



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 08:41 AM JST

PDB ID : 5YZG
EMDB ID : EMD-6864
Title : The Cryo-EM Structure of Human Catalytic Step I Spliceosome (C complex)
at 4.1 angstrom resolution
Authors : Zhan, X.; Yan, C.; Zhang, X.; Lei, J.; Shi, Y.
Deposited on : 2017-12-14
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

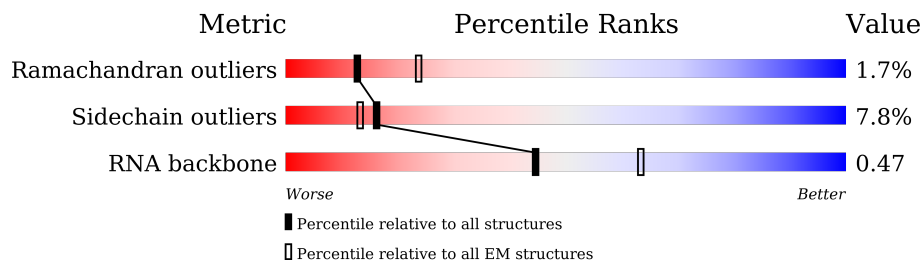
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-----------------------|
| 1 | A | 2335 | 6% 87% 9% . . |
| 2 | B | 117 | 8% 52% 16% . 28% |
| 3 | C | 972 | 79% 9% . 11% |
| 4 | D | 2136 | 74% 89% 11% |
| 5 | E | 357 | 78% 5% 16% |
| 6 | F | 107 | 7% 46% 43% . 9% |
| 7 | G | 275 | 9% 23% 68% |
| 8 | H | 188 | 17% 29% 41% . 26% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9 | I | 855 | 12% 63% 35% |
| 10 | J | 848 | 17% 63% 33% |
| 11 | K | 225 | 14% 57% 10% 32% |
| 12 | L | 802 | 9% 45% 7% 48% |
| 13 | y | 307 | 7% 32% 64% |
| 14 | M | 243 | 5% 26% 11% 63% |
| 15 | N | 144 | 92% 7% |
| 16 | O | 420 | 64% 33% |
| 17 | P | 229 | 35% 7% 58% |
| 18 | R | 536 | 32% 13% 54% |
| 19 | S | 166 | 87% 8% |
| 20 | T | 514 | 55% 5% 39% |
| 21 | Q | 1485 | 38% 89% 11% |
| 22 | U | 2752 | 99% |
| 23 | V | 908 | 8% 47% 50% |
| 24 | W | 579 | 14% 66% 9% 24% |
| 25 | X | 425 | 13% 83% |
| 26 | Y | 323 | 5% 49% 11% 37% |
| 27 | Z | 1227 | 14% 47% 48% |
| 28 | q | 504 | 14% 23% 74% |
| 28 | r | 504 | 6% 23% 74% |
| 28 | s | 504 | 36% 74% 26% |
| 28 | t | 504 | 5% 12% 87% |
| 29 | u | 411 | 44% 93% 5% |
| 30 | v | 148 | 83% 97% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 31 | w | 174 | |
| 32 | x | 703 | |
| 33 | a | 126 | |
| 33 | h | 126 | |
| 34 | b | 229 | |
| 34 | i | 229 | |
| 35 | c | 119 | |
| 35 | j | 119 | |
| 36 | d | 118 | |
| 36 | k | 118 | |
| 37 | f | 86 | |
| 37 | m | 86 | |
| 38 | e | 92 | |
| 38 | l | 92 | |
| 39 | g | 76 | |
| 39 | n | 76 | |
| 40 | o | 255 | |
| 41 | p | 225 | |
| 42 | 1 | 301 | |
| 43 | 2 | 646 | |
| 44 | 3 | 754 | |
| 45 | 4 | 37 | |

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 103906 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pre-mRNA-processing-splicing factor 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | A | 2253 | 17519 | 11136 | 3147 | 3166 | 70 | 0 | 0 |

- Molecule 2 is a RNA chain called U5 snRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | P | | |
| 2 | B | 84 | 1768 | 792 | 295 | 597 | 84 | 0 | 0 |

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | C | 862 | 6795 | 4344 | 1138 | 1281 | 32 | 0 | 0 |

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| | | | Total | C | N | O | | |
| 4 | D | 1908 | 7632 | 3816 | 1908 | 1908 | 0 | 0 |

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | E | 299 | 2338 | 1470 | 410 | 445 | 13 | 0 | 0 |

- Molecule 6 is a RNA chain called U6 snRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | P | | |
| 6 | F | 97 | 2075 | 928 | 381 | 669 | 97 | 0 | 0 |

- Molecule 7 is a RNA chain called Pre-mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7 | G | 88 | Total | C | N | O | P | 0 | 0 |
| | | | 1641 | 727 | 238 | 589 | 87 | | |

- Molecule 8 is a RNA chain called U2 snRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 8 | H | 139 | Total | C | N | O | P | 0 | 0 |
| | | | 2946 | 1317 | 507 | 983 | 139 | | |

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 9 | I | 559 | Total | C | N | O | 0 | 0 |
| | | | 2757 | 1639 | 559 | 559 | | |

- Molecule 10 is a protein called Crooked neck-like protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10 | J | 571 | Total | C | N | O | S | 0 | 0 |
| | | | 3829 | 2385 | 720 | 718 | 6 | | |

- Molecule 11 is a protein called Pre-mRNA-splicing factor SPF27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | K | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 611 | 177 | 189 | 2 | | |

- Molecule 12 is a protein called Cell division cycle 5-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12 | L | 419 | Total | C | N | O | S | 0 | 0 |
| | | | 2885 | 1809 | 534 | 537 | 5 | | |

- Molecule 13 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | y | 112 | Total | C | N | O | S | 0 | 0 |
| | | | 704 | 440 | 130 | 133 | 1 | | |

- Molecule 14 is a protein called Pre-mRNA-splicing factor SYF2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | M | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 775 | 482 | 146 | 145 | 2 | | |

- Molecule 15 is a protein called Protein BUD31 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 15 | N | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1184 | 746 | 217 | 209 | 12 | | |

- Molecule 16 is a protein called Pre-mRNA-splicing factor RBM22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16 | O | 283 | Total | C | N | O | S | 0 | 0 |
| | | | 2277 | 1430 | 403 | 424 | 20 | | |

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | P | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 829 | 508 | 162 | 157 | 2 | | |

- Molecule 18 is a protein called SNW domain-containing protein 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|-------|
| 18 | R | 245 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1962 | 1231 | 353 | 364 | 2 | 12 | | |

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | S | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1236 | 787 | 215 | 227 | 7 | | |

- Molecule 20 is a protein called Pleiotropic regulator 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20 | T | 313 | Total | C | N | O | S | 0 | 0 |
| | | | 2461 | 1554 | 447 | 452 | 8 | | |

- Molecule 21 is a protein called Intron-binding protein aquarius.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| 21 | Q | 1322 | Total | C | N | O | 0 | 0 |
| | | | 5288 | 2644 | 1322 | 1322 | | |

- Molecule 22 is a protein called Serine/arginine repetitive matrix protein 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22 | U | 26 | Total | C | N | O | S | 0 | 0 |
| | | | 193 | 120 | 36 | 36 | 1 | | |

- Molecule 23 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23 | V | 452 | Total | C | N | O | S | 0 | 0 |
| | | | 3410 | 2194 | 590 | 611 | 15 | | |

- Molecule 24 is a protein called Pre-mRNA-processing factor 17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 24 | W | 440 | Total | C | N | O | S | 0 | 0 |
| | | | 2310 | 1296 | 487 | 523 | 4 | | |

- Molecule 25 is a protein called Pre-mRNA-splicing factor CWC25 homolog.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 25 | X | 71 | Total | C | N | O | 0 | 0 |
| | | | 480 | 297 | 95 | 88 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| X | 145 | GLN | LYS | conflict | UNP Q9NXE8 |
| X | 149 | PRO | LYS | conflict | UNP Q9NXE8 |

- Molecule 26 is a protein called Coiled-coil domain-containing protein 94.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | Y | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1426 | 898 | 259 | 261 | 8 | | |

- Molecule 27 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 27 | Z | 635 | Total | C | N | O | 0 | 0 |
| | | | 2540 | 1270 | 635 | 635 | | |

- Molecule 28 is a protein called Pre-mRNA-processing factor 19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | q | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 918 | 581 | 156 | 178 | 3 | | |
| 28 | r | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 901 | 572 | 149 | 177 | 3 | | |
| 28 | s | 374 | Total | C | N | O | | 1 | 0 |
| | | | 1497 | 749 | 374 | 374 | | | |
| 28 | t | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 476 | 300 | 83 | 92 | 1 | | |

- Molecule 29 is a protein called Eukaryotic initiation factor 4A-III.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29 | u | 390 | Total | C | N | O | S | 0 | 0 |
| | | | 3126 | 1974 | 545 | 588 | 19 | | |

- Molecule 30 is a protein called Protein mago nashi homolog 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | v | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1196 | 772 | 200 | 221 | 3 | | |

- Molecule 31 is a protein called RNA-binding protein 8A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | w | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 730 | 463 | 122 | 142 | 3 | | |

- Molecule 32 is a protein called Protein CASC3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 32 | x | 25 | Total | C | N | O | 0 | 0 |
| | | | 216 | 136 | 39 | 41 | | |

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | h | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 621 | 388 | 110 | 117 | 6 | | |
| 33 | a | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 609 | 381 | 108 | 115 | 5 | | |

- Molecule 34 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | i | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 690 | 434 | 126 | 123 | 7 | | |
| 34 | b | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 426 | 123 | 119 | 7 | | |

- Molecule 35 is a protein called Small nuclear ribonucleoprotein Sm D1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | j | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 649 | 413 | 113 | 119 | 4 | | |
| 35 | c | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 641 | 409 | 112 | 116 | 4 | | |

- Molecule 36 is a protein called Small nuclear ribonucleoprotein Sm D2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | k | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 688 | 432 | 125 | 126 | 5 | | |
| 36 | d | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 768 | 482 | 141 | 140 | 5 | | |

- Molecule 37 is a protein called Small nuclear ribonucleoprotein F.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 37 | m | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 576 | 373 | 95 | 103 | 5 | | |
| 37 | f | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 576 | 373 | 95 | 103 | 5 | | |

- Molecule 38 is a protein called Small nuclear ribonucleoprotein E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | l | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 652 | 412 | 116 | 119 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | e | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 652 | 412 | 116 | 119 | 5 | | |

- Molecule 39 is a protein called Small nuclear ribonucleoprotein G.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | n | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 533 | 339 | 95 | 93 | 6 | | |
| 39 | g | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 569 | 358 | 102 | 103 | 6 | | |

- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein A'.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | o | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1277 | 817 | 219 | 238 | 3 | | |

- Molecule 41 is a protein called U2 small nuclear ribonucleoprotein B'.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | p | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 760 | 488 | 135 | 132 | 5 | | |

