UNK | GLN | conflict | UNP D0A752 |
| DD | 46 | UNK | VAL | conflict | UNP D0A752 |
| DD | 47 | UNK | GLY | conflict | UNP D0A752 |
| DD | 48 | UNK | MET | conflict | UNP D0A752 |
| DD | 49 | UNK | GLY | conflict | UNP D0A752 |
| DD | 50 | UNK | TRP | conflict | UNP D0A752 |
| DD | 51 | UNK | ARG | conflict | UNP D0A752 |
| DD | 52 | UNK | LYS | conflict | UNP D0A752 |
| DD | 53 | UNK | VAL | conflict | UNP D0A752 |
| DD | 54 | UNK | ASP | conflict | UNP D0A752 |
| DD | 55 | UNK | SER | conflict | UNP D0A752 |
| DD | 56 | UNK | PHE | conflict | UNP D0A752 |

- Molecule 31 is a protein called mS52.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | DE | 628 | 5114 | 3243 | 926 | 924 | 21 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 32 is a protein called mS53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 32 | DF | 594 | 4785 | 3001 | 904 | 855 | 25 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| DF | 18 | THR | ALA | conflict | UNP C9ZXX4 |
| DF | 372 | ASN | ASP | conflict | UNP C9ZXX4 |
| DF | 406 | ASN | SER | conflict | UNP C9ZXX4 |
| DF | 636 | UNK | GLY | conflict | UNP C9ZXX4 |
| DF | 638 | LYS | ARG | conflict | UNP C9ZXX4 |

- Molecule 33 is a protein called mS54.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | DG | 557 | 4511 | 2835 | 826 | 819 | 31 | 0 | 0 |

- Molecule 34 is a protein called mS55.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | DH | 568 | 4608 | 2888 | 858 | 840 | 22 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| DH | 75 | GLN | LYS | conflict | UNP A0A3L6LGC8 |

- Molecule 35 is a protein called mS56.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 35 | DI | 390 | 3182 | 2020 | 554 | 594 | 14 | 0 | 0 |

- Molecule 36 is a protein called mS57.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 36 | DJ | 356 | 2908 | 1855 | 511 | 528 | 14 | 0 | 0 |

- Molecule 37 is a protein called mS58.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 37 | DK | 264 | 2092 | 1317 | 375 | 395 | 5 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| DK | 97 | ASP | SER | conflict | UNP A0A3L6L3U6 |

- Molecule 38 is a protein called mS59.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 38 | DL | 234 | 1904 | 1216 | 342 | 335 | 11 | 0 | 0 |

- Molecule 39 is a protein called mS62.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 39 | DO | 194 | 1567 | 981 | 286 | 291 | 9 | 0 | 0 |

- Molecule 40 is a protein called mS63.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | DP | 210 | 1784 | 1145 | 318 | 312 | 9 | 0 | 0 |

- Molecule 41 is a protein called mS65.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | DR | 252 | 2034 | 1309 | 371 | 344 | 10 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| DR | 128 | PRO | SER | conflict | UNP C9ZPP1 |

- Molecule 42 is a protein called Rhodanese domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 42 | DT | 239 | 2058 | 1321 | 364 | 362 | 11 | 0 | 0 |

- Molecule 43 is a protein called Ubiquitin-like domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 43 | DU | 217 | 1730 | 1091 | 305 | 329 | 5 | 0 | 0 |

- Molecule 44 is a protein called mS69.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 44 | DV | 160 | 1346 | 855 | 252 | 235 | 4 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 45 is a protein called mS70.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 45 | DW | 136 | 1160 | 741 | 220 | 194 | 5 | 0 | 0 |

- Molecule 46 is a protein called mS71.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 46 | DX | 129 | 1097 | 697 | 206 | 187 | 7 | 0 | 0 |

- Molecule 47 is a protein called mS72.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 47 | DY | 154 | 1295 | 829 | 247 | 214 | 5 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 48 is a protein called mS73.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 48 | DZ | 28 | 237 | 156 | 39 | 41 | 1 | 0 | 0 |

- Molecule 49 is a protein called mS74.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 49 | Da | 36 | 320 | 202 | 70 | 46 | 2 | 0 | 0 |

- Molecule 50 is a protein called PPR_long domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 50 | F2 | 890 | 7125 | 4483 | 1254 | 1349 | 39 | 0 | 0 |

- Molecule 51 is a protein called mt-SAF3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 51 | F3 | 911 | 7039 | 4391 | 1250 | 1346 | 52 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 52 is a protein called mt-SAF5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 52 | F5 | 620 | 5056 | 3154 | 938 | 933 | 31 | 0 | 0 |

- Molecule 53 is a protein called DUF4460 domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 53 | F6 | 522 | 4195 | 2655 | 729 | 794 | 17 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F6 | 285 | ARG | HIS | conflict | UNP Q38FQ8 |
| F6 | 291 | ILE | THR | conflict | UNP Q38FQ8 |
| F6 | 602 | ALA | VAL | conflict | UNP Q38FQ8 |
| F6 | 676 | CYS | - | expression tag | UNP Q38FQ8 |

- Molecule 54 is a protein called mt-SAF7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 54 | F7 | 652 | 5166 | 3284 | 908 | 938 | 36 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 55 is a protein called mt-SAF9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 55 | F9 | 540 | 4422 | 2732 | 830 | 845 | 15 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F9 | ? | - | GLU | deletion | UNP C9ZSL5 |

- Molecule 56 is a protein called mt-SAF21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 56 | FM | 327 | 2457 | 1521 | 450 | 466 | 20 | 0 | 0 |
| 56 | FN | 320 | 2403 | 1484 | 440 | 459 | 20 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| FM | 326 | HIS | ARG | conflict | UNP C9ZJW2 |
| FM | 330 | UNK | GLY | conflict | UNP C9ZJW2 |
| FN | 326 | HIS | ARG | conflict | UNP C9ZJW2 |
| FN | 330 | UNK | GLY | conflict | UNP C9ZJW2 |

- Molecule 57 is a protein called mt-SAF22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 57 | FO | 328 | 2700 | 1692 | 513 | 481 | 14 | 0 | 0 |

- Molecule 58 is a protein called mt-SAF23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 58 | FP | 348 | 2643 | 1682 | 464 | 487 | 10 | 0 | 0 |

- Molecule 59 is a protein called LMWPc domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 59 | FW | 238 | 1960 | 1227 | 375 | 352 | 6 | 0 | 0 |

- Molecule 60 is a protein called mt-SAF27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 60 | FX | 220 | 1741 | 1093 | 318 | 316 | 14 | 0 | 0 |

- Molecule 61 is a protein called mt-SAF29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 61 | FZ | 160 | 1262 | 786 | 212 | 257 | 7 | 0 | 0 |

- Molecule 62 is a protein called mt-SAF31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 62 | Fb | 125 | 1061 | 682 | 194 | 178 | 7 | 0 | 0 |

- Molecule 63 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 63 | Fc | 83 | 660 | 421 | 104 | 134 | 1 | 0 | 0 |

- Molecule 64 is a protein called DUF4379 domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 64 | Fd | 93 | 738 | 469 | 143 | 118 | 8 | 0 | 0 |

- Molecule 65 is a protein called DNA photolyase, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 65 | Ff | 623 | 5006 | 3176 | 896 | 911 | 23 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Ff | 109 | ALA | VAL | conflict | UNP D0A9A9 |
| Ff | 127 | UNK | TYR | conflict | UNP D0A9A9 |
| Ff | 138 | GLN | ARG | conflict | UNP D0A9A9 |

- Molecule 66 is a protein called Acyl transferase-like protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 66 | Fg | 520 | 4048 | 2545 | 710 | 763 | 30 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Fg | 159 | ILE | VAL | conflict | UNP C9ZYZ4 |
| Fg | 271 | ILE | VAL | conflict | UNP C9ZYZ4 |
| Fg | 363 | MET | ARG | conflict | UNP C9ZYZ4 |
| Fg | 399 | UNK | GLU | conflict | UNP C9ZYZ4 |
| Fg | 436 | ASP | GLU | conflict | UNP C9ZYZ4 |

- Molecule 67 is a protein called mt-SAF37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 67 | Fh | 239 | 1867 | 1159 | 346 | 348 | 14 | 0 | 0 |

- Molecule 68 is a protein called mt-SAF38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 68 | Fi | 475 | 3797 | 2410 | 693 | 670 | 24 | 0 | 0 |

- Molecule 69 is a protein called Translation initiation factor IF-2, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 69 | IA | 704 | 5478 | 3433 | 986 | 1032 | 27 | 0 | 0 |

- Molecule 70 is a protein called mt-SAF39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 70 | IB | 491 | 3867 | 2415 | 723 | 712 | 17 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| IB | 98 | LYS | GLU | conflict | UNP D0A0V4 |
| IB | 206 | ILE | MET | conflict | UNP D0A0V4 |
| IB | 572 | HIS | ARG | conflict | UNP D0A0V4 |
| IB | 798 | PRO | ALA | conflict | UNP D0A0V4 |

- Molecule 71 is a protein called Unk8.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 71 | U8 | 30 | 150 | 90 | 30 | 30 | 0 | 0 |

- Molecule 72 is a protein called UnkC.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 72 | UC | 9 | 45 | 27 | 9 | 9 | 0 | 0 |

- Molecule 73 is a protein called UnkD.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 73 | UD | 13 | 65 | 39 | 13 | 13 | 0 | 0 |

- Molecule 74 is a protein called UnkF.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 74 | UF | 36 | 180 | 108 | 36 | 36 | 0 | 0 |

- Molecule 75 is a protein called UnkG.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 75 | UG | 15 | 75 | 45 | 15 | 15 | 0 | 0 |

- Molecule 76 is a protein called UnkI.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 76 | UI | 6 | 30 | 18 | 6 | 6 | 0 | 0 |

- Molecule 77 is a protein called UnkK.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 77 | UK | 24 | 120 | 72 | 24 | 24 | 0 | 0 |

- Molecule 78 is a protein called Unk.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 78 | UM | 8 | 40 | 24 | 8 | 8 | 0 | 0 |
| 78 | UN | 8 | 40 | 24 | 8 | 8 | 0 | 0 |
| 78 | UQ | 8 | 40 | 24 | 8 | 8 | 0 | 0 |

- Molecule 79 is a protein called UnkP.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 79 | UP | 32 | 160 | 96 | 32 | 32 | 0 | 0 |

- Molecule 80 is a protein called Unka.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 80 | Ua | 10 | 50 | 30 | 10 | 10 | 0 | 0 |

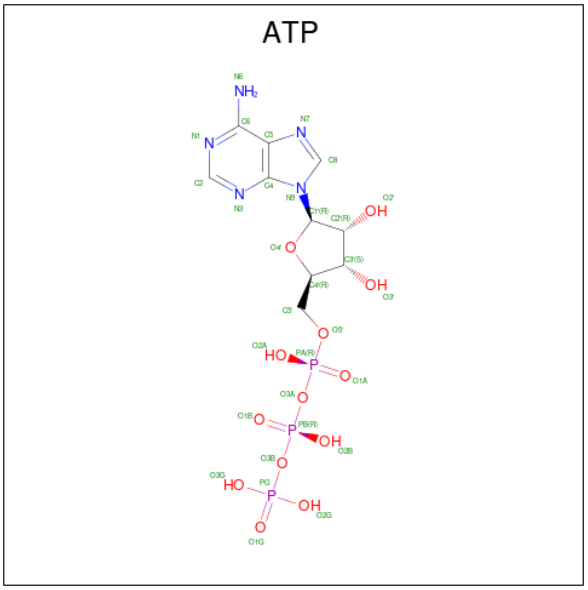
- Molecule 81 is a protein called Unkg.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 81 | Ug | 238 | 1190 | 714 | 238 | 238 | 0 | 0 |

- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

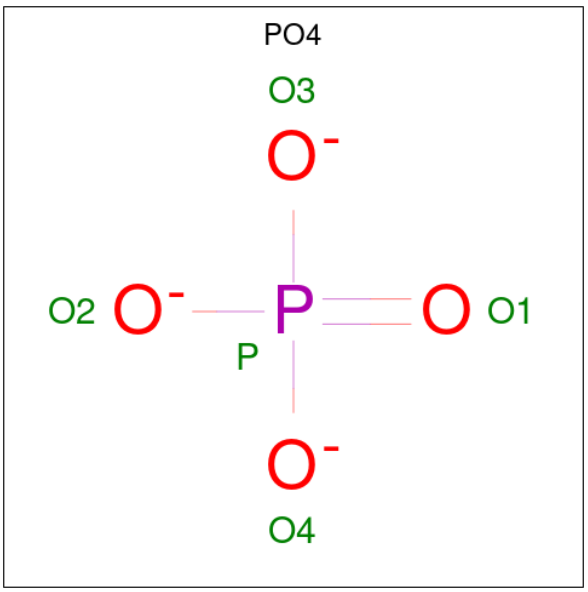
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 82 | CA | 4 | 4 | 4 | 0 |
| 82 | CQ | 1 | 1 | 1 | 0 |
| 82 | Cg | 1 | 1 | 1 | 0 |
| 82 | IA | 1 | 1 | 1 | 0 |

- Molecule 83 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



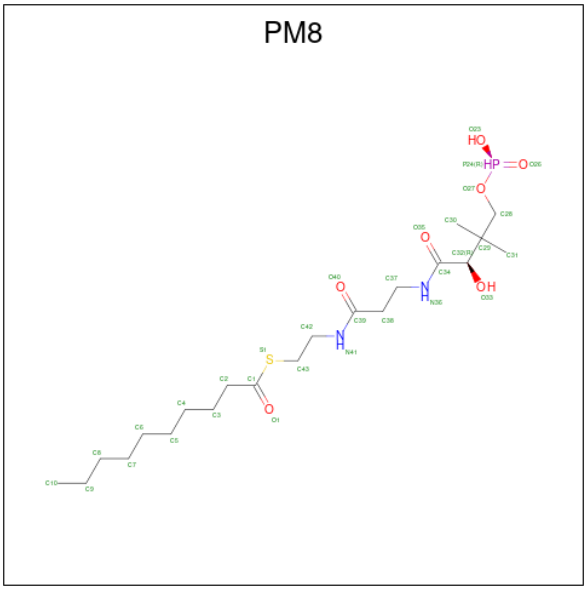

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 83 | Cg | 1 | 31 | 10 | 5 | 13 | 3 | 0 |

- Molecule 84 is PHOSPHATE ION (three-letter code: PO4) (formula: $O_4P$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | P | |
| 84 | FW | 1 | 5 | 4 | 1 | 0 |
| | | | Total | O | P | |
| 84 | IA | 1 | 5 | 4 | 1 | 0 |

- Molecule 85 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (three-letter code: PM8) (formula: $C_{21}H_{41}N_2O_7PS$).

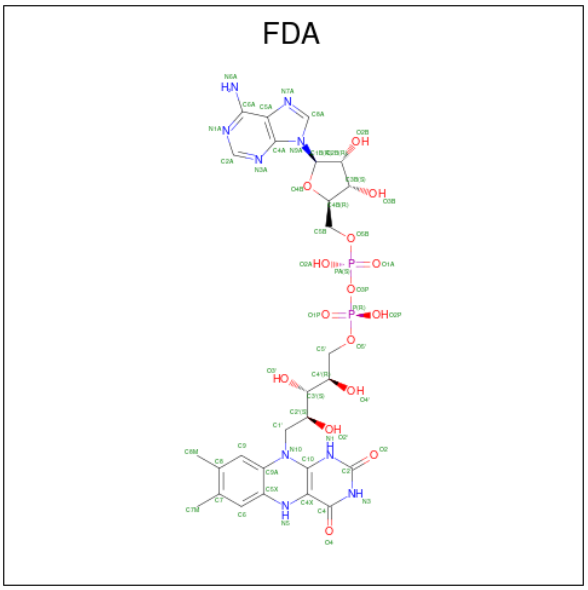


| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | |
| 85 | Fc | 1 | 32 | 21 | 2 | 7 | 1 | 1 | 0 |

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

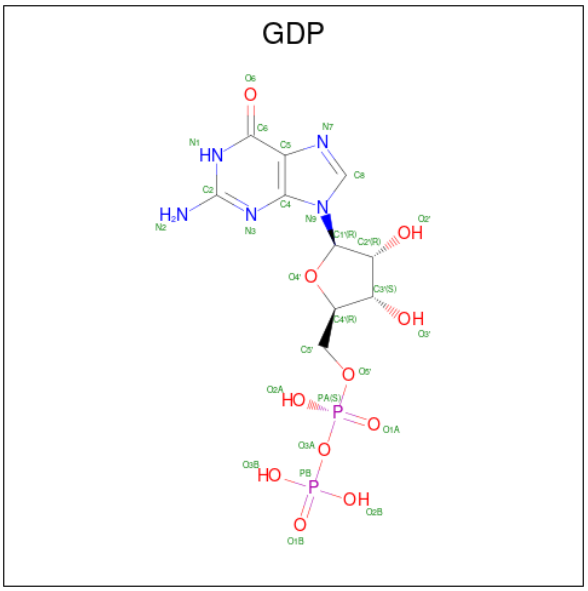
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 86 | Fd | 1 | 1 | 1 | 0 |

- Molecule 87 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 87 | Ff | 1 | 53 | 27 | 9 | 15 | 2 | 0 |

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 88 | IA | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

- Molecule 89 is water.

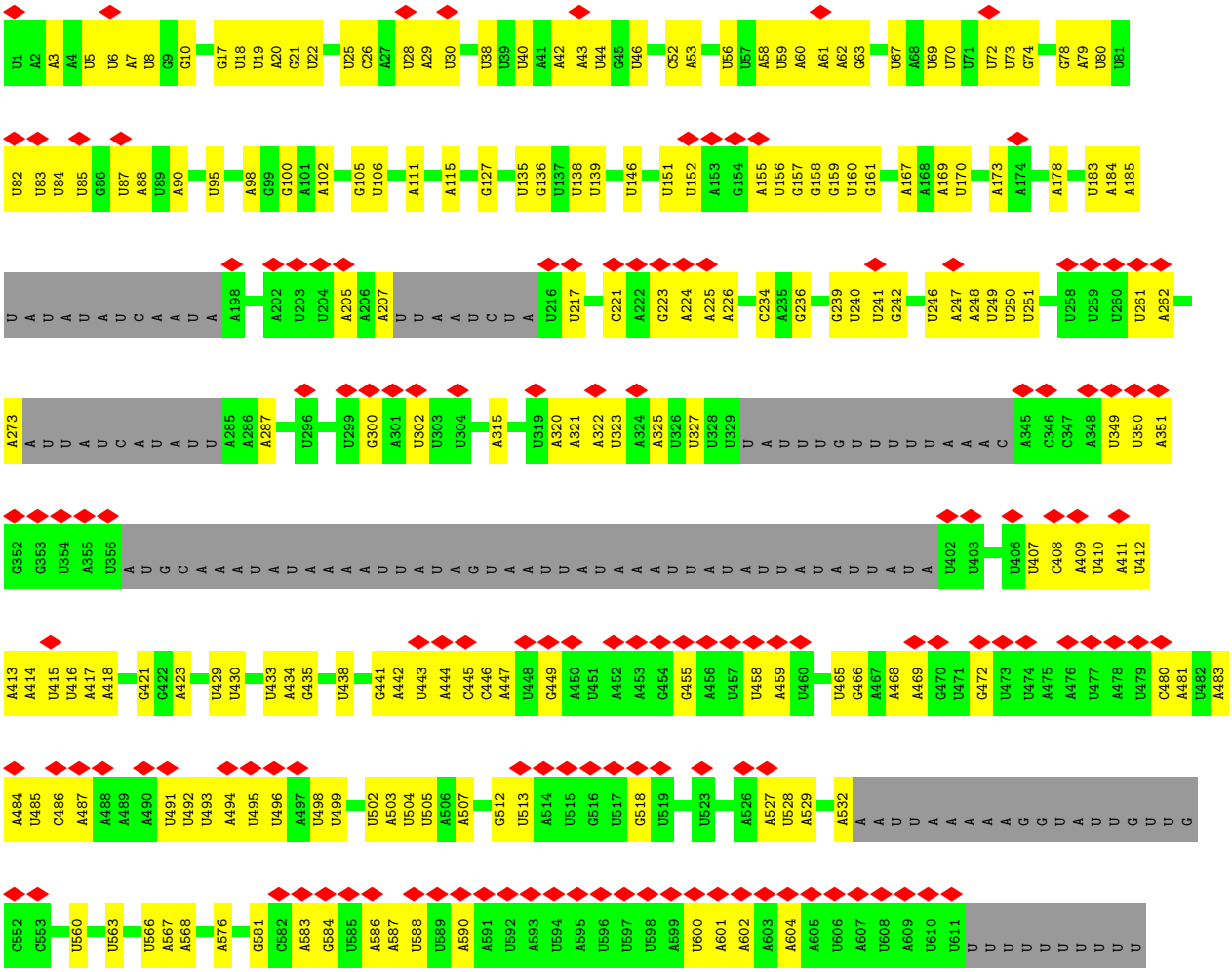
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 89 | Cg | 3 | Total | O | 0 |
| | | | 3 | 3 | |
| 89 | IA | 2 | Total | O | 0 |
| | | | 2 | 2 | |

# 3 Residue-property plots (i)

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

- Molecule 1: 9S rRNA

Chain CA:

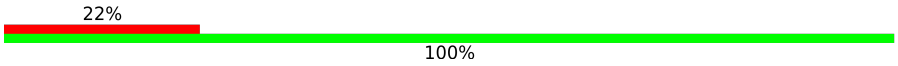


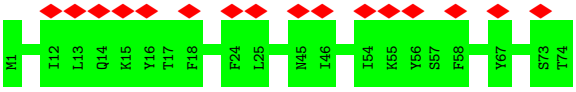
- Molecule 2: 9S rRNA

Chain CB:

- Molecule 3: uS3m

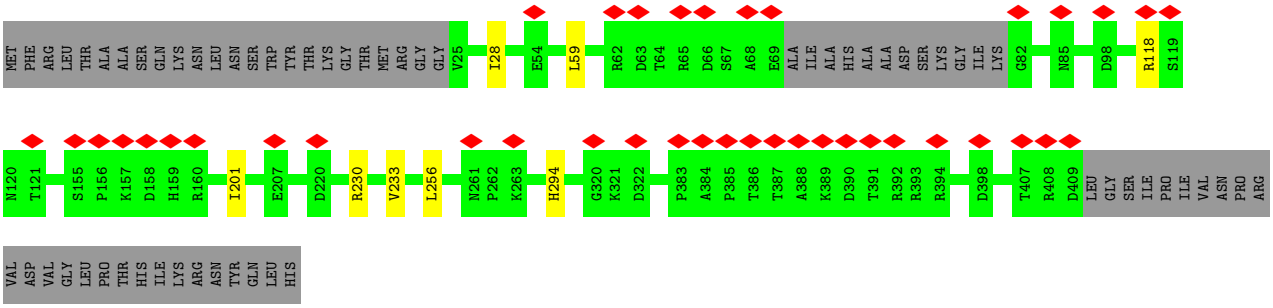
Chain CC:



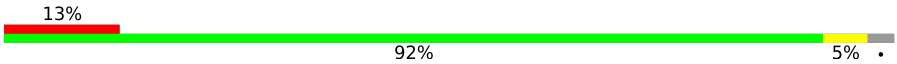

- Molecule 4: Ribosomal_S5_C domain-containing protein

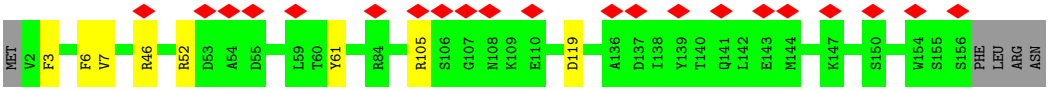
Chain CE:




- Molecule 5: bS6m

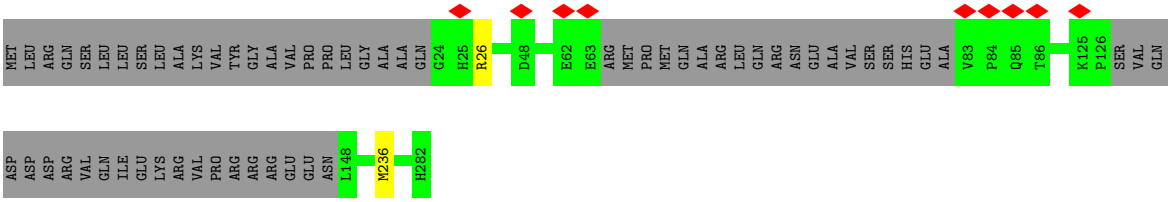
Chain CF:



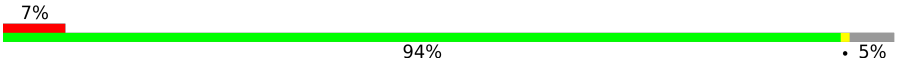

- Molecule 6: 30S ribosomal protein S8, putative

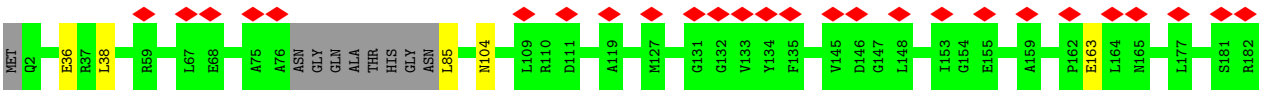
Chain CH:

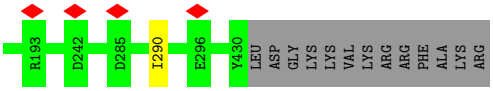



- Molecule 7: uS9m

Chain CI:

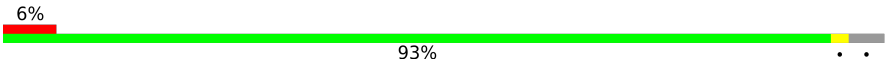


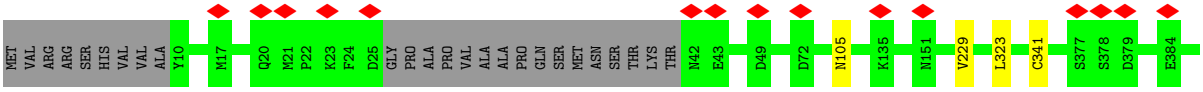



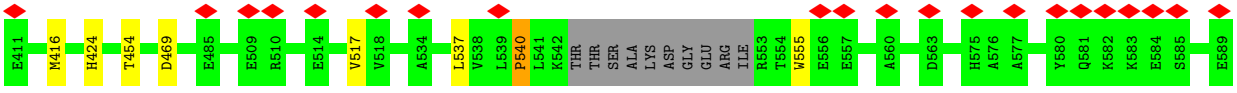


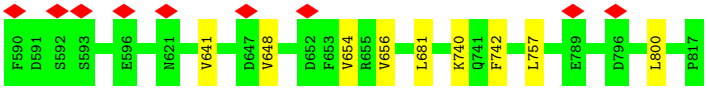

- Molecule 8: LysM domain-containing protein

Chain CJ:



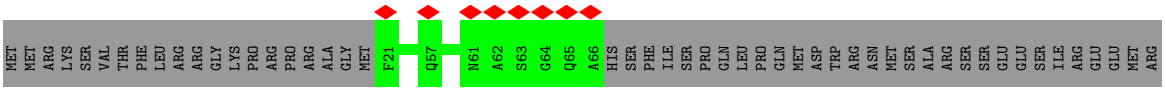



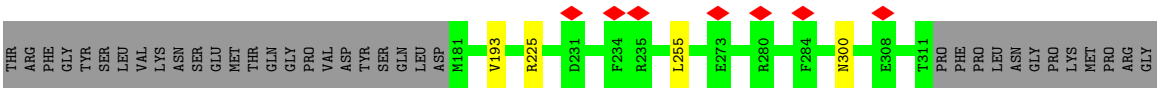




- Molecule 9: uS11m

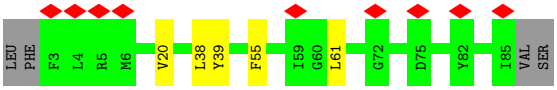
Chain CK:





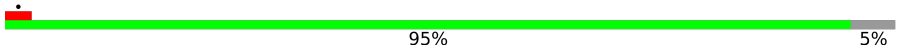
- Molecule 10: uS12m

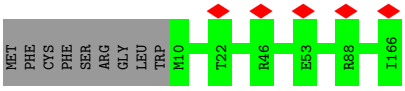
Chain CL:




- Molecule 11: uS14m

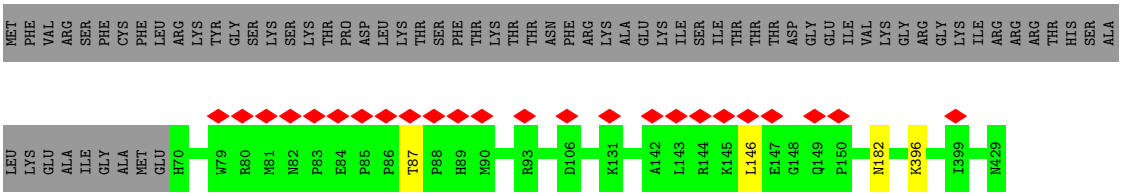
Chain CN:



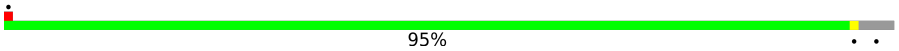

- Molecule 12: uS15m

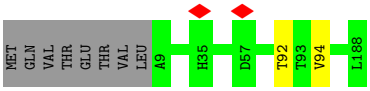
Chain CO:




- Molecule 13: bS16m

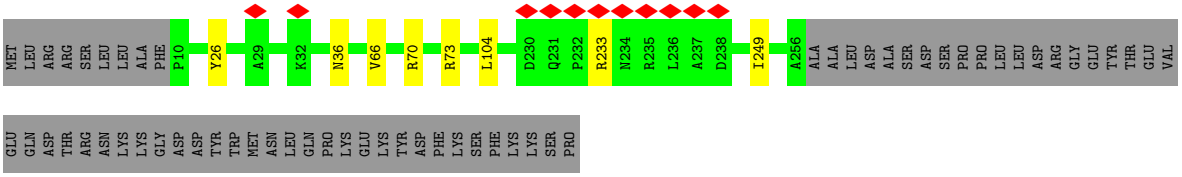
Chain CP:



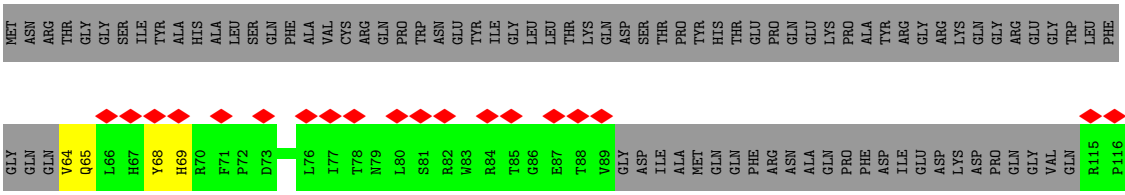

- Molecule 14: 30S Ribosomal protein S17, putative

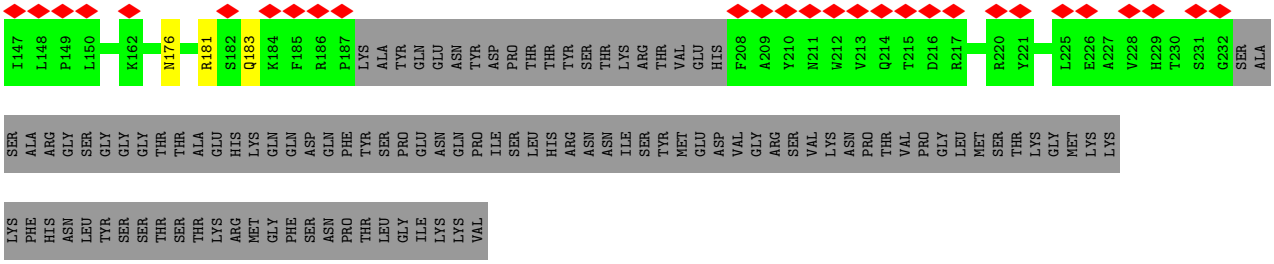
Chain CQ:




- Molecule 15: bS18m

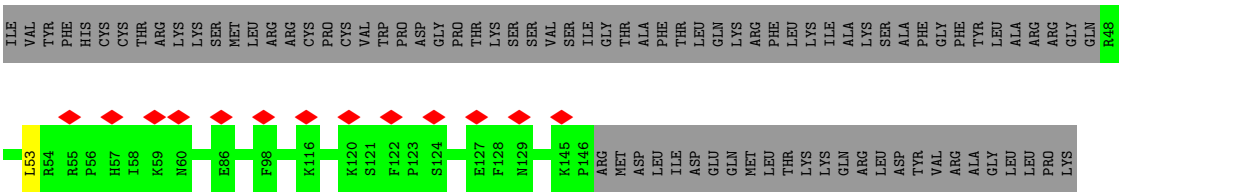
Chain CR:



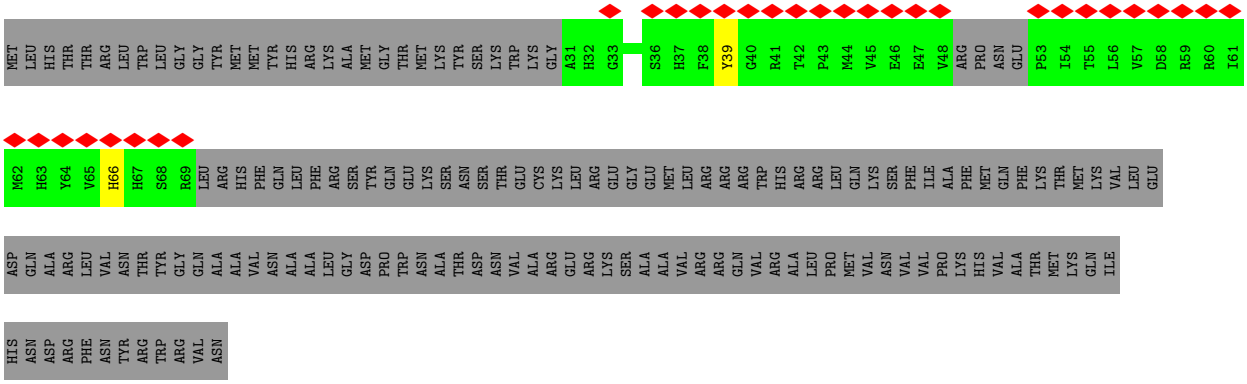

- Molecule 16: uS19m

Chain CS:



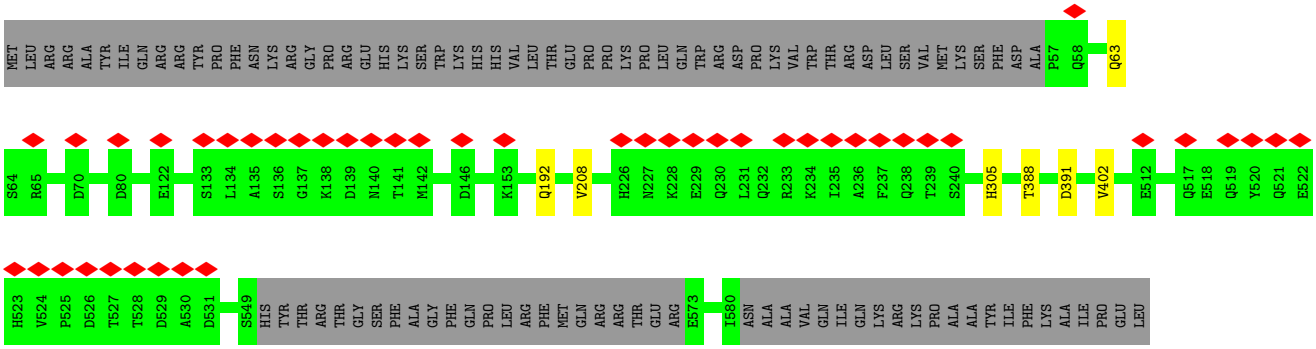

- Molecule 17: bS21m

Chain CU:



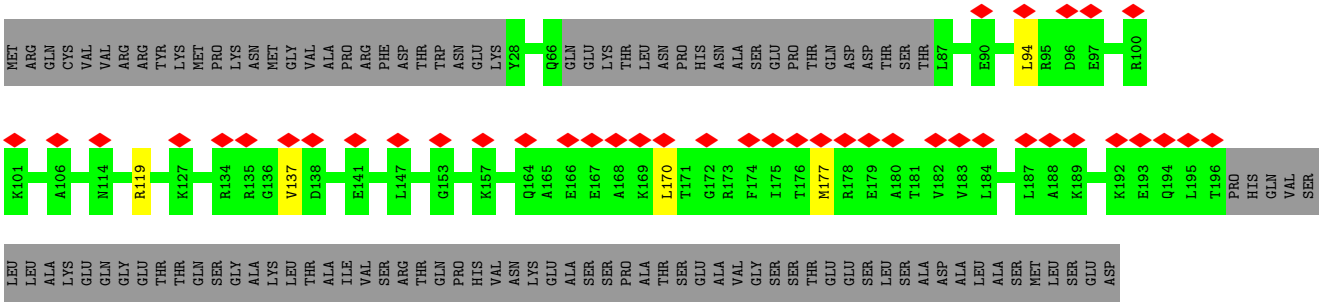

- Molecule 18: mS22

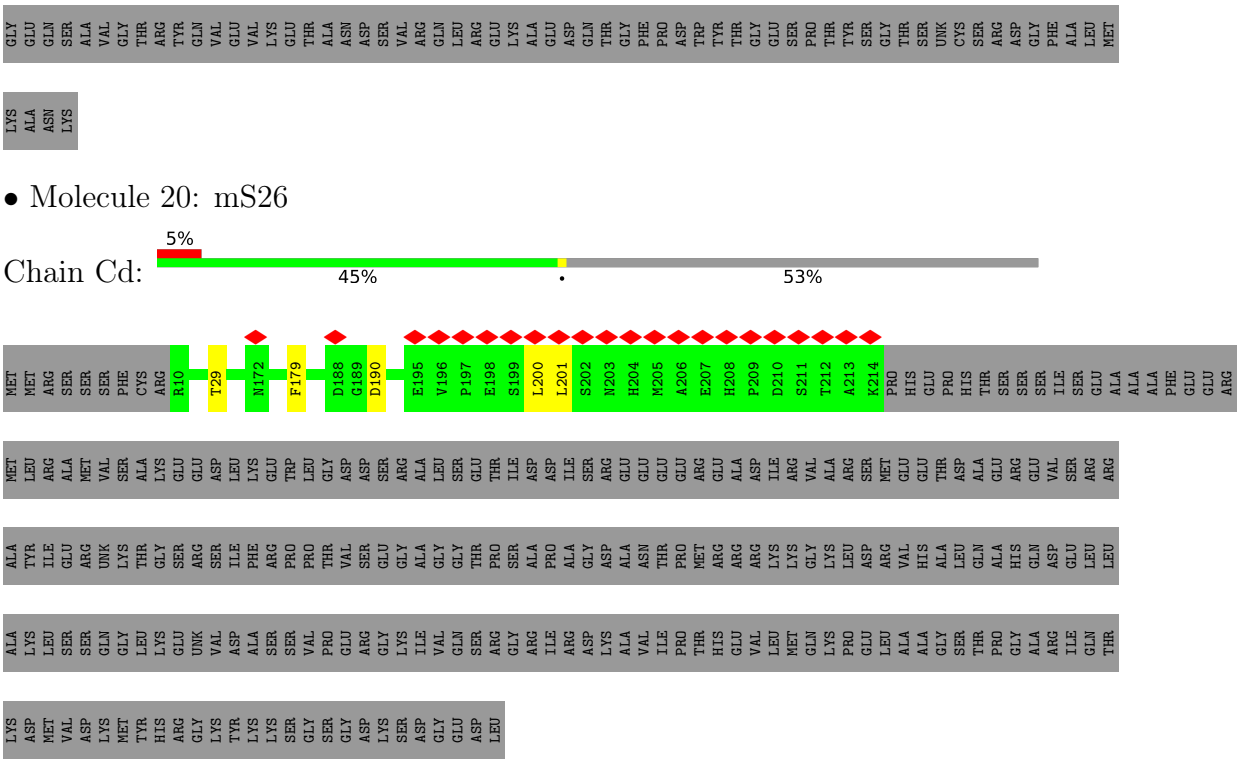
Chain Ca:

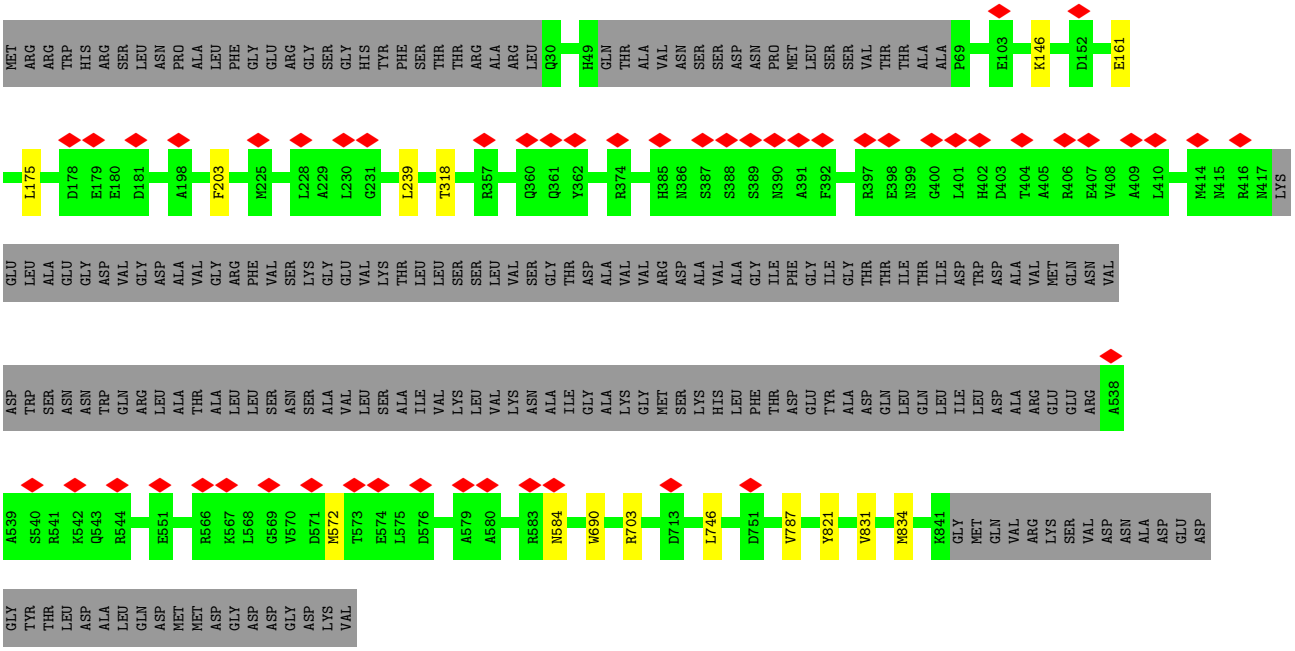



- Molecule 19: mS23

Chain Cb:

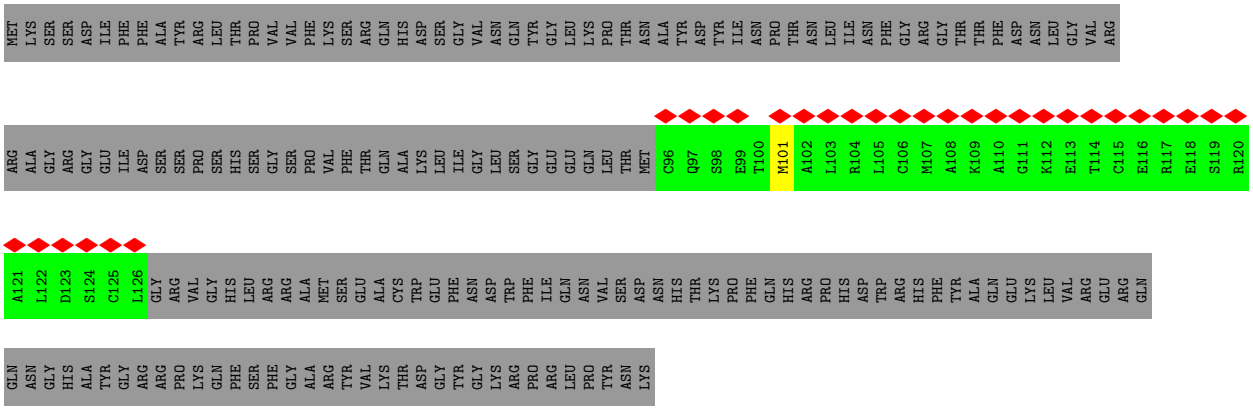



GLY GLU GLN SER ALA VAL GLY THR ARG TYR GLN VAL GLU VAL LYS GLU THR ALA ASN ASP SER VAL ARG GLN LEU ARG GLU LYS ALA GLU ASP GLN THR GLY PHE PRO ASP TRP TYR THR GLY GLU SER PRO THR TYR SER GLY THR SER UNK CYS SER ARG ASP GLY PHE ALA LEU MET
LYS ALA ASN LYS
• Molecule 20: mS26
Chain Cd:
5%
45%
53%
MET MET ARG SER SER SER PHE CYS ARG R10 T29 N172 F179 D188 G189 D190 E195 V196 P197 E198 S199 L200 L201 S202 N203 H204 M205 A206 E207 H208 P209 D210 S211 T212 A213 K214 PRO HIS GLU PRO HIS THR SER SER SER ILE SER GLU ALA ALA ALA PHE GLU GLU ARG
MET LEU ARG ALA MET VAL SER ALA LYS GLU GLU ASP LEU LYS GLU TRP LEU GLY ASP ASP SER ARG ALA LEU SER GLU THR ILE ASP ASP ILE SER ARG GLU GLU GLU GLU ARG GLU ALA ASP ILE ARG VAL ALA ARG SER MET GLU GLU THR ASP ALA GLU ARG GLU VAL SER ARG ARG
ALA TYR ILE GLU ARG UNK LYS THR GLY SER ARG SER ILE PHE ARG PRO PRO THR VAL SER GLU GLY ALA GLY GLY THR PRO SER ALA PRO ALA GLY ASP ALA ASN THR PRO MET ARG ARG ARG LYS LYS GLY LYS LEU ASP ARG VAL HIS ALA LEU GLN ALA HIS GLN ASP GLU LEU LEU
ALA LYS LEU SER SER GLN GLY LEU LYS GLU UNK VAL ASP ALA SER SER VAL PRO GLU ARG GLY LYS ILE VAL GLN SER ARG GLY ARG ILE ARG ASP LYS ALA VAL ILE PRO THR HIS GLU VAL LEU MET GLN LYS PRO GLU LEU ALA ALA GLY SER THR PRO GLY ALA ARG ILE GLN THR
LYS ASP MET VAL ASP LYS MET TYR HIS ARG GLY LYS TYR LYS LYS SER GLY SER GLY ASP LYS SER ASP GLY GLU ASP LEU
• Molecule 21: mS29
Chain Cg:
96%
MET ARG SER LYS T5 L6 K7 K8 S9 R43 K44 L45 K46 N47 G48 R52 R107 E114 T139 G236 Q262 L269 H296 D347 D468 S487 R488 G489 A490 S491 SER GLY ALA VAL GLY VAL ARG
• Molecule 22: mS33
Chain Ci:
8%
88%
9%
MET VAL LEU ARG ARG TRP PHE PRO LEU LEU G11 V15 R34 D75 G79 L84 D106 D111 H136 Q143 D146 R147 K148 L149 S150 G151 K155 K163 E170 D174 A175 THR GLU GLU GLU GLU ASP
• Molecule 23: mS34
Chain Cj:
86%
12%
MET LEU ARG CYS ALA ARG VAL ALA LEU R10 S30 R118 Y126 D167 Y209 P235 THR GLU THR ALA ASP VAL ASP LYS ASP PRO THR THR SER ASP GLY SER VAL HIS TYR ASP GLY LYS
• Molecule 24: mS35
Chain Ck:
6%
75%
23%



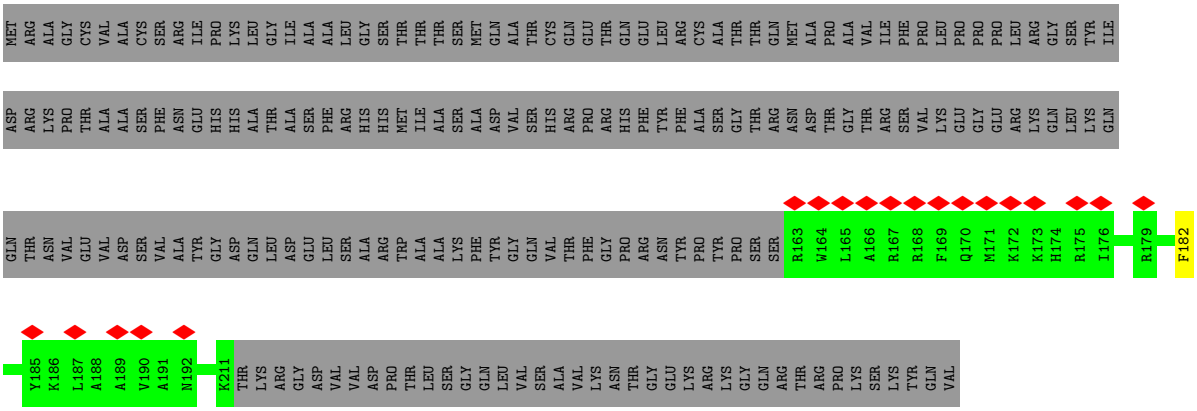

- Molecule 25: mS37

Chain Cm:




- Molecule 26: mS38

Chain Cn:



- Molecule 27: Protein FYV4, mitochondrial

Chain Cp: 89% 10%

MET LEU LYS ARG THR LEU THR VAL LEU ASP GLN THR TYR GLY P15 E148 D158 Q159 C177 E178 Q182 SER LYS LYS THR VAL

- Molecule 28: mS49

Chain DB: 91% 6%

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

THR ALA GLY GLU ASN PRO ALA SER SER GLY D71 T151 E185 R203 G229 D233 D248 D268 R274 R316 D344 R345 R361 Q370 R371 E372 Q384 V388 Q389 D390 D394 Q395 R396 T397 A410 K420 D424 D448 V556

C575 G620 S621 A622 N625 E634 R662 H670 V671 V680 L689 T741 T749 GLU THR GLY ALA V754 L755 T756 R770 M771 K772 T773 K778 V779 D780 N789 R792 L797 D802 F822 E890 Q908 N912 R942 A961 N978

K985 Y986 E987 P988 K989 R990 D1009 R1013 I1034 R1035 M1036 Q1051 A1059 E1060 R1063 Q1064 D1065 N1066 D1104 K1110 K1154 K1158 R1167 V1179 Q1180 LEU

- Molecule 29: mS50

Chain DC: 11% 92% 6%

MET PHE ARG VAL ARG ARG LEU ALA GLY PHE ILE GLN CYS SER PRO CYS GLY LYS MET GLY PRO LEU LYS GLN GLN THR ARG ARG Y29 T30 K34 S35 D36 P37 A38 A43 D47 E48 D49 E50 A53 E57 R73 K91 N94 Q95 Q96 R97 E98 K99 E100 S101

L102 L121 R153 N157 Y158 V159 G160 L161 I162 E166 V167 F168 D169 D170 E171 S172 D173 R174 P175 E176 S180 Q181 D182 T183 K197 E198 K199 E207 E216 D223 Q228 T229 Q230 T231 H242 Y243 E244 G245 E246 R247 R248 F266 L270 Q278 E279

K283 V291 L299 V335 E336 M343 M344 E345 D346 D347 V348 D349 D350 L353 D361 D372 G373 L374 L413 I430 T434 L437 G438 A439 K457 T468 T469 L475 D484 N500 H548 L576 A577 S595 G596 K602 P603 V604 E605

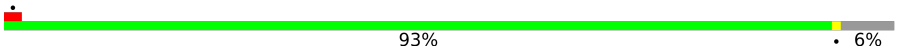
K608 L614 R618 S637 D638 A639 A640 S641 A642 V643 S644 G645 S646 S647 L648 R654 L659 E666 Q680 E683 E686 A687 K690 R697 T698 V699 R719 VAL ALA PHE PRO THR GLU THR SER THR VAL THR GLU THR THR ASN MET LYS GLU GLU THR ASN

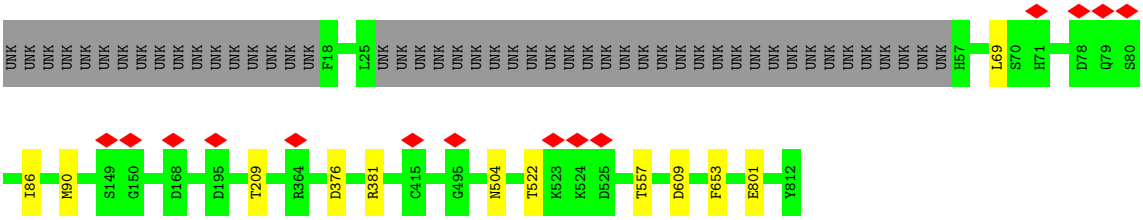
LYS PRO LEU GLU ASP SER GLU W748 A775 L779 Q782 D817 A818 L819 R828 VAL LYS ASP ALA THR ALA GLU ALA ALA GLY V839 L859 A872 G890 H894 R934 D958 T961 T968 A974 K991 E995 R996 T1019 G1024 F1076

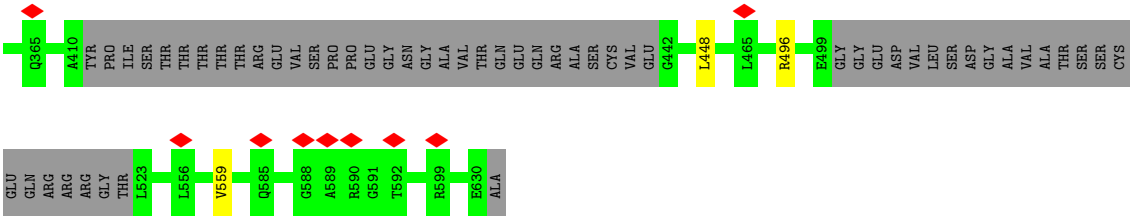
A1091 E1094 F1103 M1104 A1105 L1108 E1111 D1127 S1131 D1155 D1159 S1165

- Molecule 30: mS51

Chain DD:

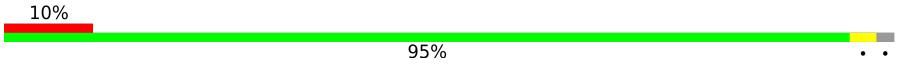


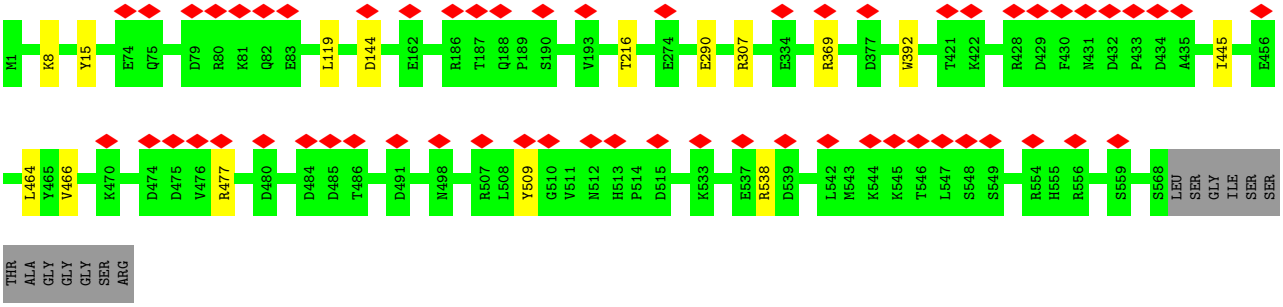


UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK F18 L25 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK




- Molecule 34: mS55

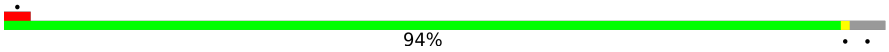
Chain DH:

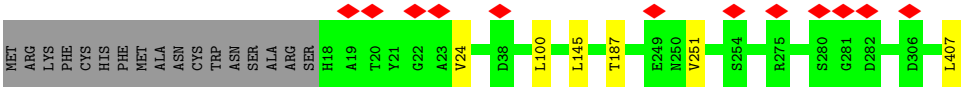



- Molecule 35: mS56

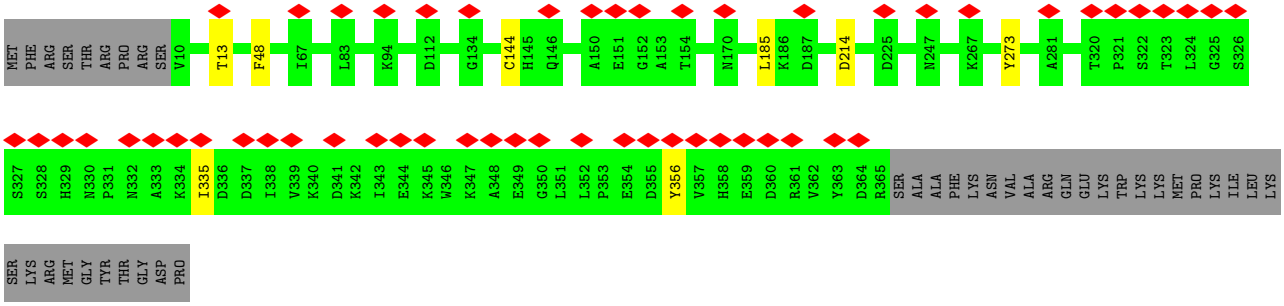
Chain DI:



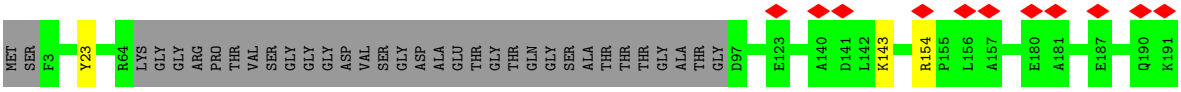

- Molecule 36: mS57

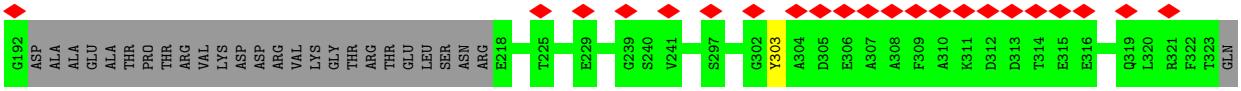
Chain DJ:




- Molecule 37: mS58

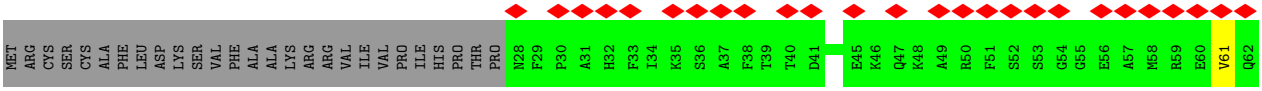
Chain DK:

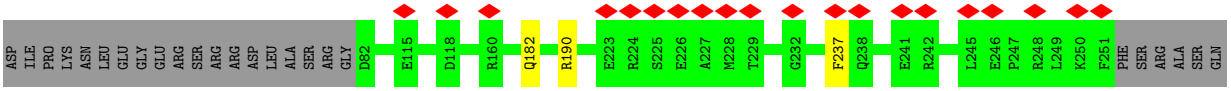


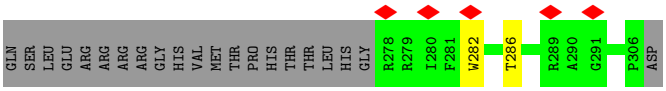



- Molecule 38: mS59

Chain DL:

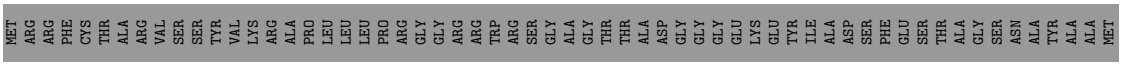


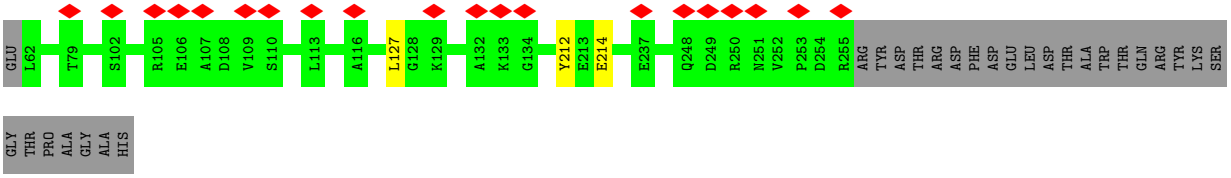




- Molecule 39: mS62

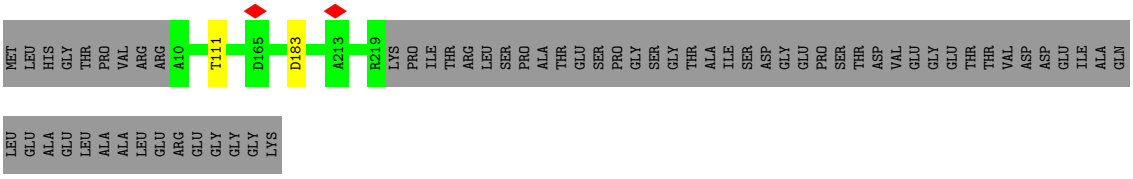
Chain DO:



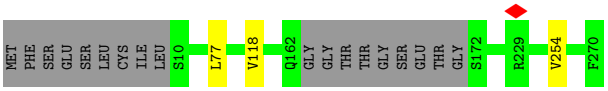

- Molecule 40: mS63

Chain DP:



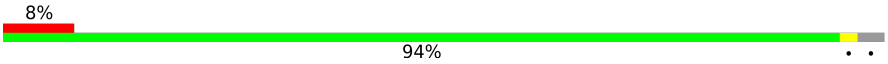

- Molecule 41: mS65

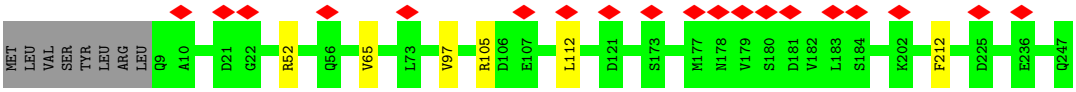
Chain DR:




- Molecule 42: Rhodanese domain-containing protein

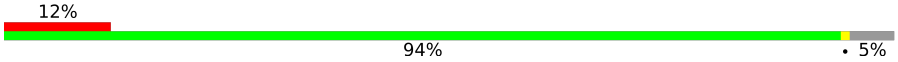
Chain DT:

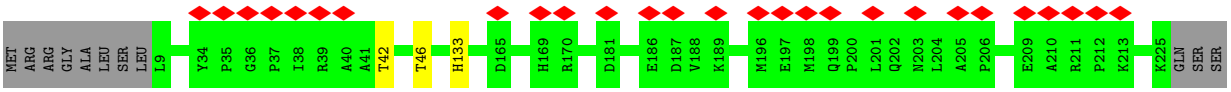



• Molecule 43: Ubiquitin-like domain-containing protein

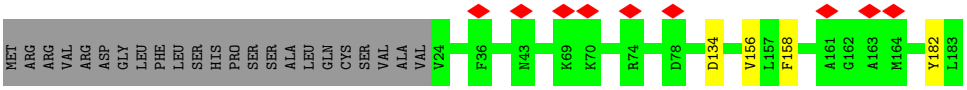
Chain DU:



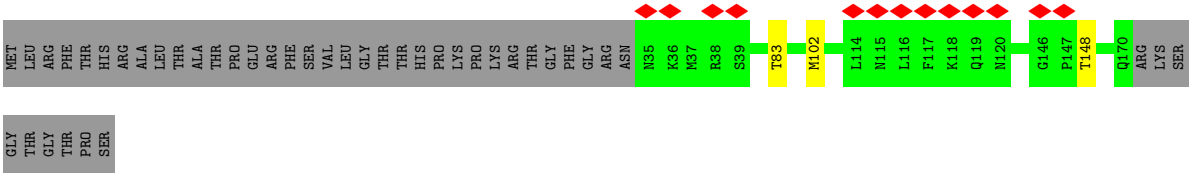

• Molecule 44: mS69

Chain DV:



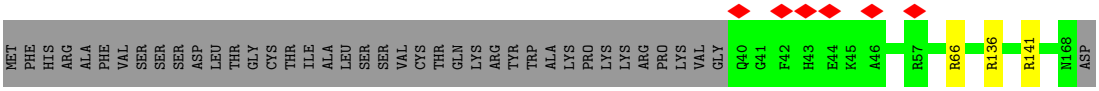

• Molecule 45: mS70

Chain DW:



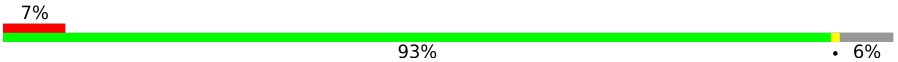

• Molecule 46: mS71

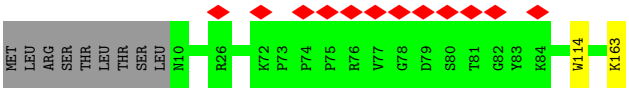
Chain DX:




• Molecule 47: mS72

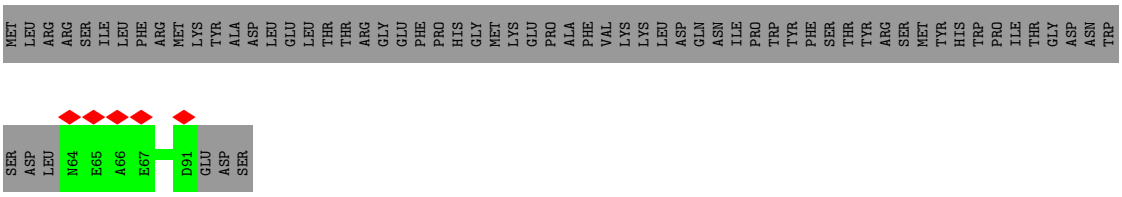
Chain DY:



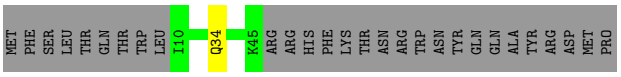

• Molecule 48: mS73

Chain DZ:



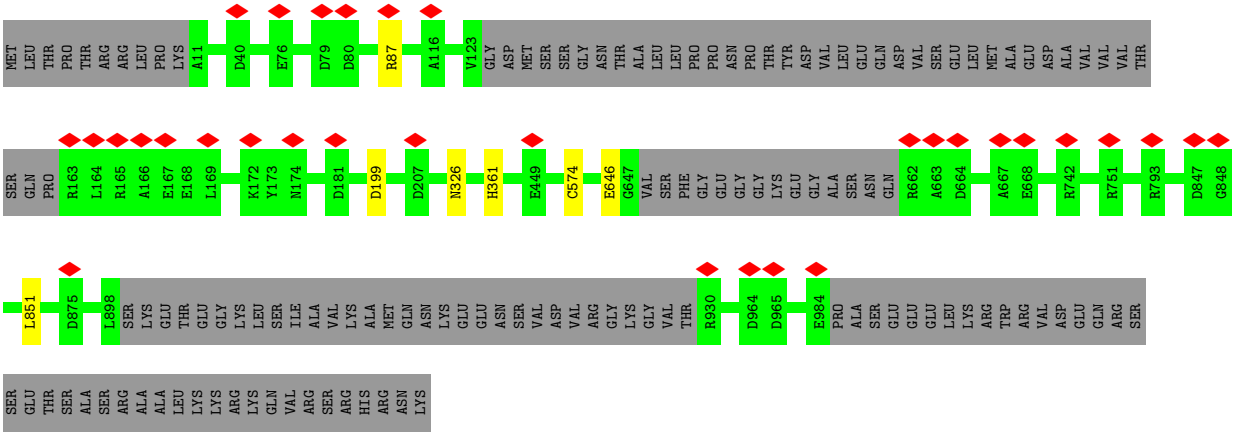

- Molecule 49: mS74

Chain Da:



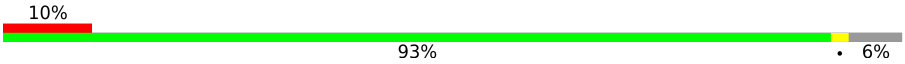

- Molecule 50: PPR_long domain-containing protein

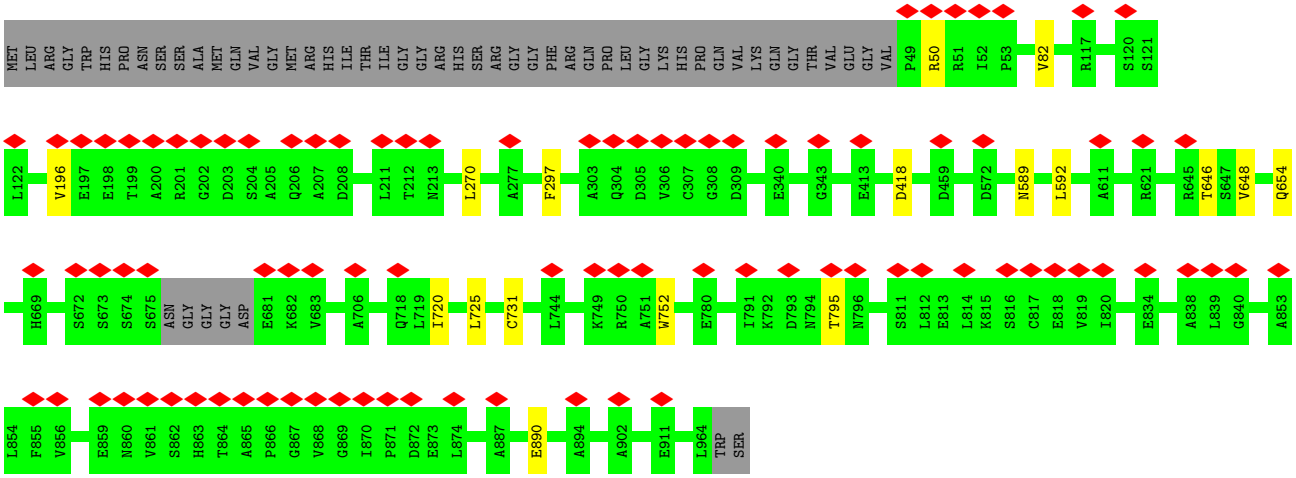
Chain F2:




- Molecule 51: mt-SAF3

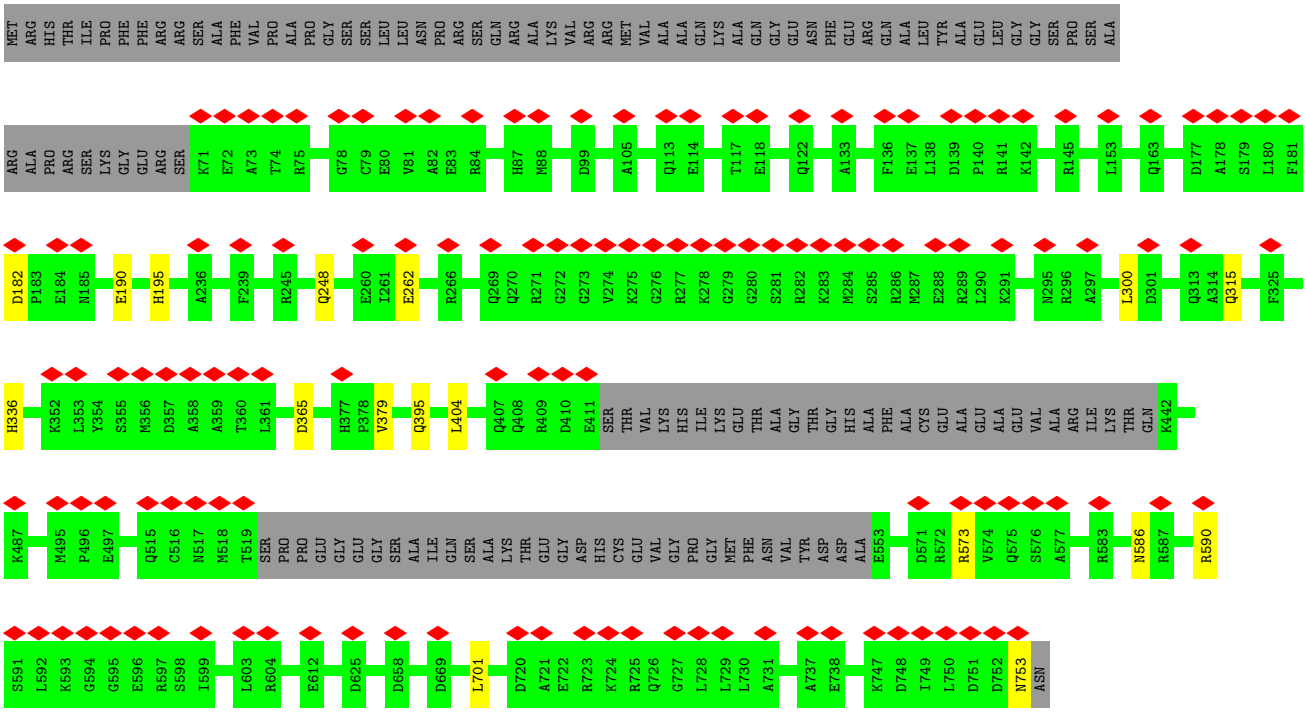
Chain F3:



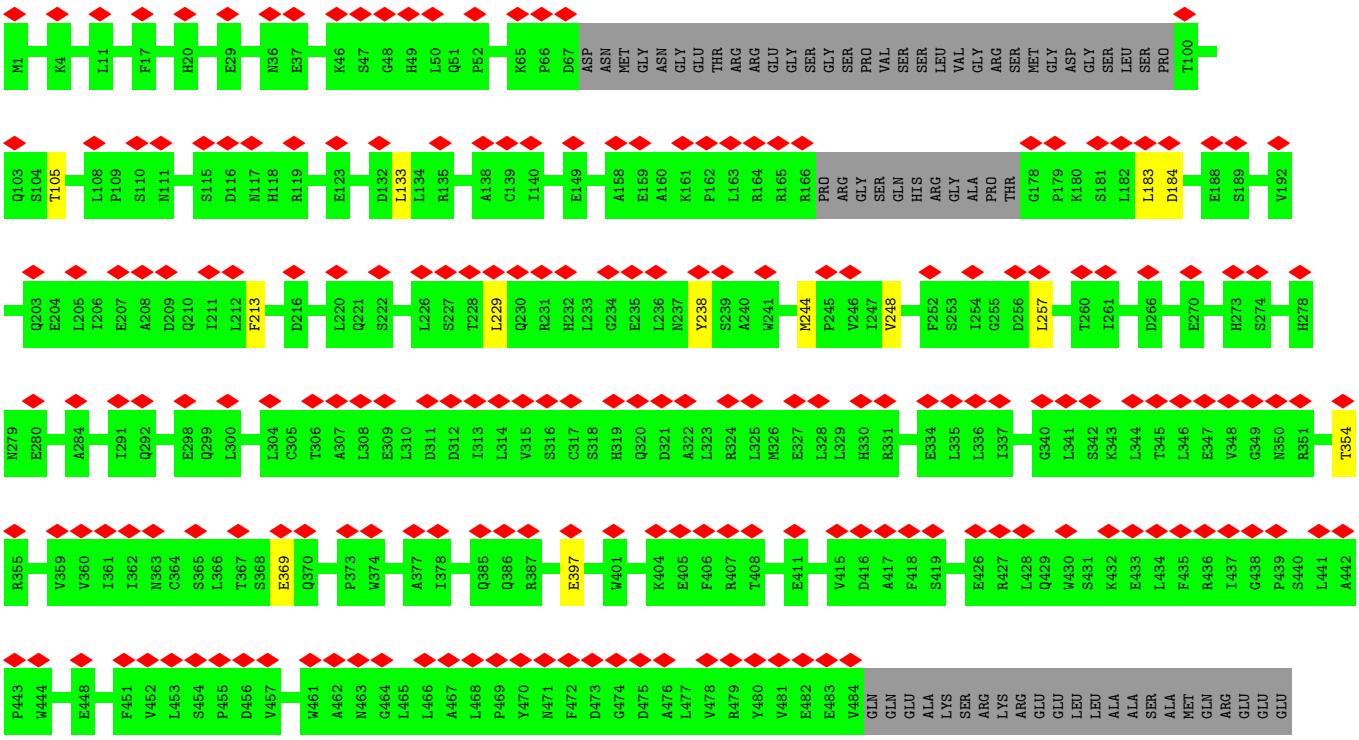

- Molecule 52: mt-SAF5

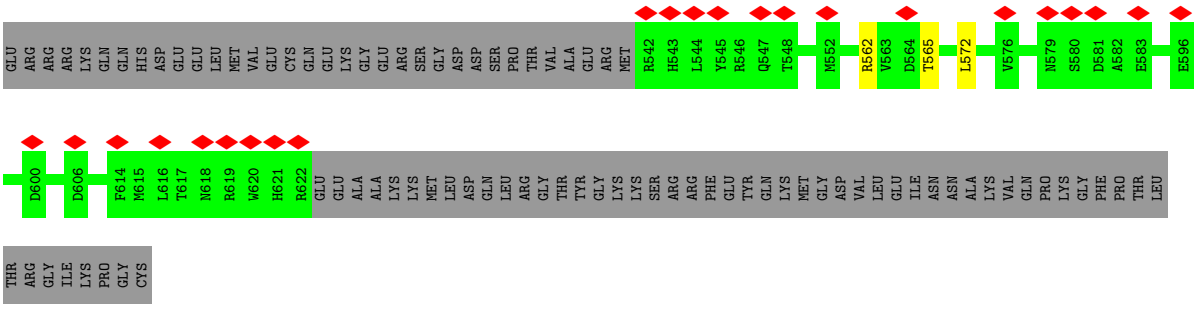
Chain F5:




- Molecule 53: DUF4460 domain-containing protein

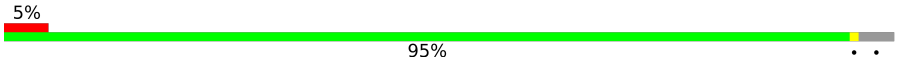
Chain F6:

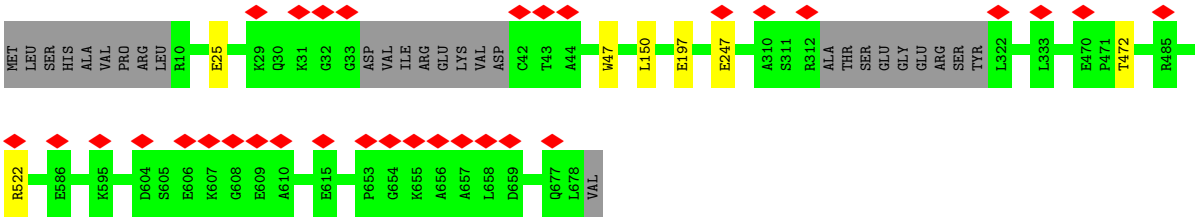





- Molecule 54: mt-SAF7

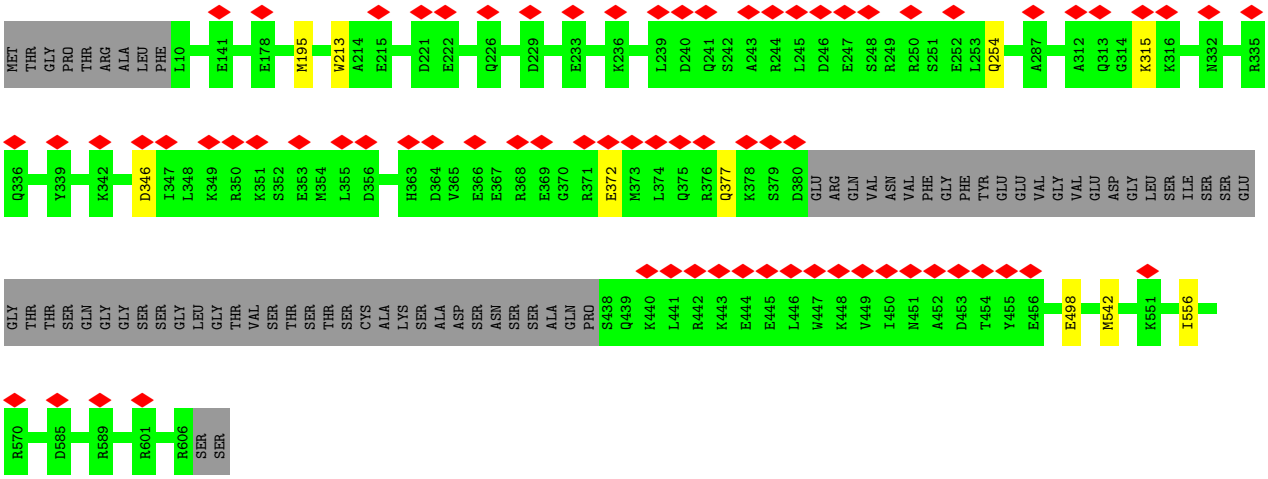
Chain F7:



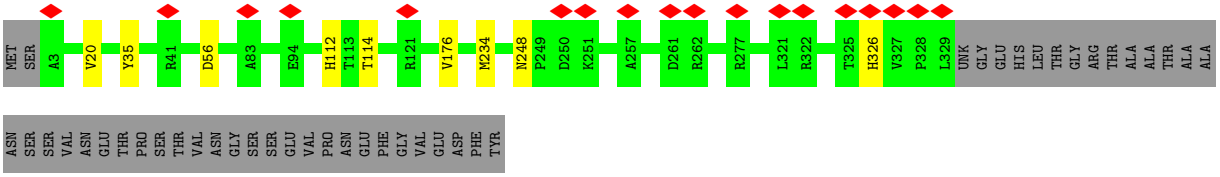

- Molecule 55: mt-SAF9

Chain F9:




- Molecule 56: mt-SAF21

Chain FM:




- Molecule 56: mt-SAF21

Chain FN: 11% 85% 14%

MET SER ALA ILE LYS R6 S7 L8 M15 G16 N17 L26 G27 F28 K29 A30 R31 S32 A33 M34 Y35 A42 L43 S44 L53 S54 A58 T64 M71 A81 K86 N102 R121 D158 L166 G180 E205 D217 A257 L270 K276