- Molecule 42 is a protein called Peptidyl-prolyl cis-trans isomerase E.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 42 | 1 | 243 | Total | C | N | O | 0 | 0 |
| | | | 972 | 486 | 243 | 243 | | |

- Molecule 43 is a protein called Peptidylprolyl isomerase domain and WD repeat-containing protein 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 43 | 2 | 416 | Total | C | N | O | 0 | 0 |
| | | | 1664 | 832 | 416 | 416 | | |

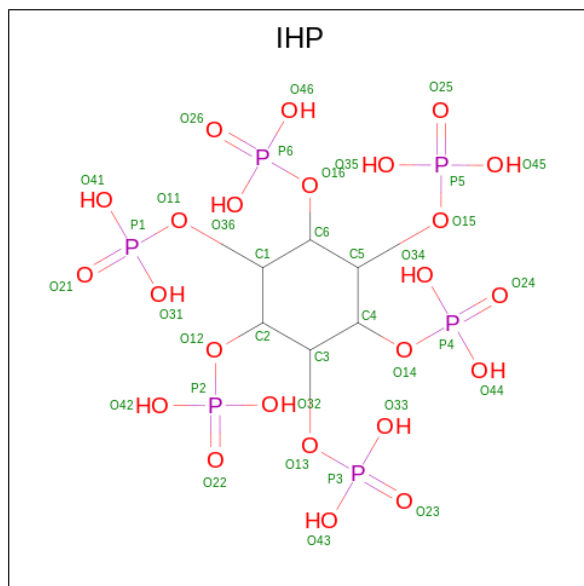
- Molecule 44 is a protein called Peptidyl-prolyl cis-trans isomerase G.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 44 | 3 | 171 | Total | C | N | O | 0 | 0 |
| | | | 684 | 342 | 171 | 171 | | |

- Molecule 45 is a protein called UNKNOWN.

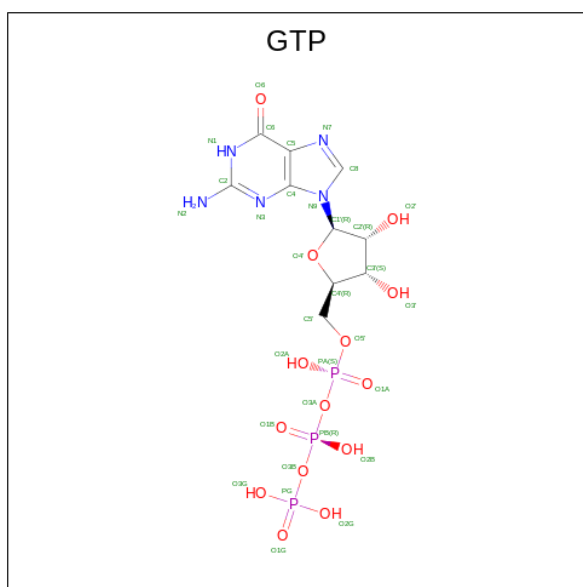
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 45 | 4 | 37 | 184 | 110 | 37 | 37 | 0 | 0 |

- Molecule 46 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---------|
| | | | Total | C | O | P | |
| 46 | A | 1 | 36 | 6 | 24 | 6 | 0 |

- Molecule 47 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

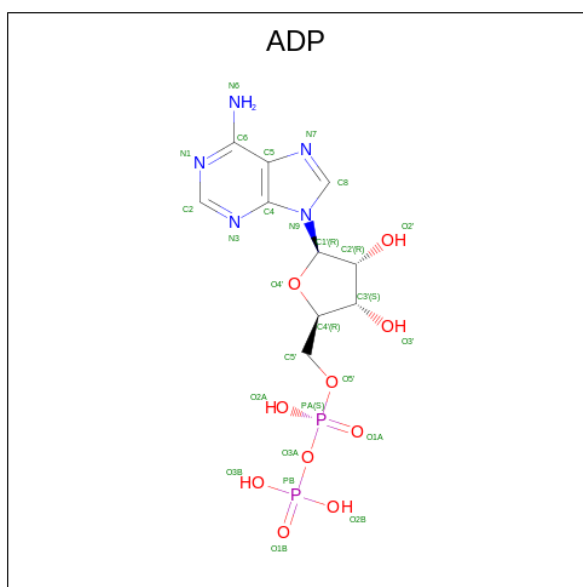


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 47 | C | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Mg | |
| 48 | C | 1 | 1 | 1 | 0 |
| 48 | F | 5 | 5 | 5 | 0 |
| 48 | u | 1 | 1 | 1 | 0 |

- Molecule 49 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

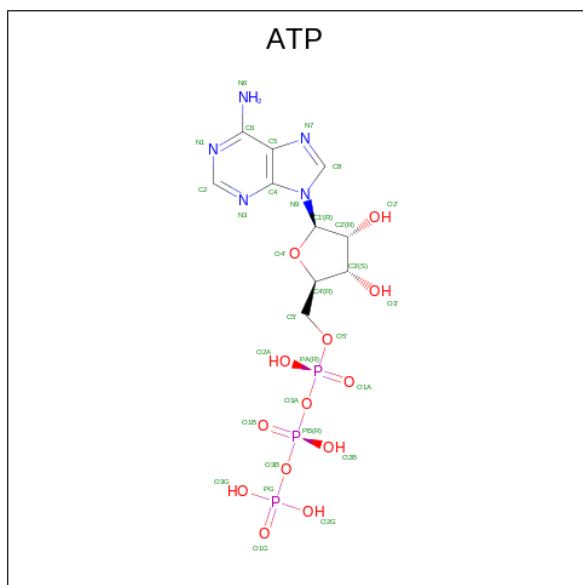


| Mol | Chain | Residues | Atoms | | | | AltConf | |
|-----|-------|----------|-------|----|----|----|---------|---|
| 49 | D | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 20 | 10 | 20 | 4 | |
| 49 | D | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 20 | 10 | 20 | 4 | |

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 50 | N | 3 | Total | Zn | 0 |
| | | | 3 | 3 | |
| 50 | O | 3 | Total | Zn | 0 |
| | | | 3 | 3 | |
| 50 | Y | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 51 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

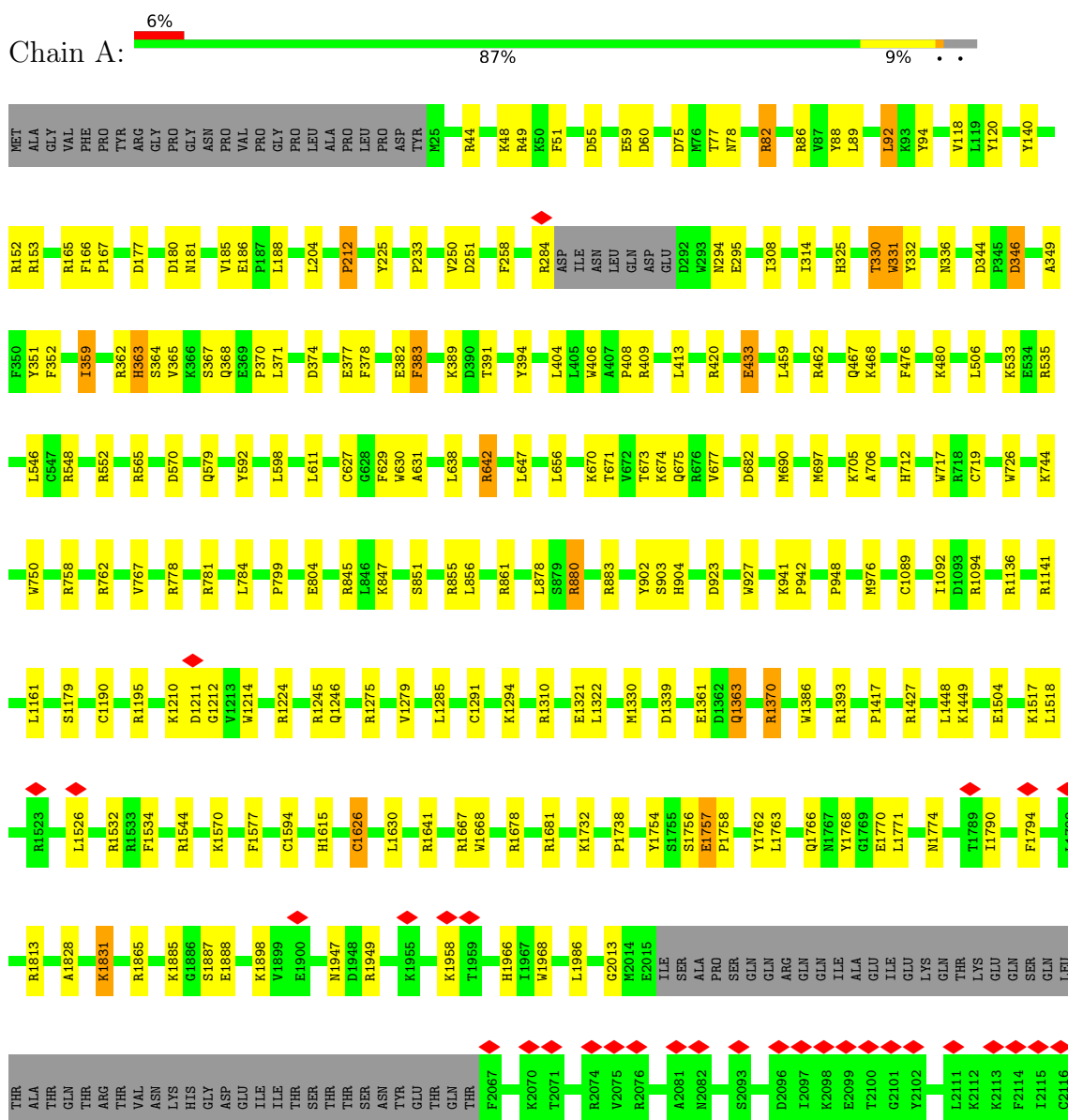


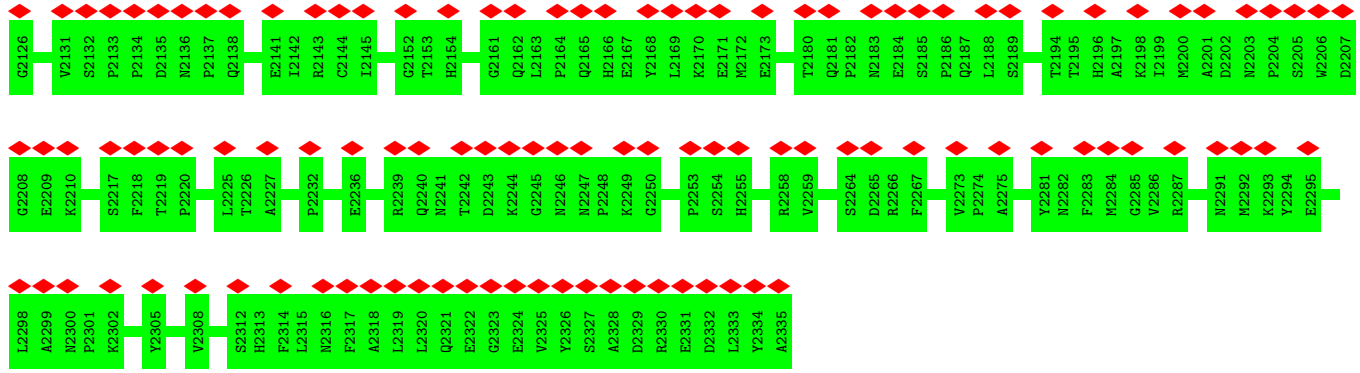
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 51 | u | 1 | 31 | 10 | 5 | 13 | 3 | 0 |