R277 G278 G279 E280 D281 D299 A319 E320 L321 R322 N323 R324 T325 HIS VAL PRO LEU UNK GLY GLU HIS LEU THR GLY ARG THR ALA ALA THR ALA ALA ASN SER SER VAL ASN GLU THR PRO SER THR VAL ASN GLY SER SER GLU VAL PRO ASN GLU PHE GLY VAL GLU ASP PHE TYR

- Molecule 57: mt-SAF22

Chain FO: 96%

MET T2 D73 L119 E219 V220 M221 N222 E223 S224 E225 G226 ASN GLY LEU ARG ARG Q232 A233 S234 S235 L236 A237 F238 A239 R244 R248 L319 R322 R333 I334

- Molecule 58: mt-SAF23

Chain FP: 9% 99%

MET V2 A3 K4 L5 Q6 A10 P11 T12 G64 D68 H84 G87 Y97 A178 E179 Q180 A181 L237 V238 G239 S240 S241 H242 S243 R244 T245 E246 E247 L248 S249 E250 T251 D252 S253 E254 T255 V256 P257 L258 V315 H349

- Molecule 59: LMWPc domain-containing protein

Chain FW: 90% 10%

MET S2 L13 L95 R108 GLU SER PHE THR VAL GLU TYR GLY ASP ASP GLY SER GLY PRO ARG GLY GLY ASP ASP P128 K245 L258 GLU GLU PHE ILE SER

- Molecule 60: mt-SAF27

Chain FX: 92% 8%

M1 Q29 D93 R199 E214 E215 V216 A217 E218 Y219 K220 GLN PHE VAL ALA VAL GLU ASP HIS LYS LEU SER LEU PRO PRO THR LEU PRO ARG GLY

- Molecule 61: mt-SAF29

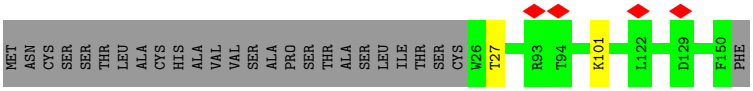
Chain FZ: 40% 86% 10%

MET ARG ARG LYS THR THR LEU ASN ILE GLY GLN VAL ILE C14 F15 D20 E23 E26 E34 E41 G44 D54 N69 V70 S71 C72 S77 G78 I79 E80 G81 A82 D83 E84 D85 E86 D87 Q88 S89 D90 M91 S92 L93 C94 S95 L96 L97 G98 V99 L100 E101

G102 E103 I104 E105 T106 D107 C108 I109 S113 P114 S115 D116 A117 E123 F124 L125 C126 D127 Y128 D129 P130 S131 D132 T133 K134 R135 M136 A137 K138 W139 V140 N141 L142 R143 S144 E145 D148 G153 A154 I155 P156 E157 G158 E159 R160 S161 L162 K172 A173 GLY LYS LYS PRO ILE

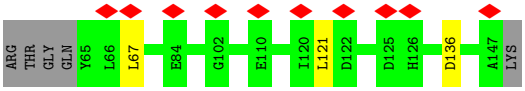
- Molecule 62: mt-SAF31

Chain Fb:



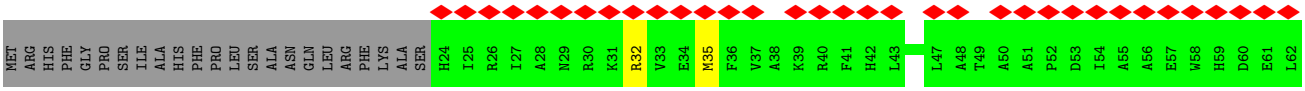

- Molecule 63: Acyl carrier protein

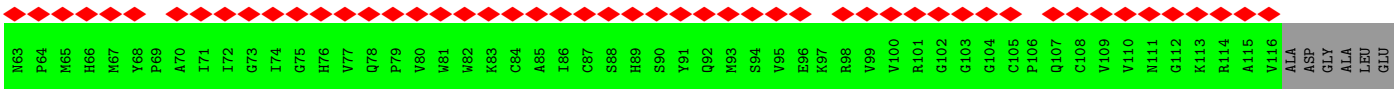
Chain Fc:




- Molecule 64: DUF4379 domain-containing protein

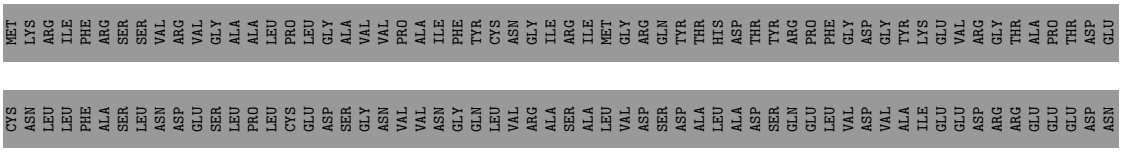
Chain Fd:

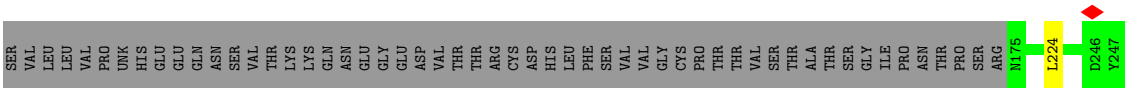


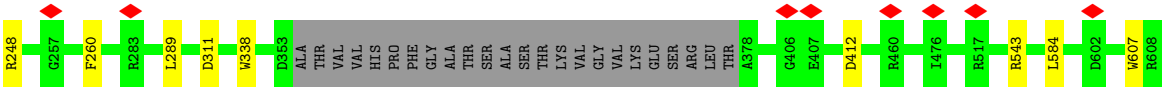



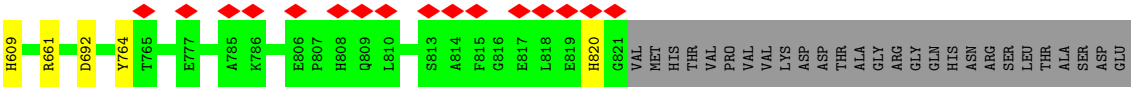
- Molecule 65: DNA photolyase, putative

Chain Ff:



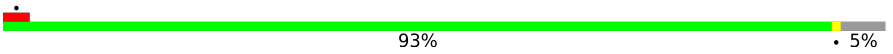



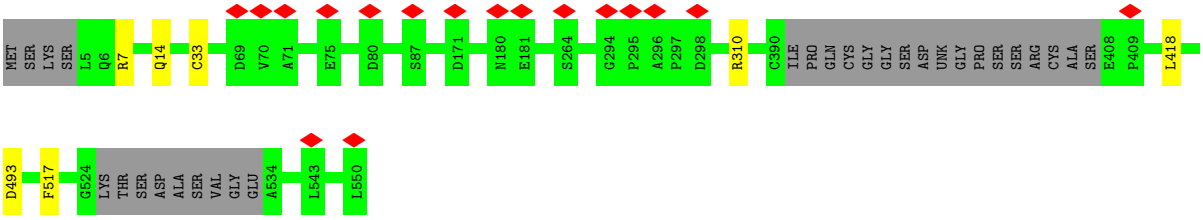



- Molecule 66: Acyl transferase-like protein, putative

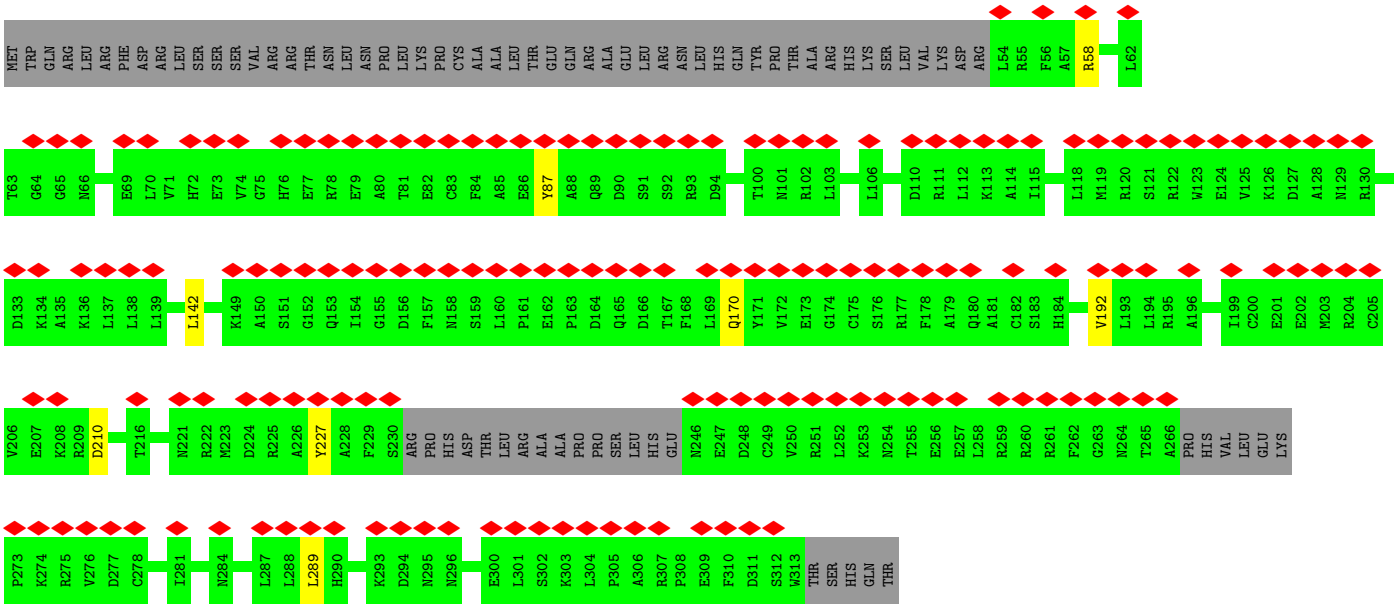
Chain Fg:



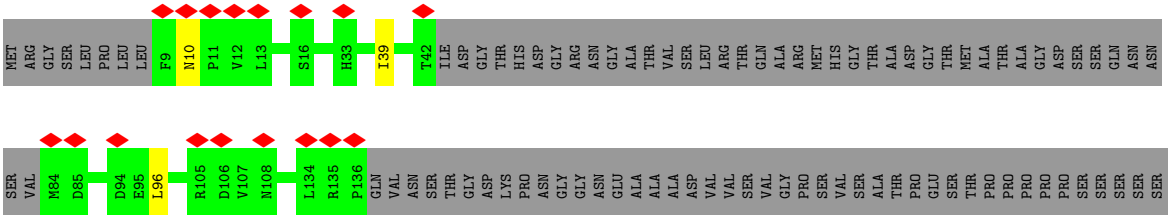

- Molecule 67: mt-SAF37

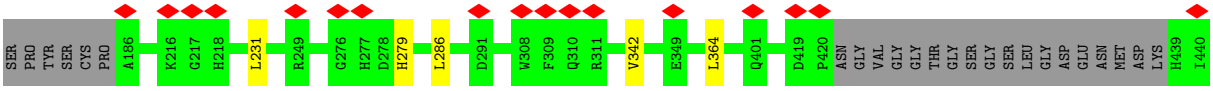
Chain Fh:

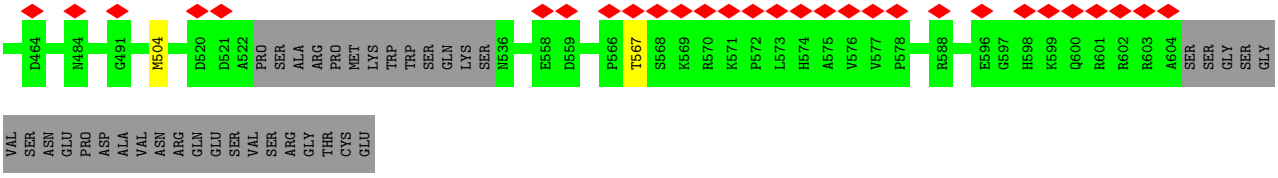



- Molecule 68: mt-SAF38

Chain Fi:

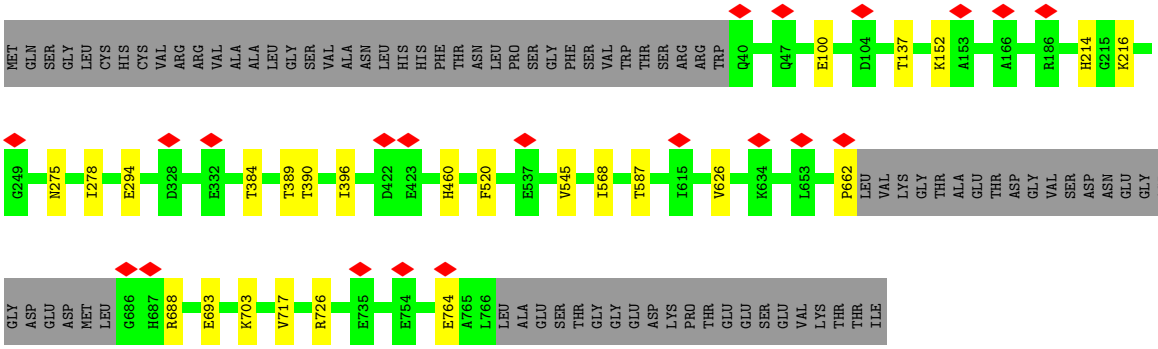




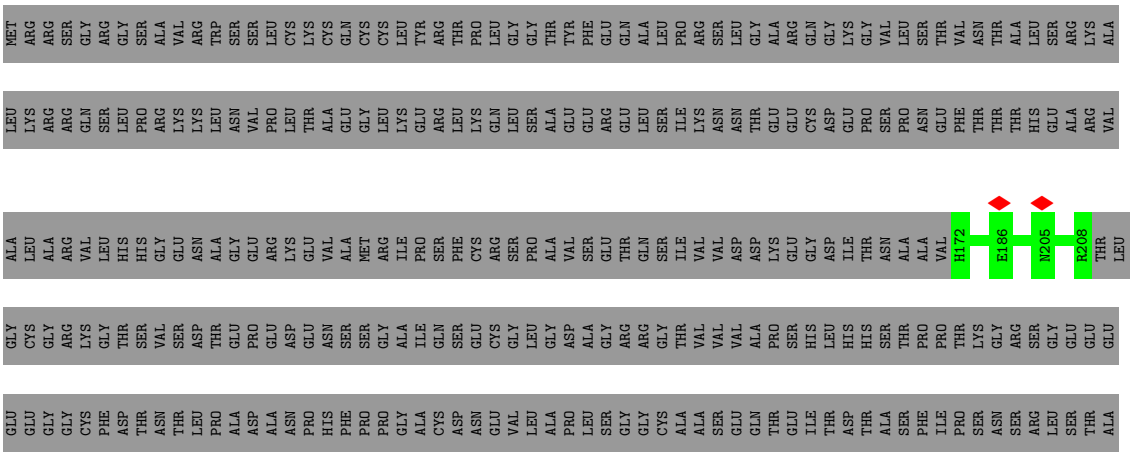

• Molecule 69: Translation initiation factor IF-2, putative

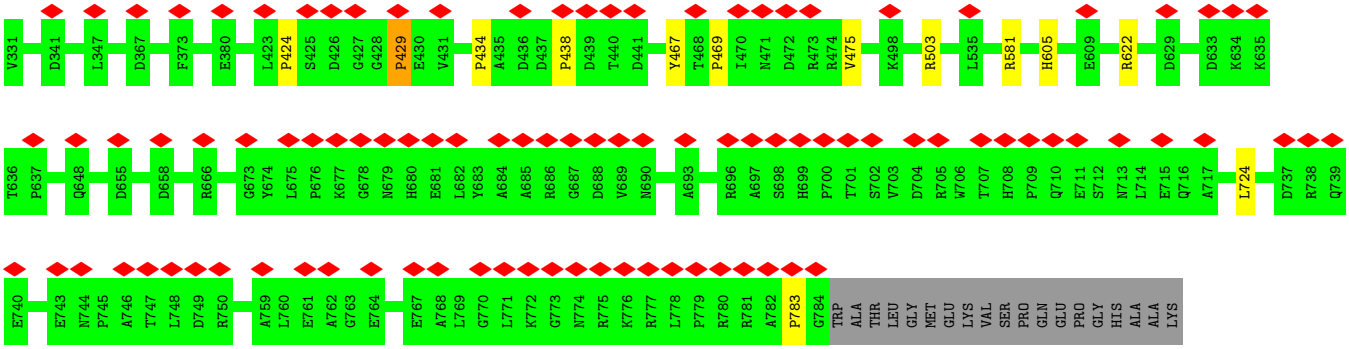
Chain IA:




• Molecule 70: mt-SAF39

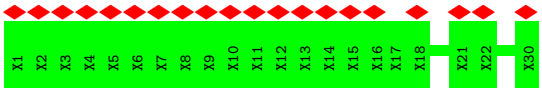
Chain IB:



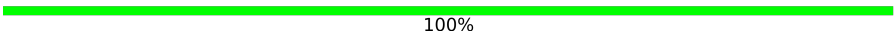




• Molecule 71: Unk8

Chain U8:

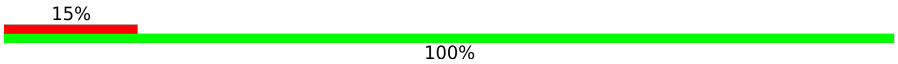




• Molecule 72: UnkC

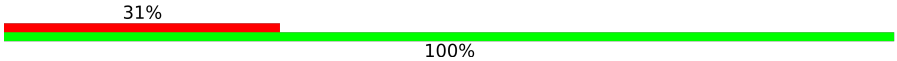
Chain UC: 

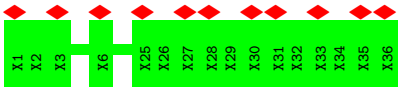

There are no outlier residues recorded for this chain.

• Molecule 73: UnkD

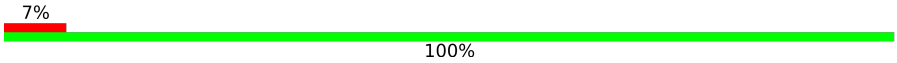
Chain UD: 

• Molecule 74: UnkF

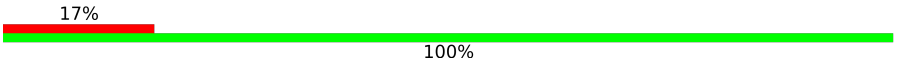
Chain UF: 

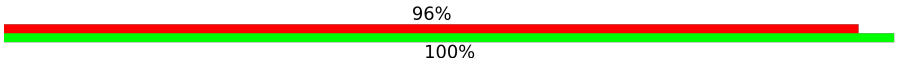

• Molecule 75: UnkG

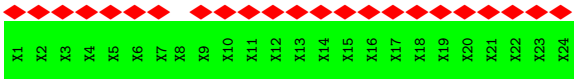
Chain UG: 

• Molecule 76: UnkI

Chain UI: 

• Molecule 77: UnkK

Chain UK: 


• Molecule 78: Unk

Chain UM: 100%

There are no outlier residues recorded for this chain.