3 Residue-property plots [i](#)

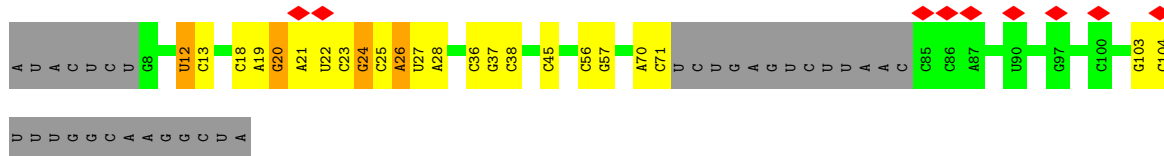
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Pre-mRNA-processing-splicing factor 8

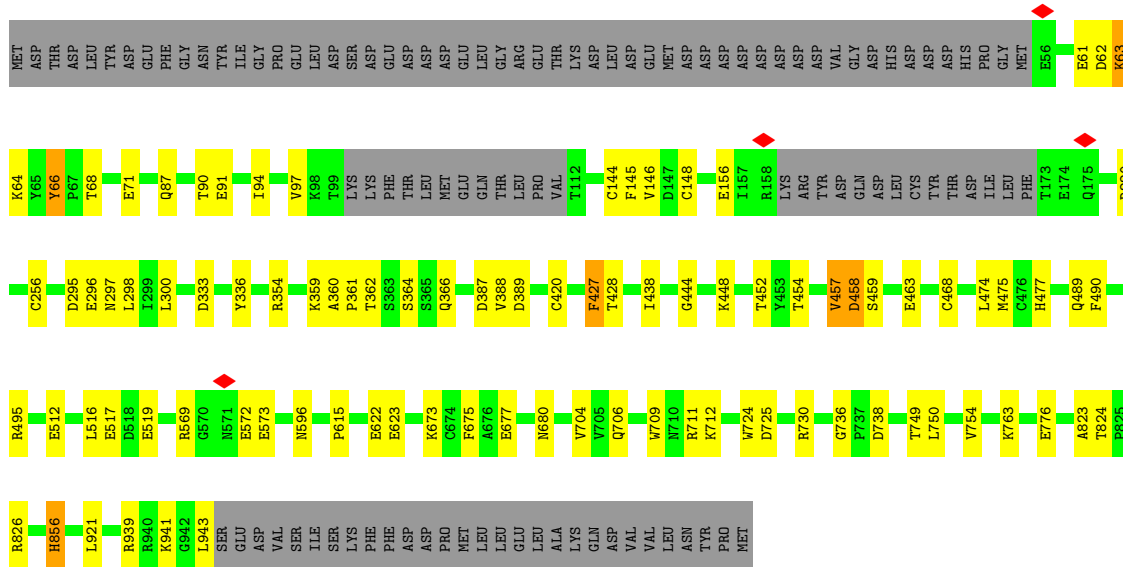
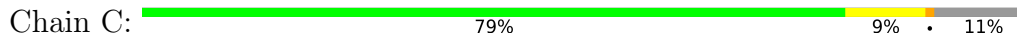




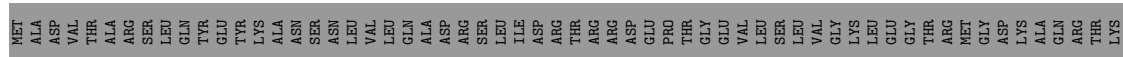
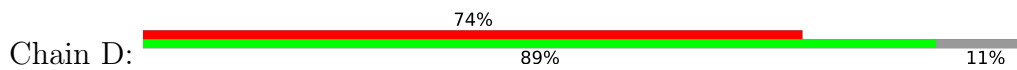
• Molecule 2: U5 snRNA



• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

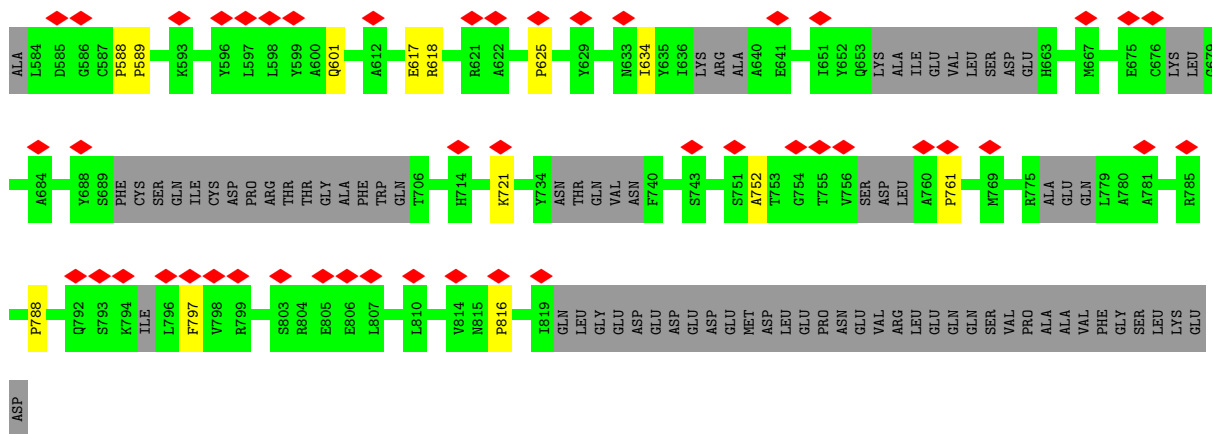


• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

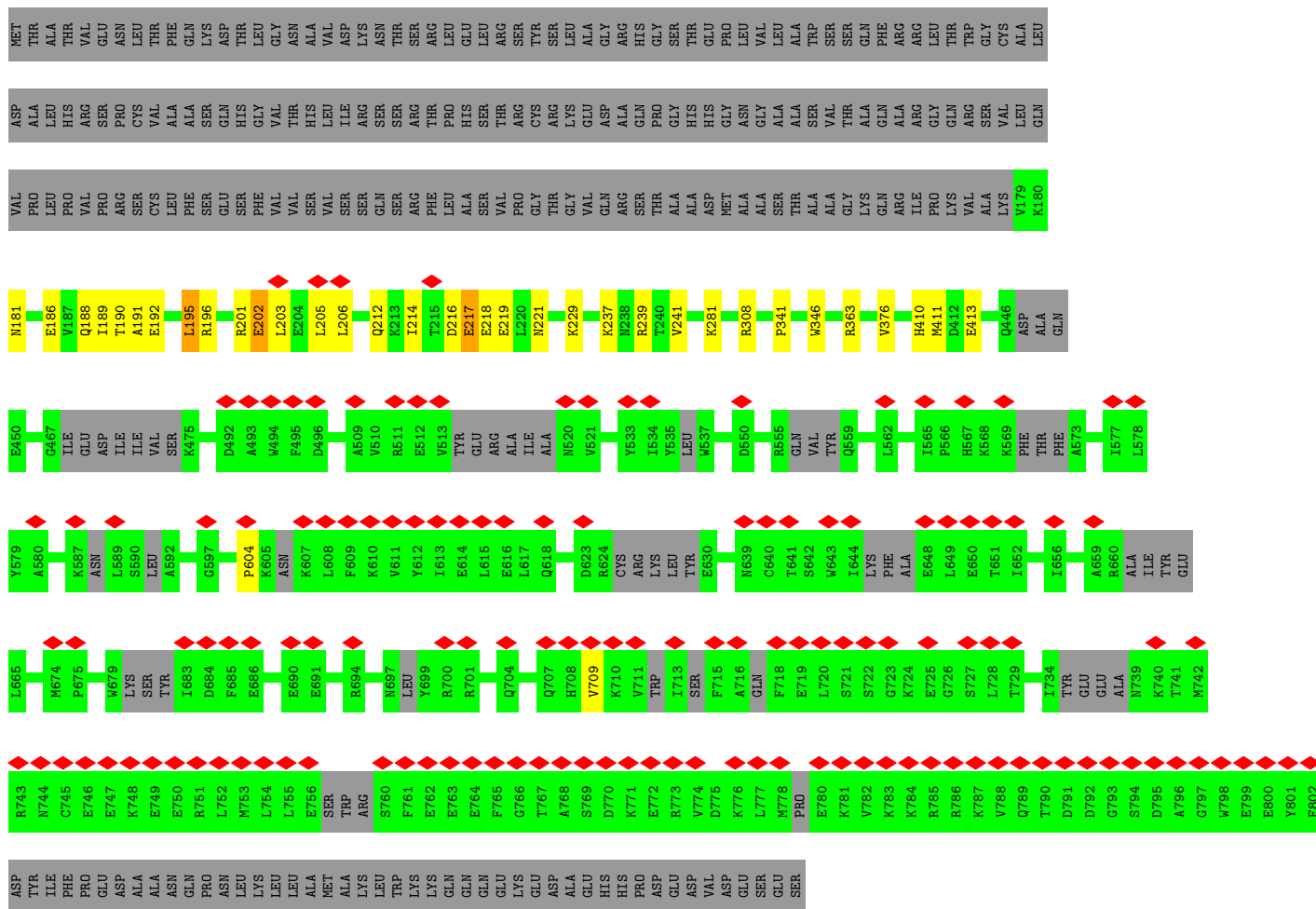


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| L869 | L870 | T871 | S872 | S873 | S874 | E875 | Y878 | Y879 | L880 | S881 | L882 | L883 | N884 | Q885 | Q886 | I889 | E890 | S891 | Q892 | A893 | H894 | S895 | K896 | L897 | P898 | D899 | M900 | E904 | I905 | V906 | L907 | G908 | N909 | V910 | Q911 | N912 | A913 | K914 | D915 | A916 | V917 | N918 | W919 | L920 | G921 | Y926 | I927 | R928 | M929 | L930 | R931 | S932 | P933 | T934 | L935 | F801 | A802 | D803 | K804 | H805 | G806 | Q807 | V808 | L809 | V810 | S811 | T814 | L815 | A816 | W817 | G818 | V819 | N820 | L821 | P822 | A823 | H824 | I827 | I828 | K829 | G830 | T831 | Q832 | V833 | Y834 | S835 | P836 | E837 | K838 | G839 | T842 | E843 | L844 | G845 | M852 | L853 | G854 | R855 | A856 | G857 | H858 | R859 | Q860 | Y861 | D862 | T863 | K864 | G865 | S932 | P933 | T934 | L935 | R546 | Q485 | S486 | K487 | L488 | Y489 | R490 | P491 | A492 | L493 | E494 | T495 | D496 | A503 | P504 | T505 | G506 | A507 | G508 | K509 | T510 | M511 | V512 | A513 | L514 | M515 | C516 | M517 | L518 | R519 | E520 | G522 | K523 | H524 | L525 | N526 | M527 | D528 | T529 | G529 | T530 | L531 | N532 | V533 | D534 | D535 | F536 | K537 | L538 | L539 | T604 | Y605 | L606 | F607 | L608 | V609 | R546 | I484 | Q485 | S486 | K487 | L488 | Y489 | R490 | P491 | A492 | L493 | E494 | T495 | D496 | A503 | P504 | T505 | G506 | A507 | G508 | K509 | T510 | M511 | V512 | A513 | L514 | M515 | C516 | M517 | L518 | R519 | E520 | G522 | K523 | H524 | L525 | N526 | M527 | D528 | T529 | G529 | T530 | L531 | N532 | V533 | D534 | D535 | F536 | K537 | L538 | L539 | T604 | Y605 | L606 | F607 | L608 | V609 | R546 | A424 | M425 | K426 | R427 | L428 | O429 | L430 | P431 | D432 | G433 | S434 | F435 | R436 | A437 | Q438 | R439 | K440 | G441 | Y442 | F443 | E444 | V445 | H446 | V447 | P448 | A449 | L450 | K451 | P452 | L453 | P454 | F455 | G456 | S457 | E458 | P459 | Q460 | L461 | L462 | P463 | V464 | E465 | R466 | L467 | V468 | L469 | L470 | A471 | Q472 | A473 | G474 | F475 | E476 | G477 | F478 | K479 | T480 | M481 | N482 | R483 | L363 | H364 | E365 | T366 | L367 | L368 | L369 | L370 | L371 | L372 | L373 | L374 | L375 | L376 | L377 | L378 | L379 | L380 | L381 | L382 | L383 | L384 | L385 | L386 | L387 | L388 | L389 | L390 | L391 | L392 | L393 | L394 | L395 | L396 | L397 | L398 | L399 | L400 | L401 | L402 | L403 | L404 | L405 | L406 | L407 | L408 | L409 | L410 | L411 | L412 | L413 | L414 | L415 | L416 | L417 | L418 | L419 | L420 | L421 | L422 | L423 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | 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S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F315 | D316 | L317 | L318 | K319 | V320 | L321 | R322 | D324 | A265 | F266 | W267 | L268 | Q269 | R270 | Q271 | R272 | L273 | S273 | R274 | L333 | L334 | A335 | S336 | A337 | Q338 | S339 | E340 | A341 | Q342 | K343 | E344 | R345 | L346 | M347 | G348 | V349 | E350 | E351 | A352 | A352 | PRD | GLU | L356 | S357 | K358 | D299 | F359 | R300 | E301 | C302 | Y361 | Q362 | E303 | R304 | Q305 | L306 | V307 | L308 | L309 | G311 | F312 | N313 | T314 | F |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|----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| Y936 | G937 | I938 | S939 | H940 | D941 | D942 | L943 | K944 | G945 | D946 | P947 | L948 | L949 | D950 | Q951 | R952 | R953 | L954 | D955 | L956 | Y957 | H958 | T959 | A960 | A961 | L962 | M963 | L964 | D965 | K966 | N967 | N968 | L969 | V970 | K971 | Y972 | D973 | K974 | K975 | T976 | G977 | N978 | F979 | Q980 | V981 | T982 | E983 | L984 | G985 | R986 | I987 | A988 | S989 | H990 | Y991 | Y992 | I993 | T994 | N995 | |
| D996 | T997 | W998 | Q999 | T1000 | Y1001 | M1002 | Q1003 | L1004 | L1005 | K1006 | P1007 | T1008 | L1009 | S1010 | E1011 | I1012 | E1013 | L1014 | V1017 | F1018 | S1019 | L1020 | S1021 | S1022 | E1023 | F1024 | K1025 | M1026 | I1027 | T1028 | V1029 | R1030 | E1031 | E1032 | E1033 | K1034 | L1035 | E1036 | L1037 | Q1038 | K1039 | L1040 | R1043 | V1044 | P1045 | V1046 | P1047 | V1048 | K1049 | E1050 | S1051 | I1052 | I1053 | E1054 | A1057 | K1058 | | | | |
| I1059 | N1060 | V1061 | L1062 | A1065 | F1066 | I1067 | L1070 | K1071 | L1072 | E1073 | G1074 | F1075 | A1076 | L1077 | M1078 | A1079 | D1080 | Y1083 | V1084 | S1087 | R1089 | A1094 | E1097 | I1098 | N1101 | R1102 | G1103 | L1107 | T1108 | T1111 | C1115 | K1116 | M1117 | I1118 | D1119 | M1122 | W1123 | P1124 | S1125 | M1126 | C1127 | P1128 | L1129 | R1130 | Q1131 | F1132 | R1133 | K1134 | | | | | | | | | | | | |
| L1135 | P1136 | E1137 | E1138 | V1139 | V1140 | K1141 | K1145 | K1146 | M1147 | F1148 | P1149 | F1150 | E1151 | R1152 | L1153 | Y1154 | D1155 | L1156 | M1157 | H1158 | I1161 | G1162 | E1163 | L1164 | I1165 | L1166 | M1167 | P1168 | M1170 | G1171 | K1172 | T1173 | I1174 | H1175 | K1176 | V1178 | H1179 | L1180 | F1181 | P1182 | K1183 | L1184 | E1185 | L1186 | S1187 | V1188 | H1189 | L1190 | Q1191 | P1192 | L1193 | T1194 | R1195 | S1196 | | | | | | |
| E1201 | L1202 | T1203 | T1204 | T1205 | F1206 | D1207 | F1208 | Q1209 | W1210 | D1211 | E1212 | K1213 | V1214 | G1215 | A1216 | S1217 | S1218 | E1219 | A1220 | I1223 | L1224 | V1225 | I1233 | Y1238 | F1239 | L1240 | L1241 | K1242 | K1243 | K1244 | Y1245 | A1246 | Q1247 | D1248 | E1249 | H1250 | L1251 | I1252 | T1253 | V1258 | F1259 | E1260 | P1261 | L1262 | P1263 | S1272 | D1273 | R1274 | M1275 | L1276 | L1277 | V1284 | | | | | | | | |
| H1288 | L1289 | I1290 | L1291 | P1292 | E1293 | K1294 | Y1295 | P1296 | P1297 | P1298 | T1299 | E1300 | L1301 | L1302 | D1303 | L1304 | Q1305 | P1306 | L1307 | P1308 | V1309 | S1310 | A1311 | L1312 | R1313 | M1314 | S1315 | A1316 | F1317 | E1318 | S1319 | L1320 | Y1321 | Q1322 | D1323 | K1324 | F1325 | P1326 | F1327 | F1328 | M1329 | P1330 | I1331 | Q1332 | T1333 | Q1334 | V1335 | F1336 | M1337 | T1338 | L1339 | Y1340 | M1341 | S1342 | D1343 | M1344 | V1346 | F1347 | | |
| V1348 | G1349 | A1350 | G1353 | S1354 | G1355 | K1356 | T1357 | L1358 | C1359 | A1360 | E1361 | F1362 | A1363 | L1364 | L1365 | R1366 | M1367 | L1368 | L1369 | Q1370 | S1371 | S1372 | E1373 | G1374 | C1376 | V1377 | Y1378 | I1379 | T1380 | P1381 | M1382 | L1385 | A1386 | E1387 | Q1388 | V1389 | M1390 | D1392 | W1393 | Y1394 | E1395 | K1396 | F1397 | Q1398 | D1399 | R1400 | L1401 | M1402 | K1403 | K1404 | V1405 | V1406 | L1407 | L1408 | T1409 | | | | | |
| G1410 | S1413 | T1414 | D1415 | L1416 | K1417 | L1418 | L1419 | G1420 | K1421 | G1422 | N1423 | I1424 | I1425 | L1426 | S1427 | T1428 | P1429 | E1430 | K1431 | W1432 | D1433 | I1434 | L1435 | S1436 | L1437 | R1438 | W1439 | K1440 | Q1441 | R1442 | K1443 | A1444 | V1445 | Q1446 | N1447 | L1448 | L1450 | F1451 | V1452 | E1455 | V1456 | H1457 | L1458 | L1459 | G1460 | G1461 | V1466 | L1467 | E1468 | V1469 | L1470 | C1471 | S1472 | R1473 | M1474 | | | | | |
| R1475 | I1477 | S1478 | S1479 | Q1480 | I1481 | E1482 | R1483 | P1484 | I1485 | R1486 | I1487 | V1488 | A1489 | L1490 | S1491 | S1492 | S1493 | L1494 | S1495 | M1496 | K1497 | K1498 | D1499 | V1500 | A1501 | H1502 | W1503 | L1504 | G1505 | C1506 | S1507 | A1508 | T1509 | S1510 | T1511 | F1512 | M1513 | F1514 | H1515 | P1516 | M1517 | V1518 | R1519 | P1520 | V1521 | P1522 | L1523 | E1524 | L1525 | H1526 | G1529 | F1530 | M1531 | I1532 | S1533 | H1534 | T1535 | | | |
| Q1536 | T1537 | R1538 | L1539 | L1540 | S1541 | M1542 | A1543 | K1544 | P1545 | V1546 | Y1547 | H1548 | A1549 | I1550 | T1551 | K1552 | H1553 | S1554 | P1555 | K1556 | K1557 | P1558 | V1559 | I1560 | F1561 | V1562 | V1563 | S1564 | S1565 | R1566 | K1567 | Q1568 | T1569 | R1570 | L1571 | V1572 | A1573 | I1574 | D1575 | I1576 | L1577 | T1578 | T1579 | C1580 | A1581 | A1582 | D1583 | I1584 | Q1585 | R1586 | Q1587 | P1588 | F1589 | L1590 | H1591 | S1592 | C1593 | L1594 | M1595 | K1596 |
| D1596 | L1597 | I1598 | P1599 | Y1600 | L1601 | E1602 | K1603 | L1604 | S1605 | D1606 | S1607 | T1608 | L1609 | K1610 | E1611 | T1612 | L1613 | L1614 | M1615 | L1616 | V1617 | G1618 | Y1619 | L1620 | H1621 | E1622 | G1623 | L1624 | S1625 | P1626 | M1627 | E1628 | R1629 | L1630 | L1631 | V1632 | E1633 | Q1634 | L1635 | F1636 | S1638 | G1639 | A1640 | I1641 | Q1642 | V1643 | V1644 | V1645 | A1646 | S1647 | R1648 | S1649 | L1650 | L1651 | C1652 | G1653 | M1654 | M1655 | V1656 | |
| A1657 | L1660 | V1661 | I1662 | L1663 | M1664 | D1665 | Y1668 | V1669 | M1670 | G1671 | K1672 | L1673 | H1674 | A1675 | Y1676 | V1677 | P1680 | I1681 | Y1682 | D1683 | V1684 | L1685 | Q1686 | M1687 | V1688 | A1691 | M1692 | R1693 | P1694 | L1695 | Q1696 | D1697 | L1698 | E1699 | C1702 | V1703 | I1704 | M1705 | C1706 | Q1707 | Q1708 | S1709 | K1710 | K1711 | D1712 | K1715 | K1716 | F1717 | L1718 | Y1719 | E1720 | P1721 | L1722 | | | | | | | |
| P1723 | V1724 | E1725 | S1726 | H1727 | L1728 | D1729 | K1730 | M1731 | M1732 | H1733 | D1734 | H1735 | A1738 | E1739 | I1740 | V1741 | T1742 | K1743 | T1744 | L1745 | E1746 | M1747 | K1748 | Q1749 | D1750 | A1751 | V1752 | D1753 | T1756 | W1757 | L1760 | Y1761 | R1762 | R1763 | M1764 | N1767 | P1768 | M1769 | Y1770 | Y1771 | M1772 | L1773 | Q1774 | G1775 | L1776 | S1777 | H1778 | R1779 | H1780 | D1783 | H1784 | L1785 | S1786 | E1787 | | | | | | |

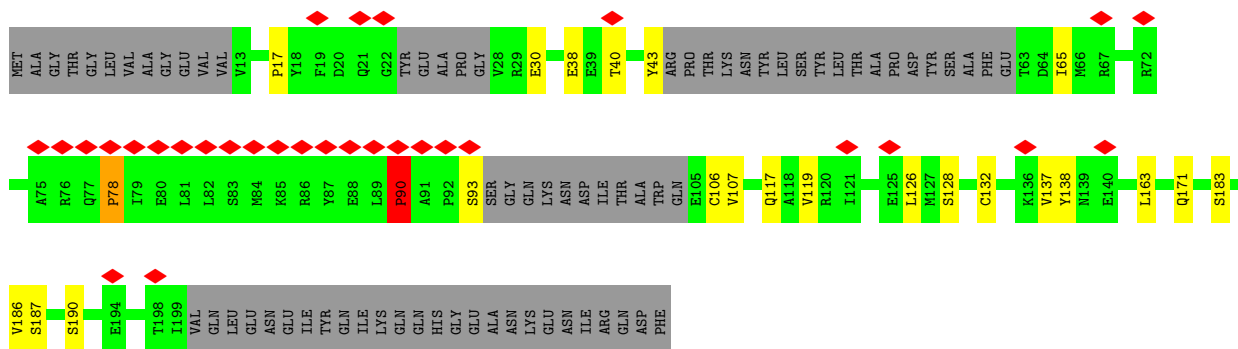


• Molecule 10: Crooked neck-like protein 1

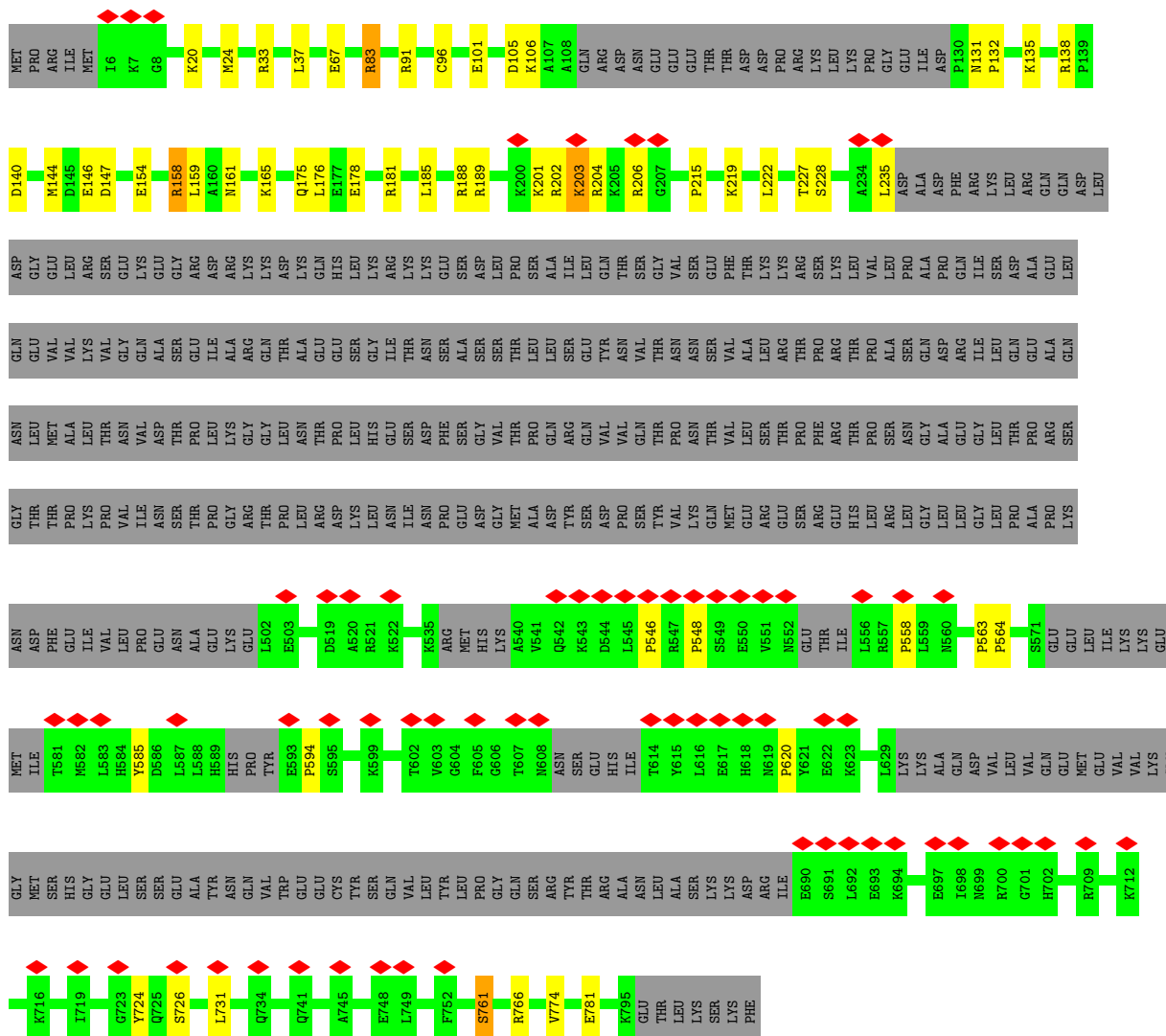
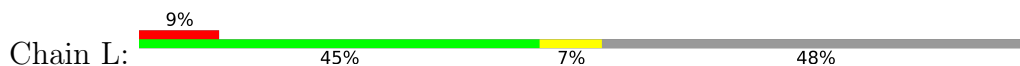