• Molecule 78: Unk

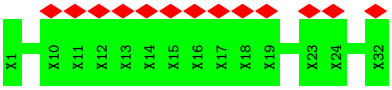
Chain UN: 25% 100%

• Molecule 78: Unk

Chain UQ: 25% 100%

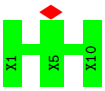
• Molecule 79: UnkP

Chain UP: 41% 100%



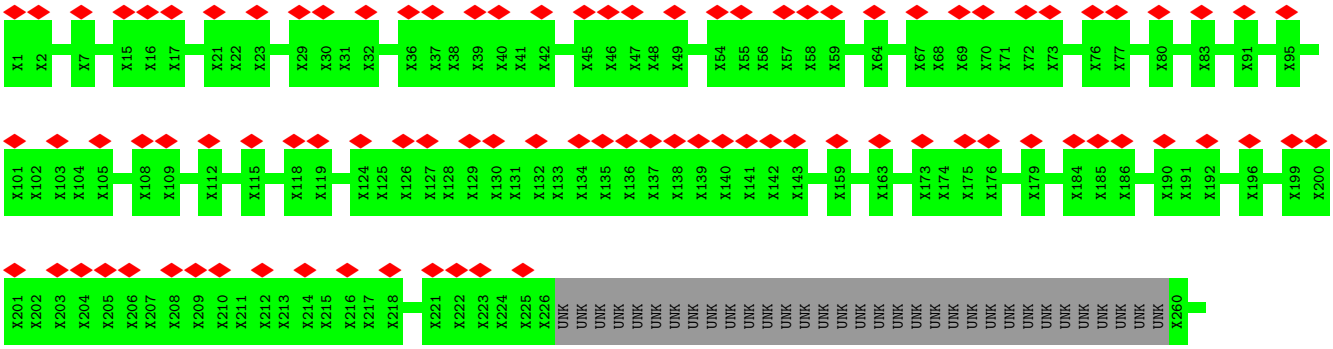

• Molecule 80: Unka

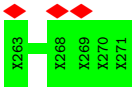
Chain Ua: 10% 100%




• Molecule 81: Unkg

Chain Ug: 35% 88% 12%


X1 X2 X7 X15 X16 X17 X21 X22 X23 X29 X30 X31 X32 X36 X37 X38 X39 X40 X41 X42 X45 X46 X47 X48 X49 X54 X55 X56 X57 X58 X59 X64 X67 X68 X69 X70 X71 X72 X73 X76 X77 X80 X83 X91 X95
X101 X102 X103 X104 X105 X108 X109 X112 X115 X118 X119 X124 X125 X126 X127 X128 X129 X130 X131 X132 X133 X134 X135 X136 X137 X138 X139 X140 X141 X142 X143 X159 X163 X173 X174 X175 X176 X179 X184 X185 X186 X190 X191 X192 X196 X199 X200
X201 X202 X203 X204 X205 X206 X207 X208 X209 X210 X211 X212 X213 X214 X215 X216 X217 X218 X221 X222 X223 X224 X225 X226
UNK UNK UNK


X263
X268
X269
X270
X271

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 38531 | 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 ($e^-/Å^2$) | 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 | 0.264 | Depositor |
| Minimum map value | -0.127 | 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 (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, FDA, GDP, PO4, PM8, ATP

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 | 0.19 | 1/11001 (0.0%) | 0.71 | 2/17084 (0.0%) |
| 2 | CB | 0.17 | 0/71 | 0.61 | 0/108 |
| 3 | CC | 0.26 | 0/666 | 0.43 | 0/900 |
| 4 | CE | 0.25 | 0/3100 | 0.51 | 0/4193 |
| 5 | CF | 0.25 | 0/1305 | 0.50 | 0/1761 |
| 6 | CH | 0.24 | 0/1839 | 0.51 | 0/2479 |
| 7 | CI | 0.24 | 0/3420 | 0.48 | 0/4619 |
| 8 | CJ | 0.25 | 0/6561 | 0.48 | 1/8927 (0.0%) |
| 9 | CK | 0.25 | 0/1468 | 0.53 | 0/1971 |
| 10 | CL | 0.30 | 0/726 | 0.51 | 0/981 |
| 11 | CN | 0.24 | 0/1361 | 0.48 | 0/1840 |
| 12 | CO | 0.25 | 0/3070 | 0.49 | 0/4145 |
| 13 | CP | 0.25 | 0/1533 | 0.49 | 0/2074 |
| 14 | CQ | 0.26 | 0/2072 | 0.50 | 0/2808 |
| 15 | CR | 0.25 | 0/1083 | 0.49 | 0/1467 |
| 16 | CS | 0.25 | 0/851 | 0.47 | 0/1150 |
| 17 | CU | 0.22 | 0/296 | 0.48 | 0/397 |
| 18 | Ca | 0.25 | 0/4378 | 0.47 | 0/5921 |
| 19 | Cb | 0.25 | 0/1273 | 0.48 | 0/1711 |
| 20 | Cd | 0.26 | 0/1818 | 0.45 | 0/2447 |
| 21 | Cg | 0.25 | 0/4064 | 0.45 | 0/5518 |
| 22 | Ci | 0.25 | 0/1388 | 0.48 | 0/1878 |
| 23 | Cj | 0.25 | 0/1842 | 0.48 | 0/2511 |
| 24 | Ck | 0.23 | 0/5469 | 0.48 | 0/7396 |
| 25 | Cm | 0.23 | 0/231 | 0.49 | 0/305 |
| 26 | Cn | 0.24 | 0/434 | 0.52 | 0/573 |
| 27 | Cp | 0.25 | 0/1472 | 0.49 | 0/1996 |
| 28 | DB | 0.24 | 0/9332 | 0.50 | 0/12641 |
| 29 | DC | 0.24 | 0/8971 | 0.47 | 0/12172 |
| 30 | DD | 0.26 | 0/6494 | 0.48 | 0/8808 |
| 31 | DE | 0.24 | 0/5246 | 0.48 | 0/7111 |
| 32 | DF | 0.24 | 0/4895 | 0.51 | 0/6635 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | DG | 0.25 | 0/4608 | 0.49 | 0/6242 |
| 34 | DH | 0.24 | 0/4716 | 0.49 | 0/6392 |
| 35 | DI | 0.25 | 0/3248 | 0.47 | 0/4401 |
| 36 | DJ | 0.25 | 0/2993 | 0.46 | 0/4063 |
| 37 | DK | 0.24 | 0/2132 | 0.46 | 0/2877 |
| 38 | DL | 0.25 | 0/1952 | 0.49 | 0/2629 |
| 39 | DO | 0.24 | 0/1597 | 0.50 | 0/2153 |
| 40 | DP | 0.24 | 0/1837 | 0.46 | 0/2488 |
| 41 | DR | 0.26 | 0/2099 | 0.50 | 0/2861 |
| 42 | DT | 0.25 | 0/2133 | 0.46 | 0/2889 |
| 43 | DU | 0.25 | 0/1772 | 0.49 | 0/2404 |
| 44 | DV | 0.25 | 0/1382 | 0.51 | 0/1871 |
| 45 | DW | 0.24 | 0/1202 | 0.47 | 0/1639 |
| 46 | DX | 0.24 | 0/1128 | 0.49 | 0/1516 |
| 47 | DY | 0.25 | 0/1337 | 0.51 | 0/1814 |
| 48 | DZ | 0.24 | 0/246 | 0.39 | 0/332 |
| 49 | Da | 0.24 | 0/332 | 0.52 | 0/441 |
| 50 | F2 | 0.25 | 0/7281 | 0.46 | 0/9837 |
| 51 | F3 | 0.24 | 0/7158 | 0.47 | 0/9686 |
| 52 | F5 | 0.24 | 0/5144 | 0.48 | 1/6918 (0.0%) |
| 53 | F6 | 0.24 | 0/4297 | 0.46 | 0/5841 |
| 54 | F7 | 0.25 | 0/5281 | 0.46 | 0/7149 |
| 55 | F9 | 0.25 | 0/4497 | 0.49 | 0/6031 |
| 56 | FM | 0.24 | 0/2497 | 0.47 | 0/3376 |
| 56 | FN | 0.24 | 0/2441 | 0.47 | 0/3299 |
| 57 | FO | 0.24 | 0/2763 | 0.52 | 0/3735 |
| 58 | FP | 0.25 | 0/2710 | 0.46 | 0/3709 |
| 59 | FW | 0.24 | 0/2002 | 0.52 | 0/2704 |
| 60 | FX | 0.25 | 0/1783 | 0.46 | 0/2410 |
| 61 | FZ | 0.23 | 0/1287 | 0.43 | 0/1737 |
| 62 | Fb | 0.25 | 0/1092 | 0.45 | 0/1471 |
| 63 | Fc | 0.24 | 0/670 | 0.44 | 0/912 |
| 64 | Fd | 0.23 | 0/759 | 0.48 | 0/1028 |
| 65 | Ff | 0.25 | 0/5149 | 0.48 | 0/7008 |
| 66 | Fg | 0.24 | 0/4129 | 0.47 | 0/5595 |
| 67 | Fh | 0.24 | 0/1902 | 0.48 | 0/2566 |
| 68 | Fi | 0.25 | 0/3899 | 0.50 | 0/5296 |
| 69 | IA | 0.26 | 0/5577 | 0.49 | 1/7550 (0.0%) |
| 70 | IB | 0.24 | 0/3944 | 0.55 | 5/5333 (0.1%) |
| 73 | UD | 0.25 | 0/64 | 0.42 | 0/88 |
| 75 | UG | 0.24 | 0/74 | 0.39 | 0/102 |
| All | All | 0.24 | 1/208844 (0.0%) | 0.50 | 10/284920 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | CA | 302 | U | C1'-N1 | 6.06 | 1.57 | 1.48 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 70 | IB | 429 | PRO | N-CA-CB | 6.89 | 111.57 | 103.30 |
| 70 | IB | 424 | PRO | N-CA-CB | 6.48 | 111.08 | 103.30 |
| 8 | CJ | 540 | PRO | N-CA-CB | 6.41 | 110.99 | 103.30 |
| 1 | CA | 70 | U | C2-N1-C1' | 6.38 | 125.35 | 117.70 |
| 69 | IA | 662 | PRO | N-CA-CB | 5.96 | 110.45 | 103.30 |

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 | |
|---|---|---|---|---|---|---|---|
| 3 | CC | 72/74 (97%) | 68 (94%) | 4 (6%) | 0 | 100 | 100 |
| 4 | CE | 369/435 (85%) | 357 (97%) | 12 (3%) | 0 | 100 | 100 |
| 5 | CF | 153/160 (96%) | 150 (98%) | 3 (2%) | 0 | 100 | 100 |
| 6 | CH | 213/282 (76%) | 208 (98%) | 5 (2%) | 0 | 100 | 100 |
| 7 | CI | 417/443 (94%) | 406 (97%) | 11 (3%) | 0 | 100 | 100 |
| 8 | CJ | 776/817 (95%) | 748 (96%) | 27 (4%) | 1 (0%) | 51 | 83 |
| 9 | CK | 173/326 (53%) | 170 (98%) | 3 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 10 | CL | 81/87 (93%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 11 | CN | 155/166 (93%) | 147 (95%) | 8 (5%) | 0 | 100 | 100 |
| 12 | CO | 358/429 (83%) | 341 (95%) | 17 (5%) | 0 | 100 | 100 |
| 13 | CP | 178/188 (95%) | 168 (94%) | 10 (6%) | 0 | 100 | 100 |
| 14 | CQ | 245/307 (80%) | 239 (98%) | 6 (2%) | 0 | 100 | 100 |
| 15 | CR | 118/320 (37%) | 110 (93%) | 8 (7%) | 0 | 100 | 100 |
| 16 | CS | 97/244 (40%) | 88 (91%) | 9 (9%) | 0 | 100 | 100 |
| 17 | CU | 31/193 (16%) | 30 (97%) | 1 (3%) | 0 | 100 | 100 |
| 18 | Ca | 497/602 (83%) | 486 (98%) | 11 (2%) | 0 | 100 | 100 |
| 19 | Cb | 145/325 (45%) | 141 (97%) | 4 (3%) | 0 | 100 | 100 |
| 20 | Cd | 203/440 (46%) | 199 (98%) | 4 (2%) | 0 | 100 | 100 |
| 21 | Cg | 485/498 (97%) | 472 (97%) | 13 (3%) | 0 | 100 | 100 |
| 22 | Ci | 163/181 (90%) | 157 (96%) | 6 (4%) | 0 | 100 | 100 |
| 23 | Cj | 224/257 (87%) | 220 (98%) | 4 (2%) | 0 | 100 | 100 |
| 24 | Ck | 667/874 (76%) | 650 (98%) | 17 (2%) | 0 | 100 | 100 |
| 25 | Cm | 29/215 (14%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 26 | Cn | 47/250 (19%) | 47 (100%) | 0 | 0 | 100 | 100 |
| 27 | Cp | 166/187 (89%) | 163 (98%) | 3 (2%) | 0 | 100 | 100 |
| 28 | DB | 1102/1181 (93%) | 1061 (96%) | 41 (4%) | 0 | 100 | 100 |
| 29 | DC | 1093/1165 (94%) | 1049 (96%) | 44 (4%) | 0 | 100 | 100 |
| 30 | DD | 760/812 (94%) | 733 (96%) | 27 (4%) | 0 | 100 | 100 |
| 31 | DE | 620/747 (83%) | 600 (97%) | 20 (3%) | 0 | 100 | 100 |
| 32 | DF | 592/666 (89%) | 567 (96%) | 25 (4%) | 0 | 100 | 100 |
| 33 | DG | 549/631 (87%) | 533 (97%) | 16 (3%) | 0 | 100 | 100 |
| 34 | DH | 566/581 (97%) | 549 (97%) | 17 (3%) | 0 | 100 | 100 |
| 35 | DI | 388/407 (95%) | 378 (97%) | 10 (3%) | 0 | 100 | 100 |
| 36 | DJ | 354/396 (89%) | 341 (96%) | 13 (4%) | 0 | 100 | 100 |
| 37 | DK | 258/324 (80%) | 247 (96%) | 11 (4%) | 0 | 100 | 100 |
| 38 | DL | 228/307 (74%) | 226 (99%) | 2 (1%) | 0 | 100 | 100 |
| 39 | DO | 192/282 (68%) | 188 (98%) | 4 (2%) | 0 | 100 | 100 |
| 40 | DP | 208/274 (76%) | 201 (97%) | 7 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 41 | DR | 248/270 (92%) | 239 (96%) | 9 (4%) | 0 | 100 | 100 |
| 42 | DT | 237/247 (96%) | 232 (98%) | 5 (2%) | 0 | 100 | 100 |
| 43 | DU | 215/228 (94%) | 209 (97%) | 6 (3%) | 0 | 100 | 100 |
| 44 | DV | 158/183 (86%) | 149 (94%) | 9 (6%) | 0 | 100 | 100 |
| 45 | DW | 134/179 (75%) | 132 (98%) | 2 (2%) | 0 | 100 | 100 |
| 46 | DX | 127/169 (75%) | 117 (92%) | 10 (8%) | 0 | 100 | 100 |
| 47 | DY | 152/163 (93%) | 144 (95%) | 8 (5%) | 0 | 100 | 100 |
| 48 | DZ | 26/94 (28%) | 24 (92%) | 2 (8%) | 0 | 100 | 100 |
| 49 | Da | 34/64 (53%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 50 | F2 | 882/1024 (86%) | 866 (98%) | 16 (2%) | 0 | 100 | 100 |
| 51 | F3 | 907/966 (94%) | 877 (97%) | 30 (3%) | 0 | 100 | 100 |
| 52 | F5 | 614/754 (81%) | 600 (98%) | 14 (2%) | 0 | 100 | 100 |
| 53 | F6 | 514/676 (76%) | 507 (99%) | 7 (1%) | 0 | 100 | 100 |
| 54 | F7 | 646/679 (95%) | 614 (95%) | 32 (5%) | 0 | 100 | 100 |
| 55 | F9 | 536/607 (88%) | 523 (98%) | 13 (2%) | 0 | 100 | 100 |
| 56 | FM | 325/370 (88%) | 316 (97%) | 9 (3%) | 0 | 100 | 100 |
| 56 | FN | 318/370 (86%) | 309 (97%) | 9 (3%) | 0 | 100 | 100 |
| 57 | FO | 324/334 (97%) | 312 (96%) | 12 (4%) | 0 | 100 | 100 |
| 58 | FP | 346/349 (99%) | 335 (97%) | 11 (3%) | 0 | 100 | 100 |
| 59 | FW | 234/263 (89%) | 229 (98%) | 5 (2%) | 0 | 100 | 100 |
| 60 | FX | 218/239 (91%) | 212 (97%) | 6 (3%) | 0 | 100 | 100 |
| 61 | FZ | 158/178 (89%) | 153 (97%) | 5 (3%) | 0 | 100 | 100 |
| 62 | Fb | 123/151 (82%) | 117 (95%) | 6 (5%) | 0 | 100 | 100 |
| 63 | Fc | 81/148 (55%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 64 | Fd | 91/143 (64%) | 89 (98%) | 2 (2%) | 0 | 100 | 100 |
| 65 | Ff | 619/848 (73%) | 587 (95%) | 32 (5%) | 0 | 100 | 100 |
| 66 | Fg | 514/550 (94%) | 493 (96%) | 21 (4%) | 0 | 100 | 100 |
| 67 | Fh | 233/318 (73%) | 226 (97%) | 7 (3%) | 0 | 100 | 100 |
| 68 | Fi | 465/629 (74%) | 447 (96%) | 18 (4%) | 0 | 100 | 100 |
| 69 | IA | 700/787 (89%) | 678 (97%) | 22 (3%) | 0 | 100 | 100 |
| 70 | IB | 487/803 (61%) | 466 (96%) | 19 (4%) | 2 (0%) | 34 | 71 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 73 | UD | 11/13 (85%) | 11 (100%) | 0 | 0 | 100 | 100 |
| 75 | UG | 13/15 (87%) | 10 (77%) | 3 (23%) | 0 | 100 | 100 |
| All | All | 23662/28884 (82%) | 22880 (97%) | 779 (3%) | 3 (0%) | 100 | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 70 | IB | 429 | PRO |
| 70 | IB | 783 | PRO |
| 8 | CJ | 540 | PRO |

### 5.3.2 Protein sidechains (i)

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 | |
|---|---|---|---|---|---|---|
| 3 | CC | 73/73 (100%) | 73 (100%) | 0 | 100 | 100 |
| 4 | CE | 314/372 (84%) | 306 (98%) | 8 (2%) | 47 | 75 |
| 5 | CF | 139/144 (96%) | 131 (94%) | 8 (6%) | 20 | 55 |
| 6 | CH | 192/246 (78%) | 190 (99%) | 2 (1%) | 76 | 88 |
| 7 | CI | 354/371 (95%) | 348 (98%) | 6 (2%) | 60 | 82 |
| 8 | CJ | 691/723 (96%) | 671 (97%) | 20 (3%) | 42 | 72 |
| 9 | CK | 150/283 (53%) | 146 (97%) | 4 (3%) | 44 | 73 |
| 10 | CL | 75/79 (95%) | 70 (93%) | 5 (7%) | 16 | 50 |
| 11 | CN | 142/150 (95%) | 142 (100%) | 0 | 100 | 100 |
| 12 | CO | 316/377 (84%) | 312 (99%) | 4 (1%) | 69 | 86 |
| 13 | CP | 160/168 (95%) | 158 (99%) | 2 (1%) | 69 | 86 |
| 14 | CQ | 216/270 (80%) | 208 (96%) | 8 (4%) | 34 | 66 |
| 15 | CR | 111/279 (40%) | 104 (94%) | 7 (6%) | 18 | 53 |
| 16 | CS | 90/220 (41%) | 89 (99%) | 1 (1%) | 73 | 88 |
| 17 | CU | 31/169 (18%) | 29 (94%) | 2 (6%) | 17 | 51 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 18 | Ca | 440/543 (81%) | 433 (98%) | 7 (2%) | 62 | 83 |
| 19 | Cb | 128/277 (46%) | 123 (96%) | 5 (4%) | 32 | 65 |
| 20 | Cd | 186/381 (49%) | 181 (97%) | 5 (3%) | 44 | 73 |
| 21 | Cg | 429/437 (98%) | 420 (98%) | 9 (2%) | 53 | 78 |
| 22 | Ci | 144/160 (90%) | 139 (96%) | 5 (4%) | 36 | 68 |
| 23 | Cj | 193/219 (88%) | 187 (97%) | 6 (3%) | 40 | 71 |
| 24 | Ck | 583/746 (78%) | 568 (97%) | 15 (3%) | 46 | 74 |
| 25 | Cm | 26/184 (14%) | 25 (96%) | 1 (4%) | 33 | 66 |
| 26 | Cn | 43/210 (20%) | 42 (98%) | 1 (2%) | 50 | 76 |
| 27 | Cp | 157/175 (90%) | 156 (99%) | 1 (1%) | 86 | 94 |
| 28 | DB | 972/1030 (94%) | 936 (96%) | 36 (4%) | 34 | 66 |
| 29 | DC | 929/985 (94%) | 907 (98%) | 22 (2%) | 49 | 75 |
| 30 | DD | 673/673 (100%) | 661 (98%) | 12 (2%) | 59 | 81 |
| 31 | DE | 552/642 (86%) | 536 (97%) | 16 (3%) | 42 | 72 |
| 32 | DF | 504/560 (90%) | 496 (98%) | 8 (2%) | 62 | 83 |
| 33 | DG | 483/543 (89%) | 470 (97%) | 13 (3%) | 44 | 73 |
| 34 | DH | 496/504 (98%) | 481 (97%) | 15 (3%) | 41 | 71 |
| 35 | DI | 350/365 (96%) | 344 (98%) | 6 (2%) | 60 | 82 |
| 36 | DJ | 312/347 (90%) | 304 (97%) | 8 (3%) | 46 | 74 |
| 37 | DK | 218/261 (84%) | 214 (98%) | 4 (2%) | 59 | 81 |
| 38 | DL | 199/263 (76%) | 193 (97%) | 6 (3%) | 41 | 71 |
| 39 | DO | 163/229 (71%) | 160 (98%) | 3 (2%) | 59 | 81 |
| 40 | DP | 189/239 (79%) | 187 (99%) | 2 (1%) | 73 | 88 |
| 41 | DR | 221/235 (94%) | 218 (99%) | 3 (1%) | 67 | 85 |
| 42 | DT | 220/228 (96%) | 214 (97%) | 6 (3%) | 44 | 73 |
| 43 | DU | 179/201 (89%) | 176 (98%) | 3 (2%) | 60 | 82 |
| 44 | DV | 145/165 (88%) | 141 (97%) | 4 (3%) | 43 | 72 |
| 45 | DW | 126/163 (77%) | 123 (98%) | 3 (2%) | 49 | 75 |
| 46 | DX | 114/149 (76%) | 111 (97%) | 3 (3%) | 46 | 74 |
| 47 | DY | 137/146 (94%) | 135 (98%) | 2 (2%) | 65 | 84 |
| 48 | DZ | 23/84 (27%) | 23 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 49 | Da | 32/59 (54%) | 31 (97%) | 1 (3%) | 40 | 71 |
| 50 | F2 | 752/867 (87%) | 745 (99%) | 7 (1%) | 78 | 90 |
| 51 | F3 | 767/809 (95%) | 750 (98%) | 17 (2%) | 52 | 77 |
| 52 | F5 | 533/642 (83%) | 517 (97%) | 16 (3%) | 41 | 71 |
| 53 | F6 | 462/590 (78%) | 446 (96%) | 16 (4%) | 36 | 68 |
| 54 | F7 | 553/577 (96%) | 546 (99%) | 7 (1%) | 69 | 86 |
| 55 | F9 | 449/503 (89%) | 439 (98%) | 10 (2%) | 52 | 77 |
| 56 | FM | 258/292 (88%) | 249 (96%) | 9 (4%) | 36 | 68 |
| 56 | FN | 252/292 (86%) | 248 (98%) | 4 (2%) | 62 | 83 |
| 57 | FO | 285/290 (98%) | 278 (98%) | 7 (2%) | 47 | 75 |
| 58 | FP | 270/286 (94%) | 266 (98%) | 4 (2%) | 65 | 84 |
| 59 | FW | 214/234 (92%) | 213 (100%) | 1 (0%) | 88 | 95 |
| 60 | FX | 178/195 (91%) | 177 (99%) | 1 (1%) | 86 | 94 |
| 61 | FZ | 140/156 (90%) | 133 (95%) | 7 (5%) | 24 | 59 |
| 62 | Fb | 113/135 (84%) | 111 (98%) | 2 (2%) | 59 | 81 |
| 63 | Fc | 77/127 (61%) | 74 (96%) | 3 (4%) | 32 | 65 |
| 64 | Fd | 77/119 (65%) | 75 (97%) | 2 (3%) | 46 | 74 |
| 65 | Ff | 524/715 (73%) | 509 (97%) | 15 (3%) | 42 | 72 |
| 66 | Fg | 446/469 (95%) | 439 (98%) | 7 (2%) | 62 | 83 |
| 67 | Fh | 189/281 (67%) | 181 (96%) | 8 (4%) | 30 | 63 |
| 68 | Fi | 413/536 (77%) | 403 (98%) | 10 (2%) | 49 | 75 |
| 69 | IA | 590/661 (89%) | 566 (96%) | 24 (4%) | 30 | 64 |
| 70 | IB | 393/675 (58%) | 386 (98%) | 7 (2%) | 59 | 81 |
| All | All | 20555/24778 (83%) | 20063 (98%) | 492 (2%) | 51 | 75 |