• Molecule 11: Pre-mRNA-splicing factor SPF27



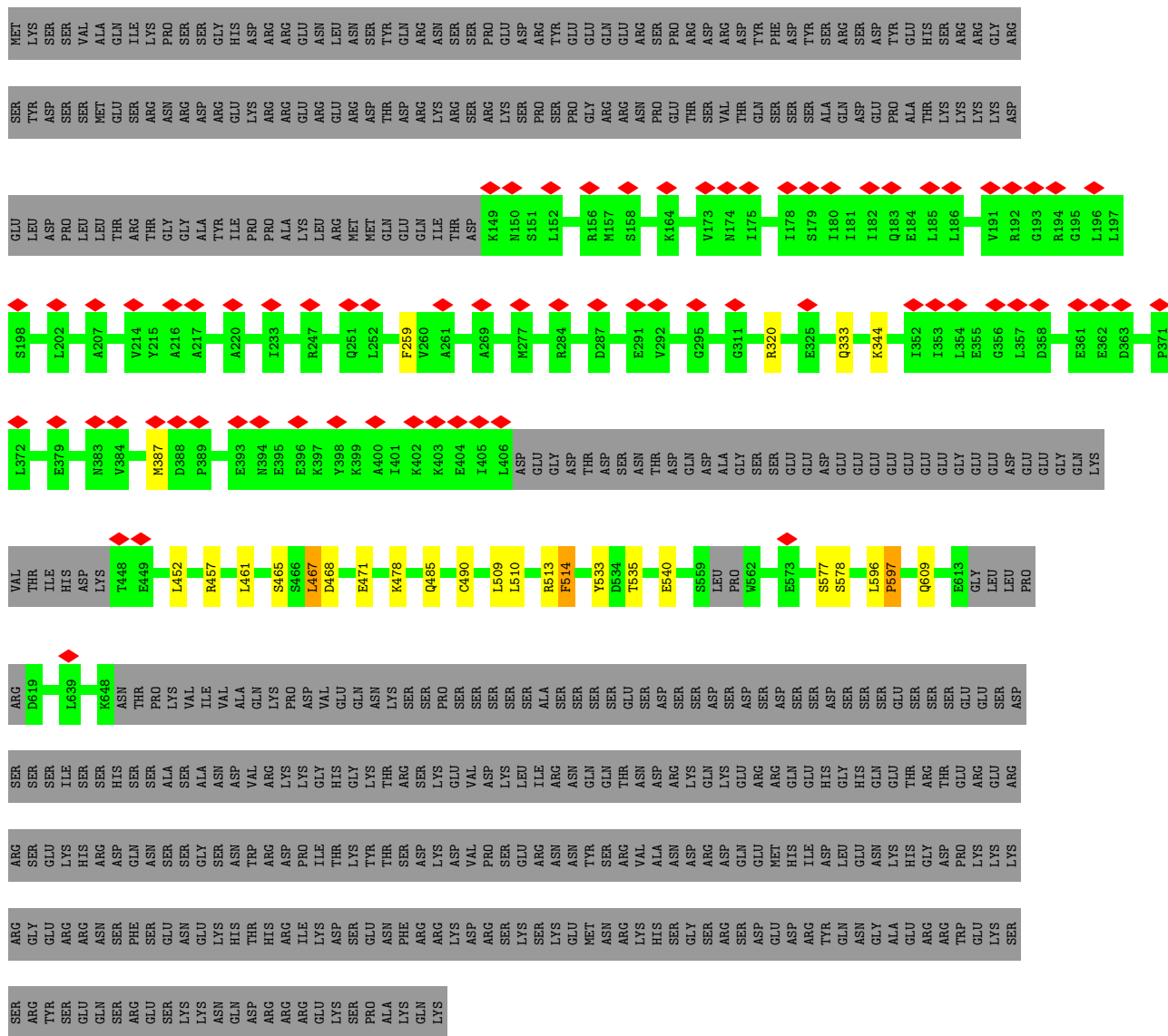


• Molecule 12: Cell division cycle 5-like protein

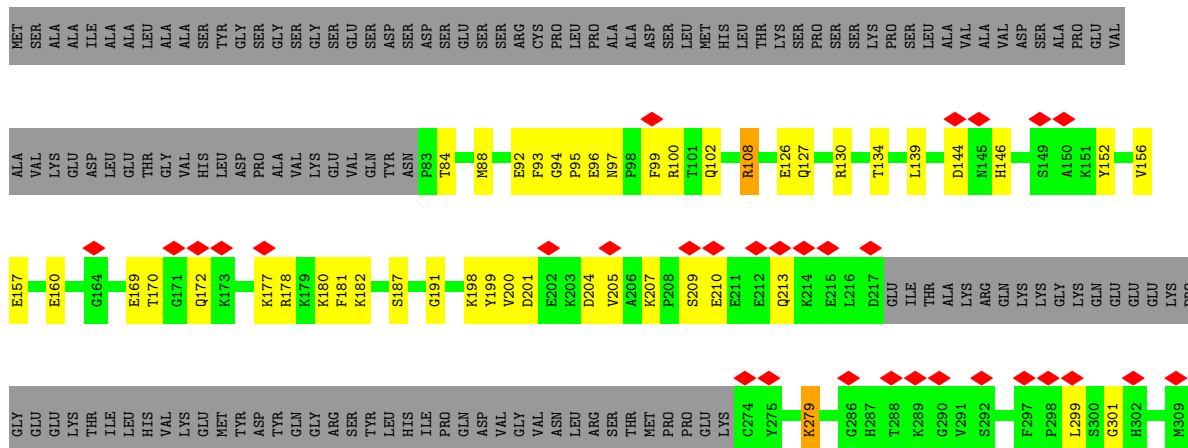


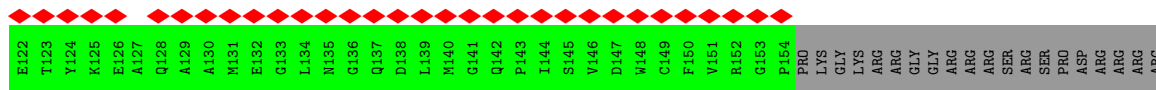
• Molecule 13: Pre-mRNA-splicing factor ISY1 homolog





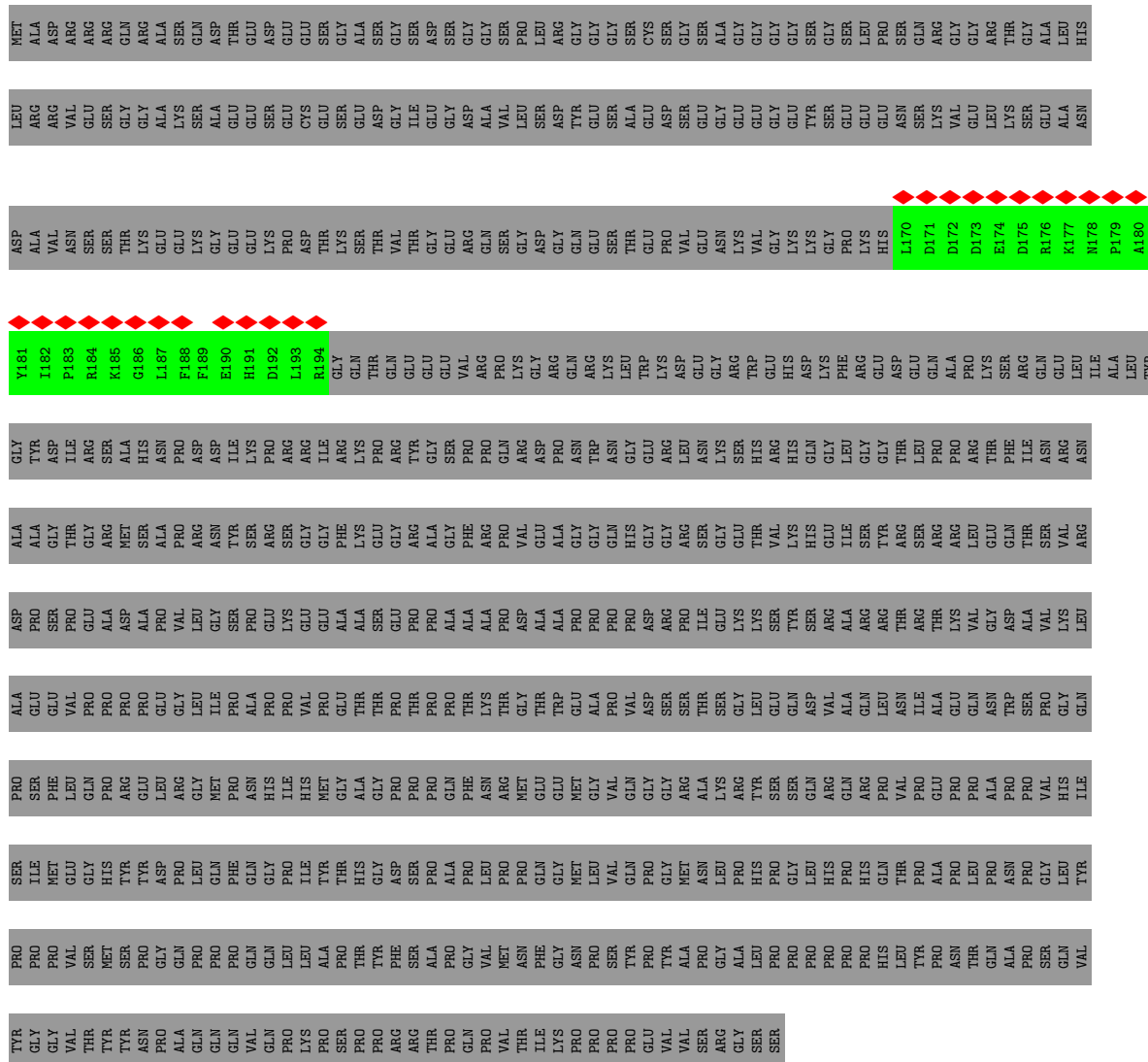
● Molecule 24: Pre-mRNA-processing factor 17





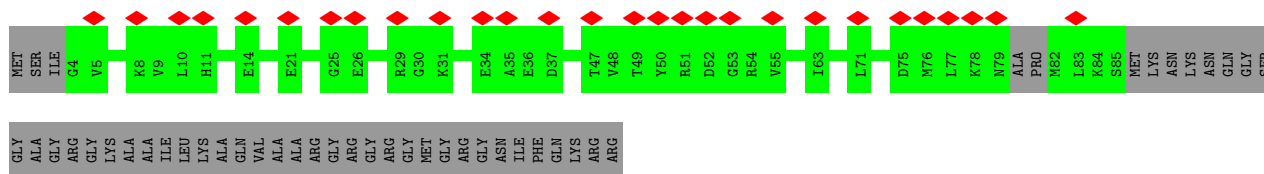
• Molecule 32: Protein CASC3

Chain x: 96%



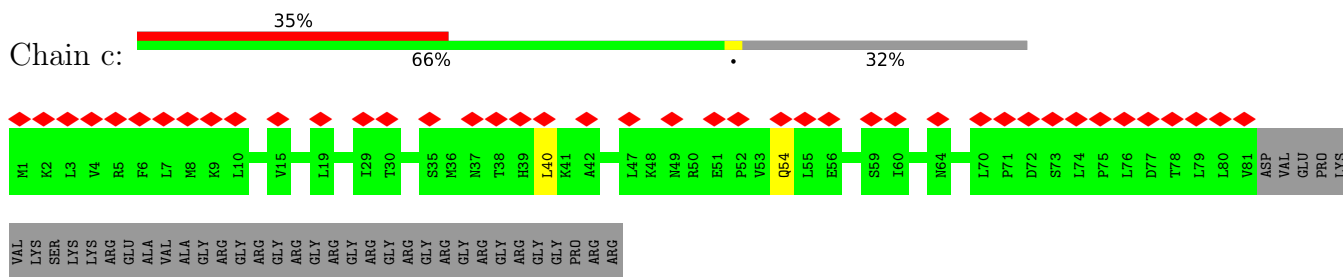
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

Chain h: 22% 63% 37%

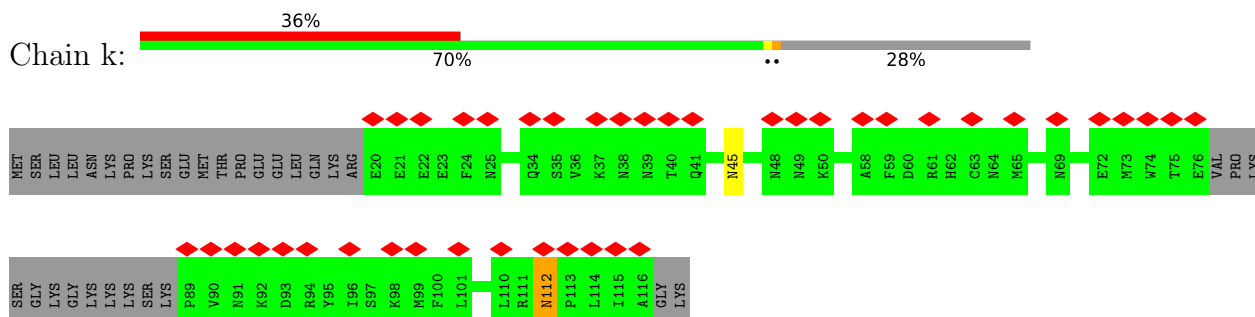


• Molecule 33: Small nuclear ribonucleoprotein Sm D3

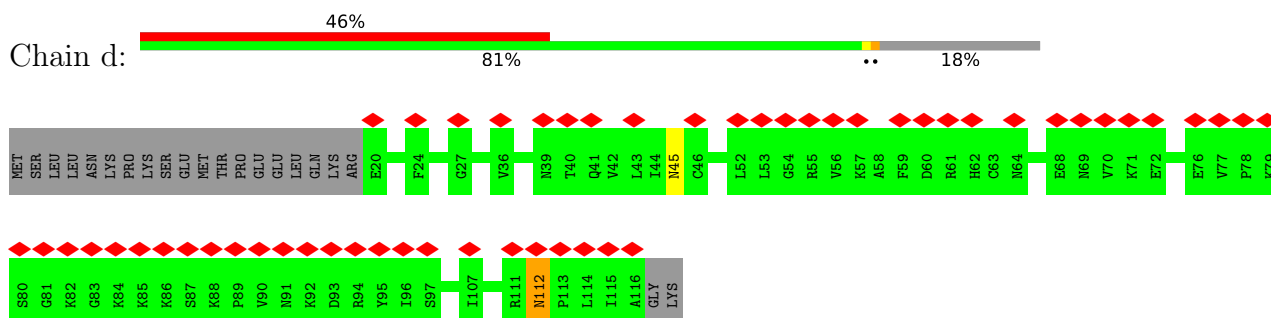
• Molecule 35: Small nuclear ribonucleoprotein Sm D1