5 of 492 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | DG | 186 | ARG |
| 67 | Fh | 58 | ARG |
| 42 | DT | 52 | ARG |
| 66 | Fg | 33 | CYS |
| 69 | IA | 460 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 421 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DP | 116 | HIS |
| 51 | F3 | 432 | GLN |
| 69 | IA | 40 | GLN |
| 41 | DR | 62 | HIS |
| 46 | DX | 130 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | CA | 494/621 (79%) | 188 (38%) | 5 (1%) |
| 2 | CB | 2/3 (66%) | 2 (100%) | 0 |
| All | All | 496/624 (79%) | 190 (38%) | 5 (1%) |

5 of 190 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CA | 3 | A |
| 1 | CA | 5 | U |
| 1 | CA | 6 | U |
| 1 | CA | 7 | A |
| 1 | CA | 8 | U |

All (5) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | CA | 151 | U |
| 1 | CA | 169 | A |
| 1 | CA | 349 | U |
| 1 | CA | 465 | U |
| 1 | CA | 566 | U |

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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 | $\#\|Z\| > 2$ |
| 85 | PM8 | Fc | 201 | 63 | 25,31,31 | 0.20 | 0 | 30,38,38 | 0.46 | 0 |
| 88 | GDP | IA | 1000 | 82 | 24,30,30 | 1.17 | 2 (8%) | 31,47,47 | 2.01 | 8 (25%) |
| 83 | ATP | Cg | 1000 | 82 | 26,33,33 | 0.60 | 0 | 31,52,52 | 0.76 | 1 (3%) |
| 84 | PO4 | IA | 1001 | 82 | 4,4,4 | 0.94 | 0 | 6,6,6 | 0.46 | 0 |
| 87 | FDA | Ff | 901 | - | 51,58,58 | 1.21 | 6 (11%) | 60,89,89 | 2.23 | 8 (13%) |
| 84 | PO4 | FW | 301 | - | 4,4,4 | 0.97 | 0 | 6,6,6 | 0.41 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 87 | FDA | Ff | 901 | - | - | 12/30/50/50 | 0/6/6/6 |
| 83 | ATP | Cg | 1000 | 82 | - | 2/18/38/38 | 0/3/3/3 |
| 85 | PM8 | Fc | 201 | 63 | - | 7/36/38/38 | - |
| 88 | GDP | IA | 1000 | 82 | - | 0/12/32/32 | 0/3/3/3 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 87 | Ff | 901 | FDA | C4X-C10 | 5.55 | 1.44 | 1.38 |
| 88 | IA | 1000 | GDP | C5-C6 | 4.14 | 1.48 | 1.41 |
| 87 | Ff | 901 | FDA | C4-N3 | 2.98 | 1.38 | 1.33 |
| 88 | IA | 1000 | GDP | C5-C4 | 2.44 | 1.47 | 1.40 |
| 87 | Ff | 901 | FDA | C4X-C4 | 2.27 | 1.45 | 1.41 |

The worst 5 of 17 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 87 | Ff | 901 | FDA | C2-N3-C4 | 13.00 | 126.12 | 115.14 |
| 87 | Ff | 901 | FDA | C4X-C4-N3 | -6.99 | 113.87 | 123.43 |
| 88 | IA | 1000 | GDP | C2-N3-C4 | 4.95 | 121.01 | 115.36 |
| 87 | Ff | 901 | FDA | C10-C4X-N5 | 4.72 | 124.52 | 121.26 |
| 88 | IA | 1000 | GDP | C2-N1-C6 | 3.99 | 122.27 | 115.93 |

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

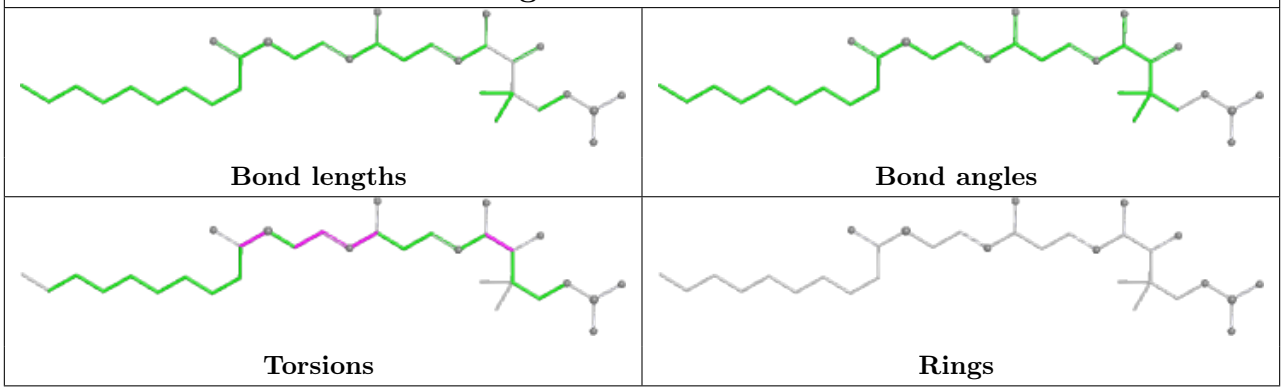
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 83 | Cg | 1000 | ATP | O4'-C4'-C5'-O5' |
| 85 | Fc | 201 | PM8 | O1-C1-S1-C43 |
| 85 | Fc | 201 | PM8 | C2-C1-S1-C43 |
| 87 | Ff | 901 | FDA | C5B-O5B-PA-O1A |
| 87 | Ff | 901 | FDA | C5B-O5B-PA-O2A |

There are no ring outliers.

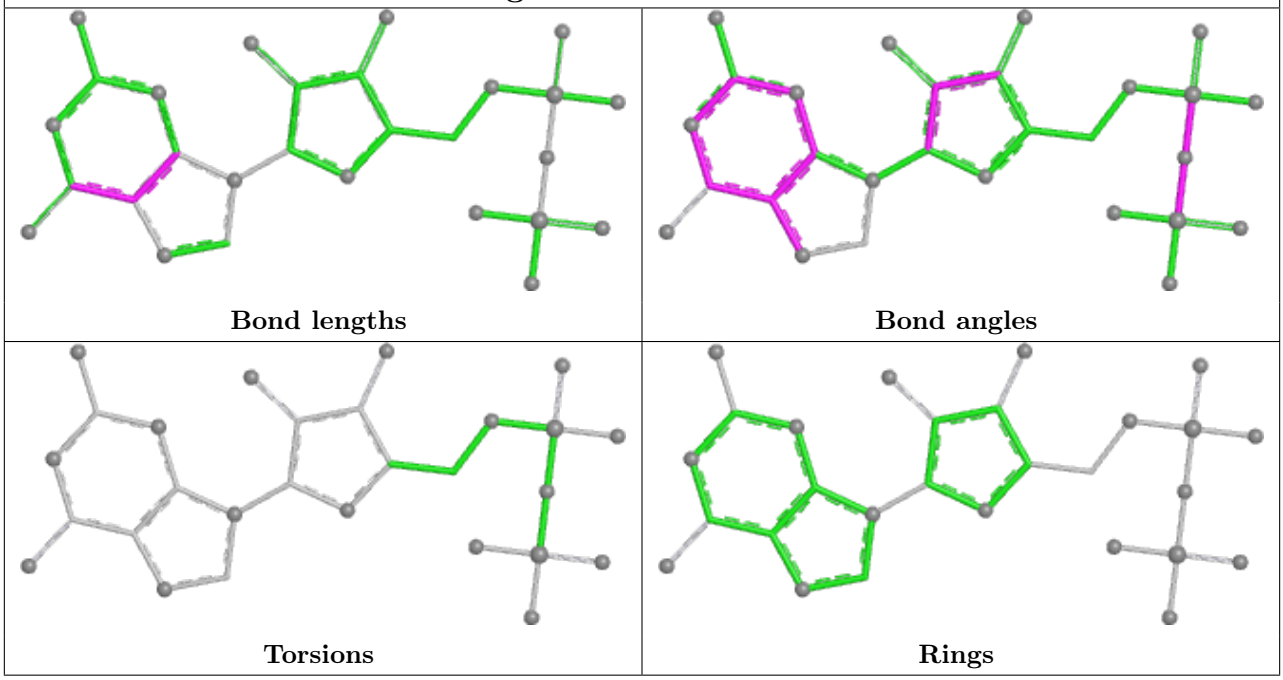
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

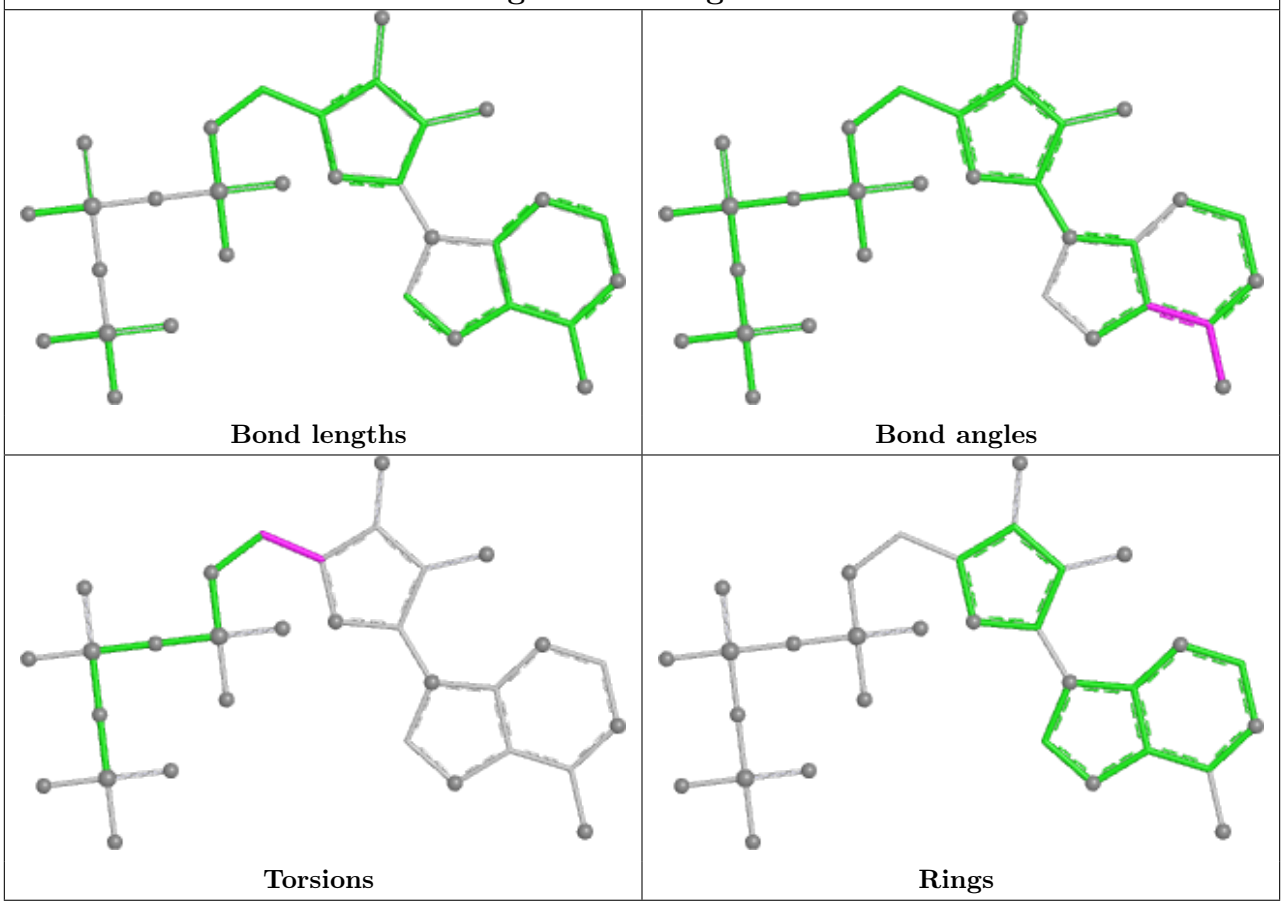
**Ligand PM8 Fc 201**

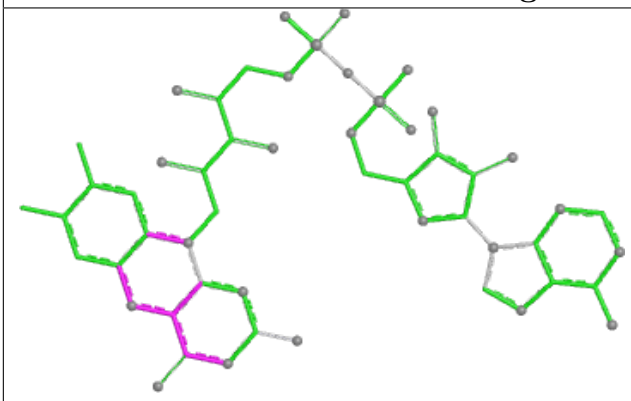
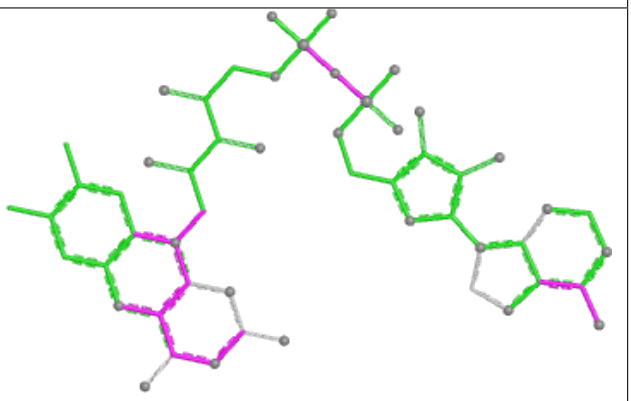
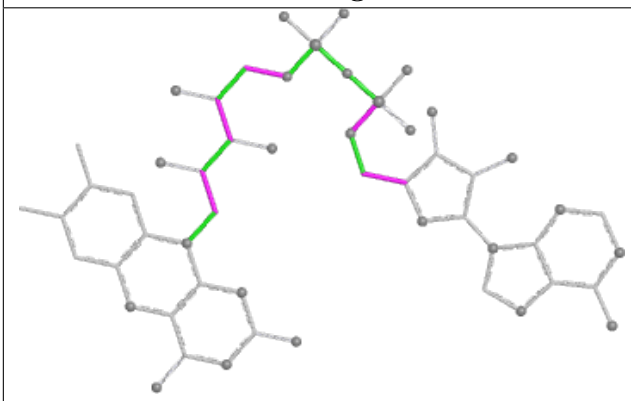
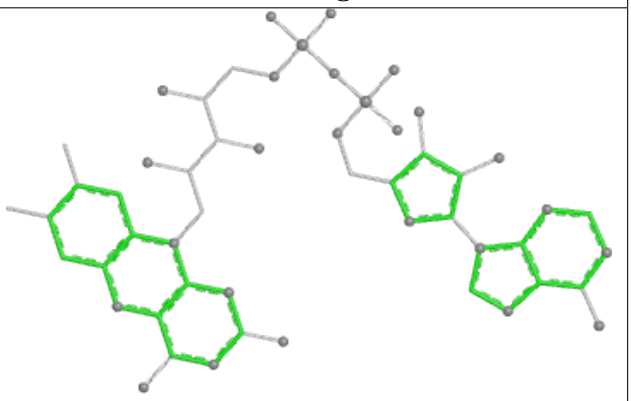


## Ligand GDP IA 1000




## Ligand ATP Cg 1000



| Ligand FDA Ff 901 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

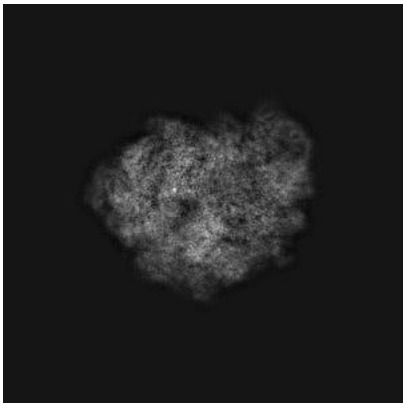
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13660. These allow visual inspection of the internal detail of the map and identification of artifacts.