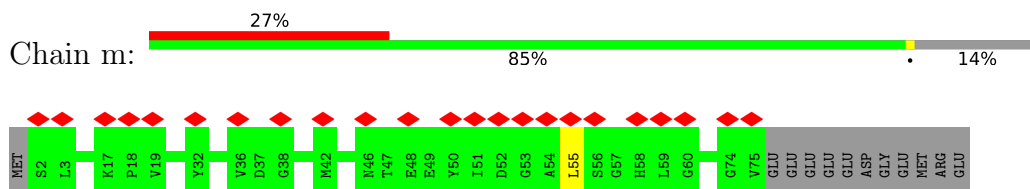
• Molecule 36: Small nuclear ribonucleoprotein Sm D2



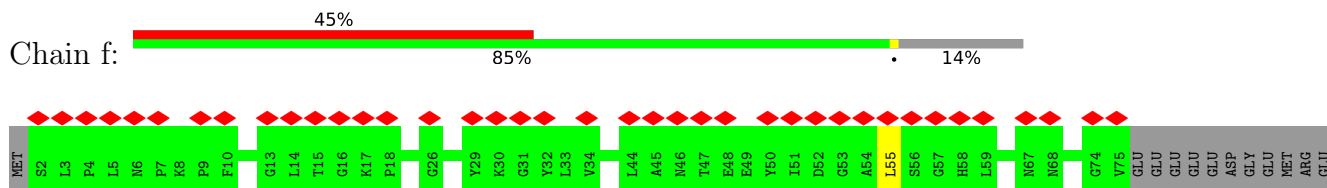
• Molecule 36: Small nuclear ribonucleoprotein Sm D2



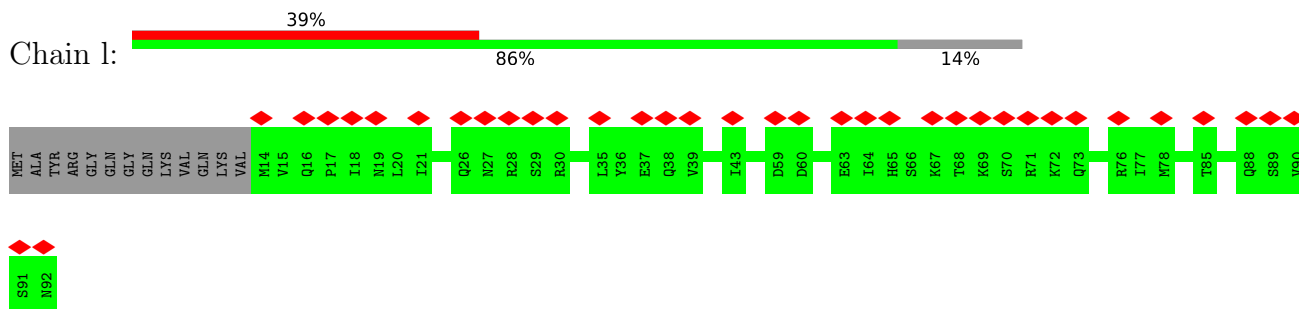
• Molecule 37: Small nuclear ribonucleoprotein F



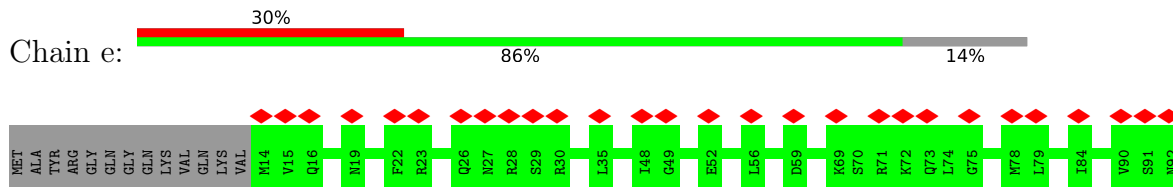
• Molecule 37: Small nuclear ribonucleoprotein F



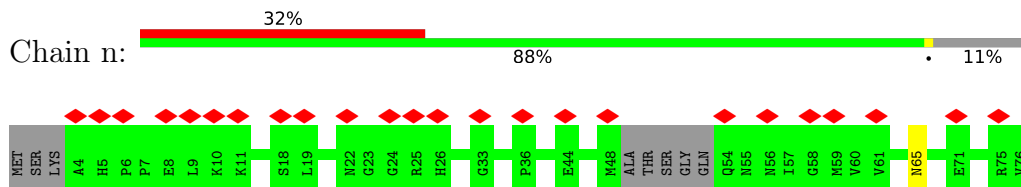
• Molecule 38: Small nuclear ribonucleoprotein E



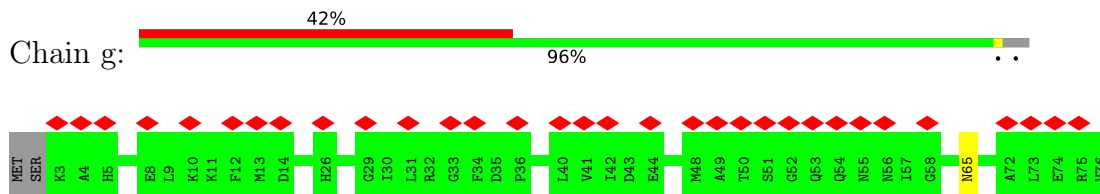
• Molecule 38: Small nuclear ribonucleoprotein E



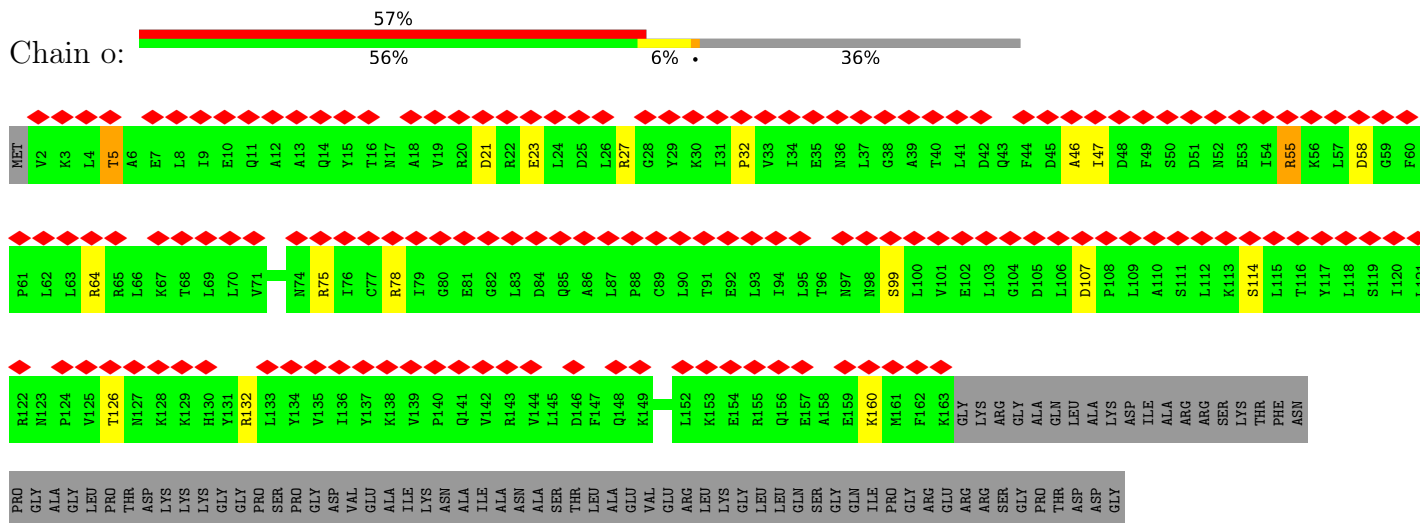
• Molecule 39: Small nuclear ribonucleoprotein G



• Molecule 39: Small nuclear ribonucleoprotein G

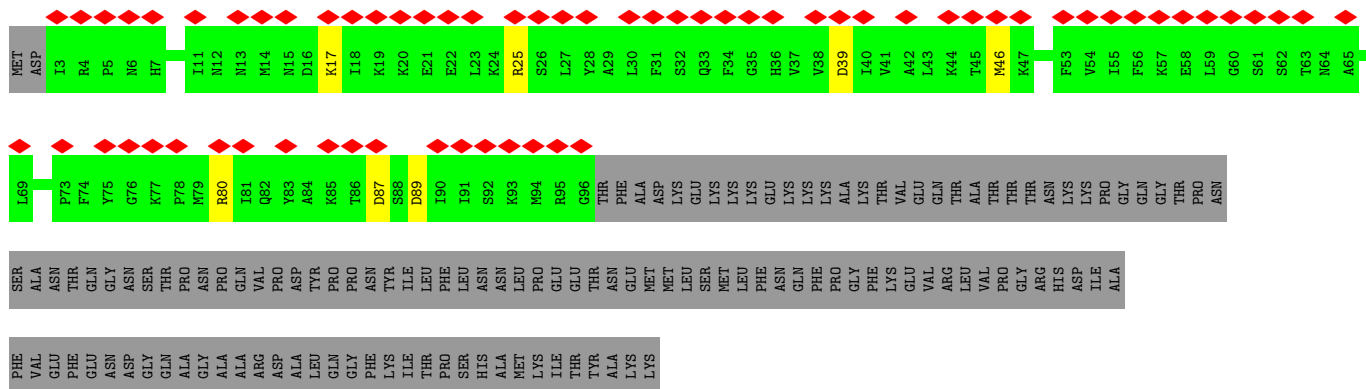


• Molecule 40: U2 small nuclear ribonucleoprotein A'

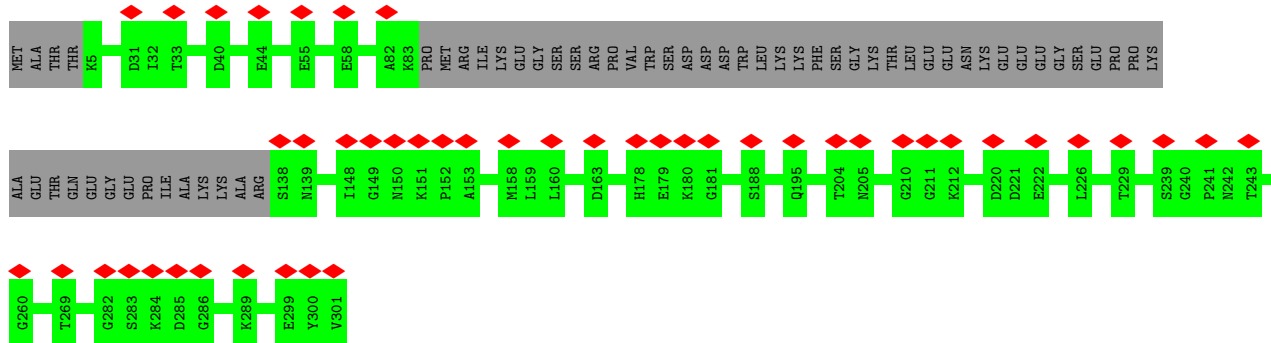
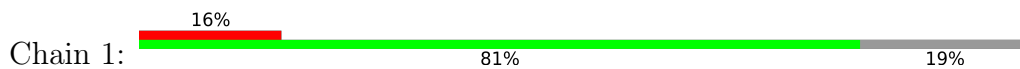