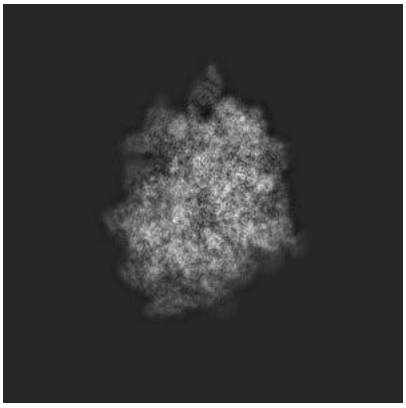
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

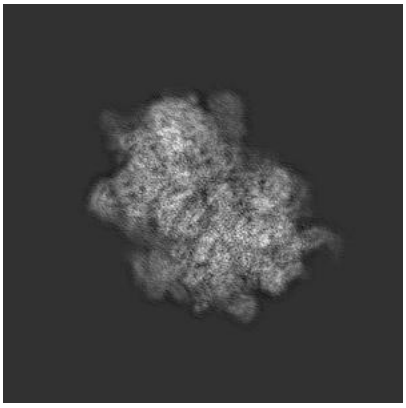
### 6.1.1 Primary map



X



Y

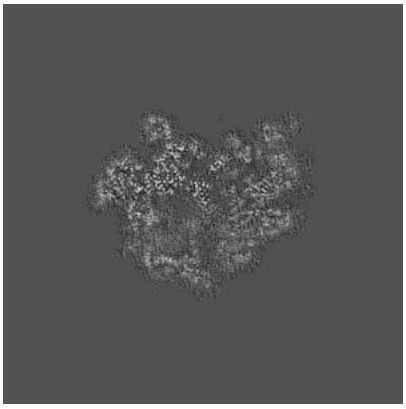


Z

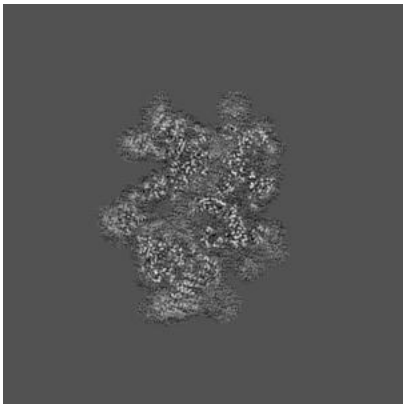
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

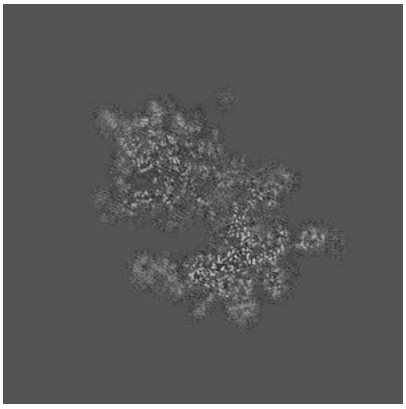
### 6.2.1 Primary map



X Index: 180



Y Index: 180

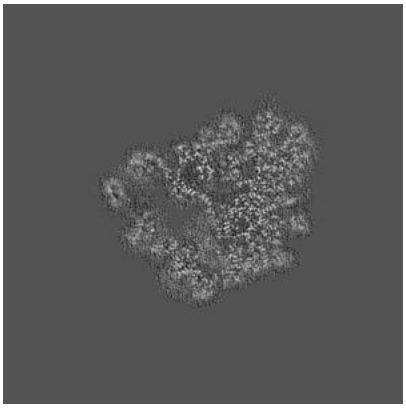


Z Index: 180

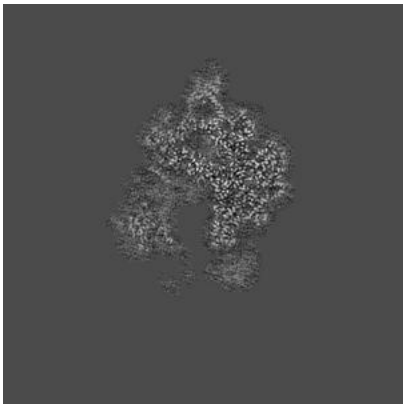
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

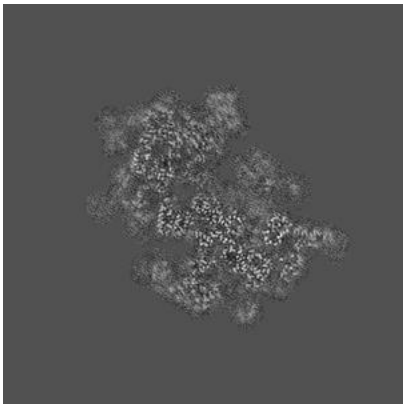
### 6.3.1 Primary map



X Index: 157



Y Index: 154

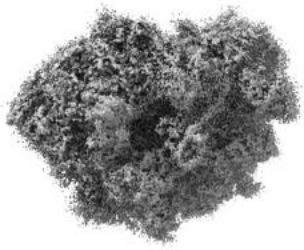


Z Index: 192

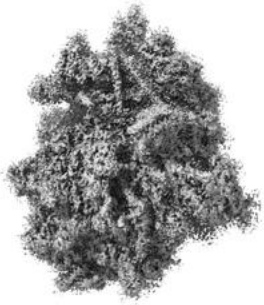
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

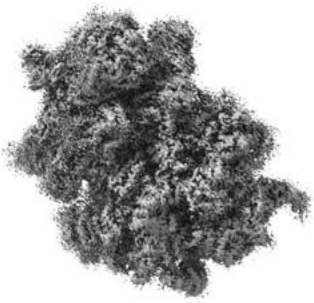
### 6.4.1 Primary map



X



Y



Z

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.

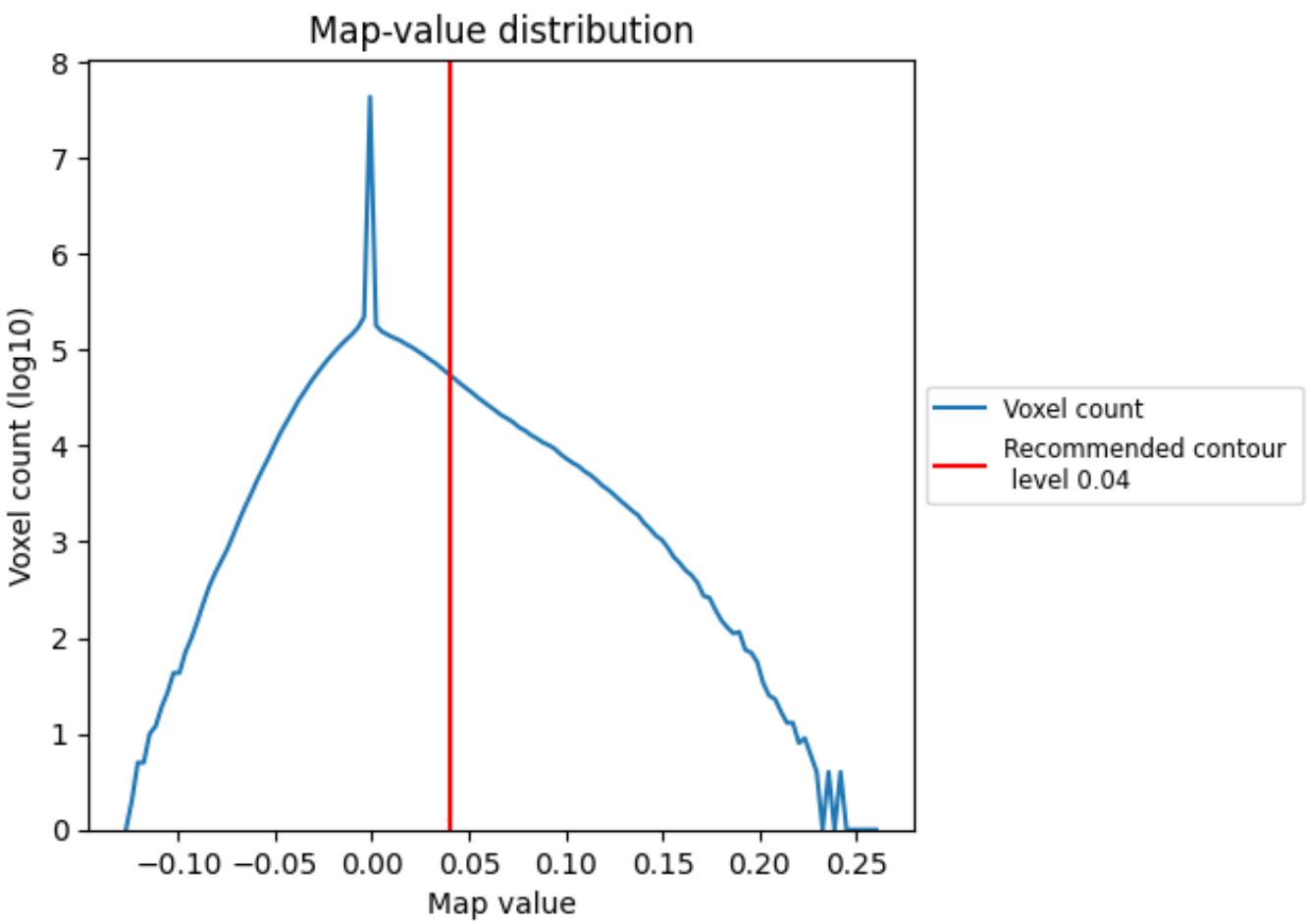
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

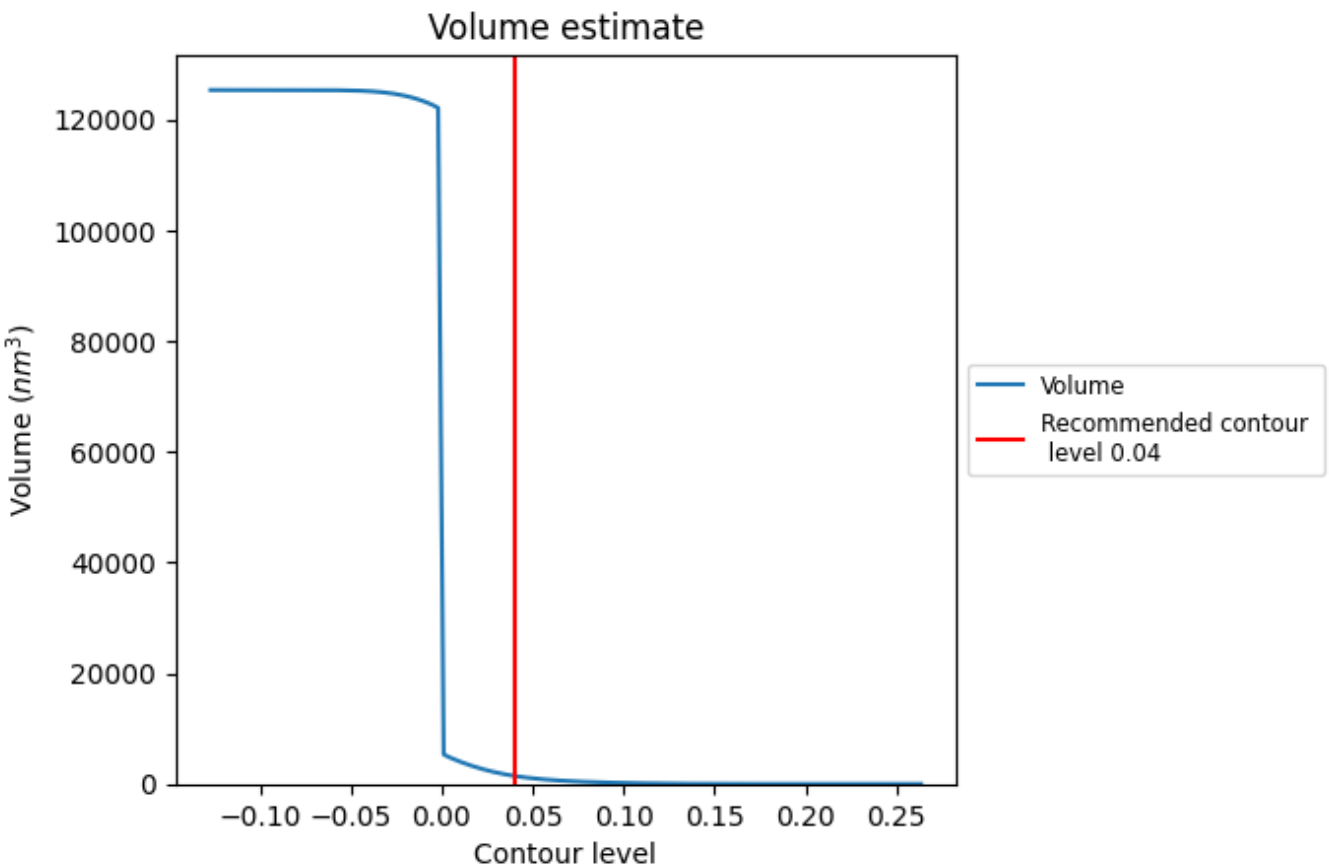
This section contains the results of statistical analysis of the map.

## 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.

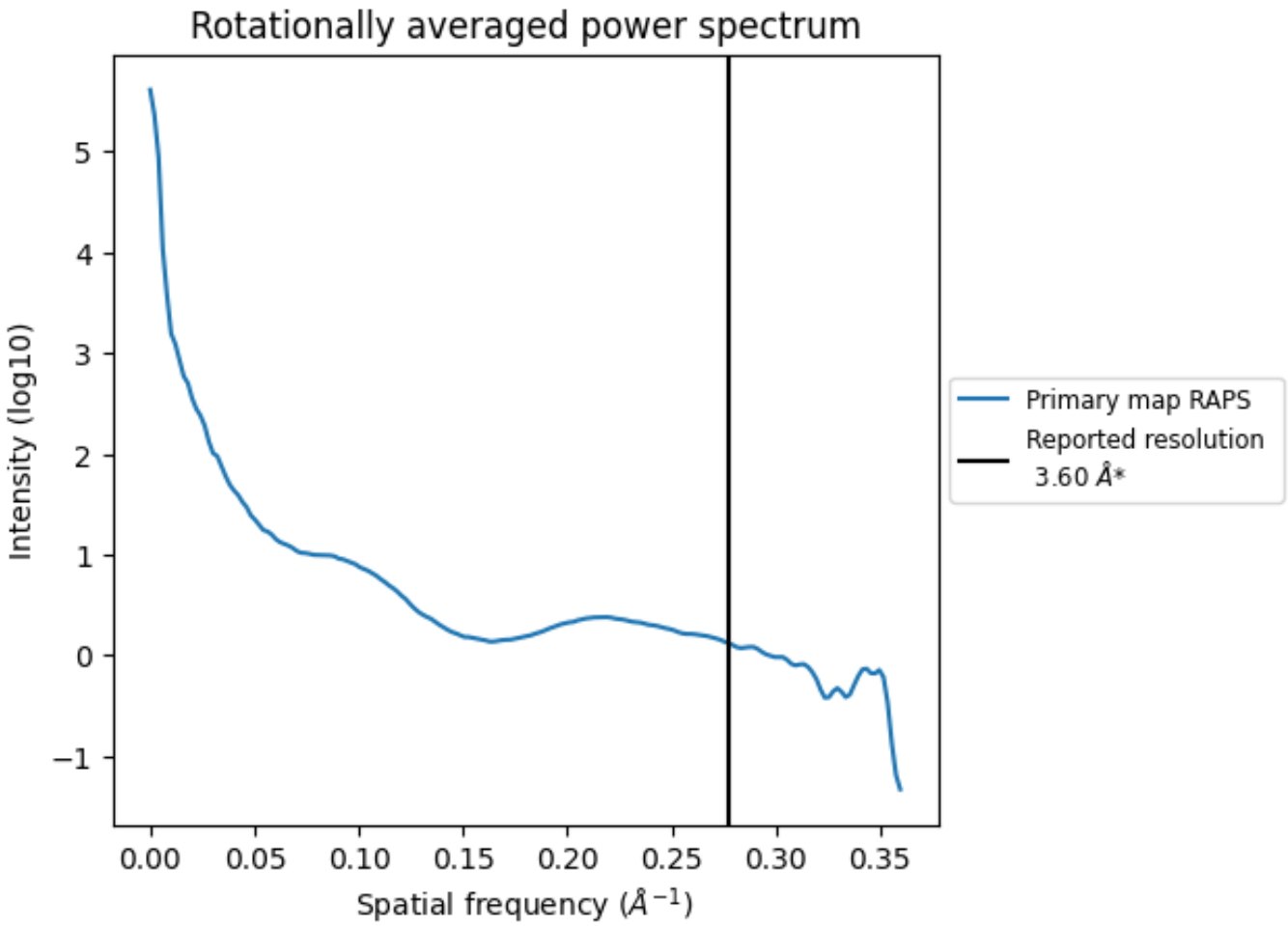
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 1447 $nm^3$; this corresponds to an approximate mass of 1307 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 (i)




*Reported resolution corresponds to spatial frequency of 0.278 Å$^{-1}$

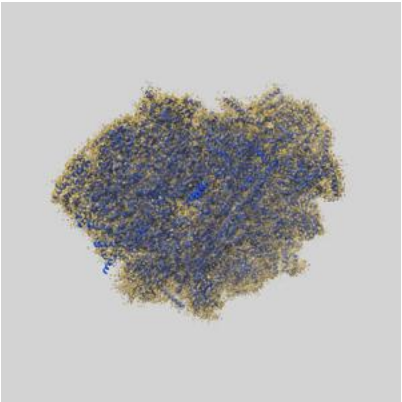
# 8 Fourier-Shell correlation (i)

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

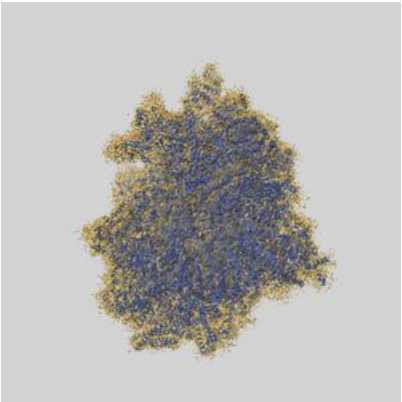
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13660 and PDB model 7PUA. Per-residue inclusion information can be found in section 3 on page 28.

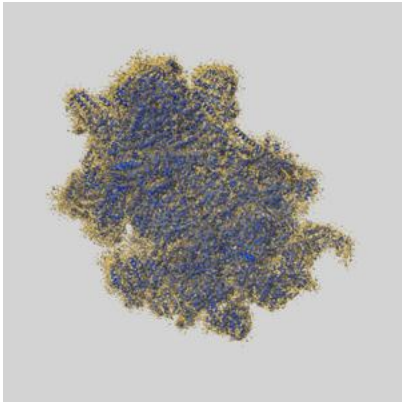
## 9.1 Map-model overlay (i)



X



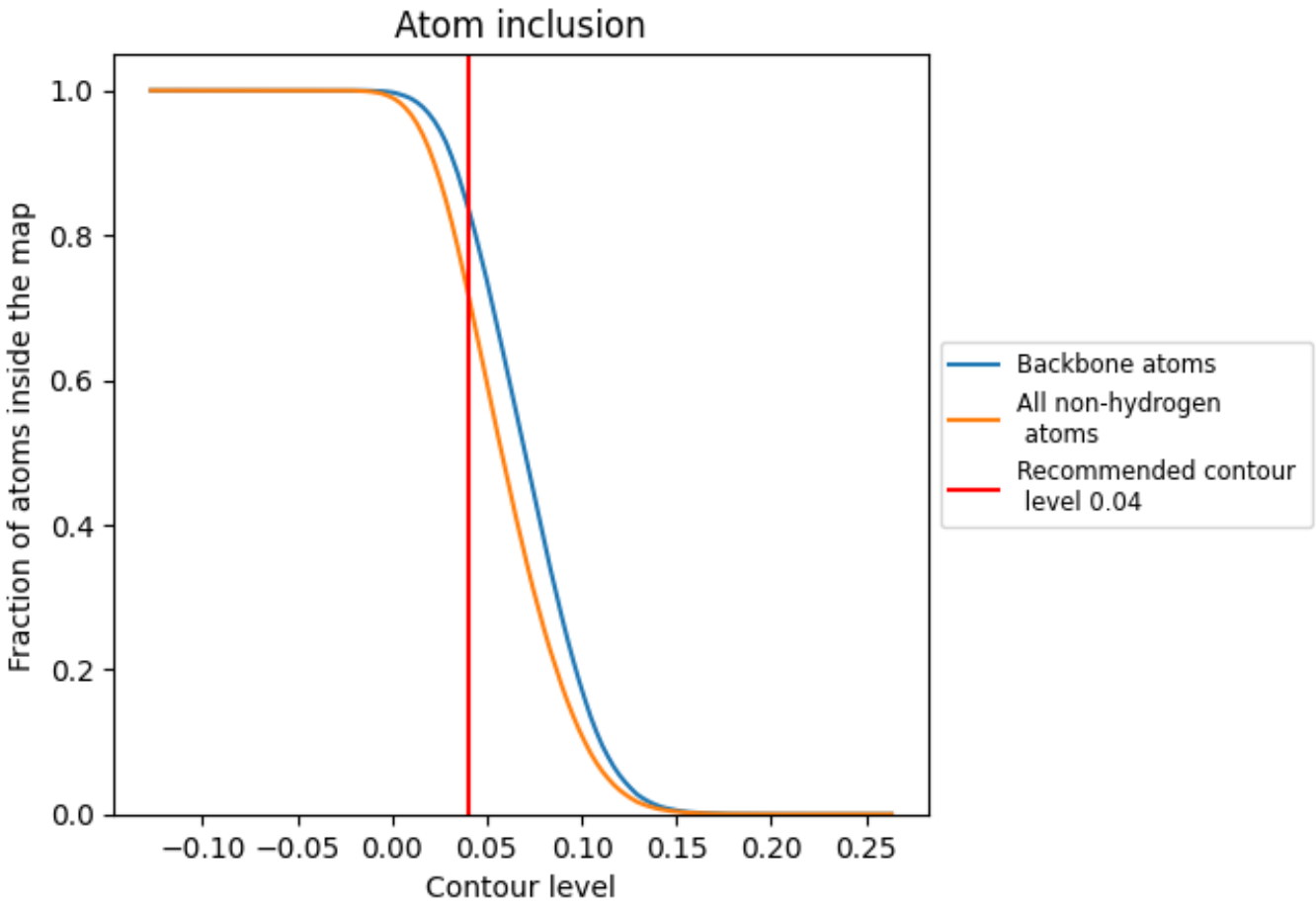
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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 Atom inclusion (i)




At the recommended contour level, 84% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.