GLU
GLU
GLU
MET
GLU
GLU
ASP
THR
VAL
THR
THR
ASN
GLY
SER

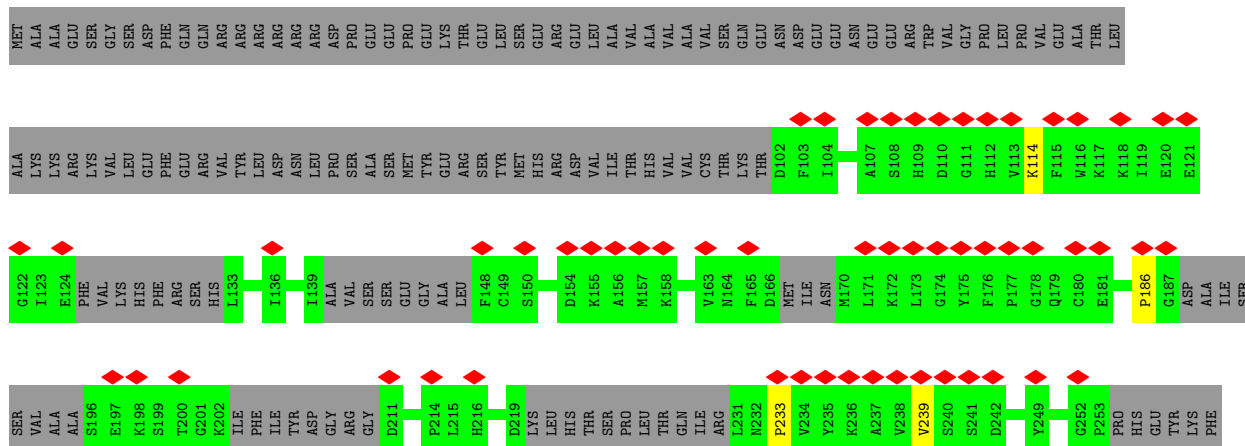
● Molecule 41: U2 small nuclear ribonucleoprotein B''

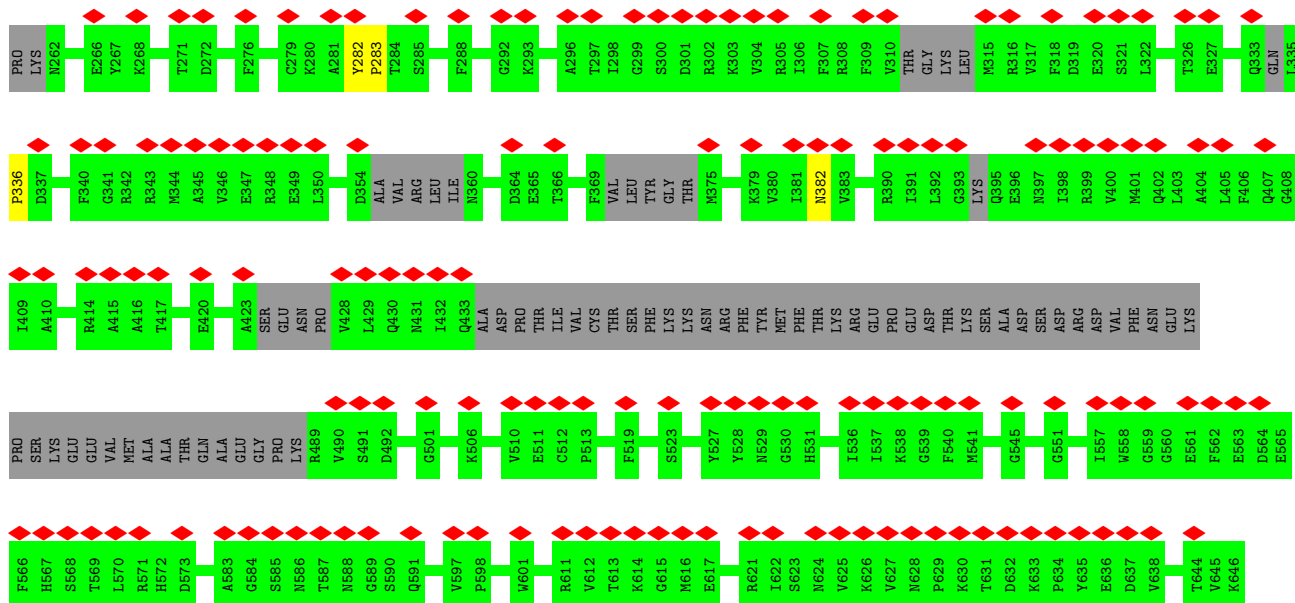


● Molecule 42: Peptidyl-prolyl cis-trans isomerase E

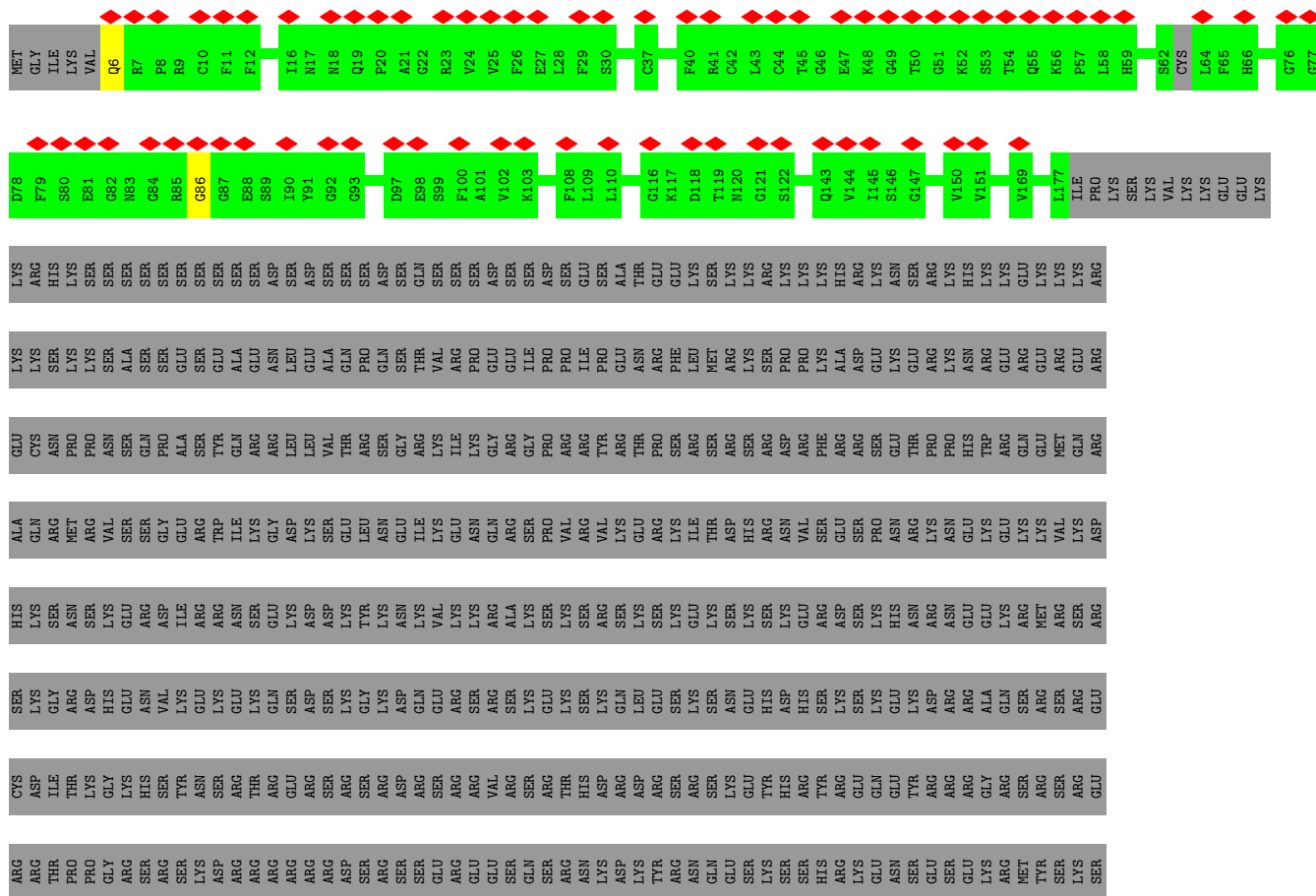


● Molecule 43: Peptidylprolyl isomerase domain and WD repeat-containing protein 1





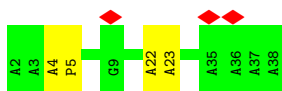
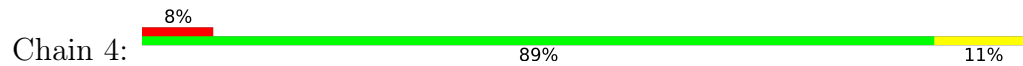
• Molecule 44: Peptidyl-prolyl cis-trans isomerase G



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

● Molecule 45: UNKNOWN



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 53633 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.209 | Depositor |
| Minimum map value | -0.105 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.008 | Depositor |
| Recommended contour level | 0.029 | Depositor |
| Map size (\AA) | 535.2, 535.2, 535.2 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.338, 1.338, 1.338 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, ADP, IHP, SEP, ATP, ZN

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 1.00 | 25/17966 (0.1%) | 1.07 | 63/24251 (0.3%) |
| 2 | B | 0.78 | 3/1970 (0.2%) | 0.91 | 6/3060 (0.2%) |
| 3 | C | 0.80 | 1/6946 (0.0%) | 0.97 | 10/9436 (0.1%) |
| 4 | D | 0.32 | 0/7628 | 0.56 | 0/9528 |
| 5 | E | 0.64 | 0/2392 | 0.79 | 0/3242 |
| 6 | F | 0.68 | 3/2323 (0.1%) | 0.86 | 3/3619 (0.1%) |
| 7 | G | 0.76 | 8/1820 (0.4%) | 0.90 | 2/2819 (0.1%) |
| 8 | H | 0.98 | 28/3283 (0.9%) | 1.65 | 117/5096 (2.3%) |
| 9 | I | 0.39 | 0/2724 | 0.56 | 17/3738 (0.5%) |
| 10 | J | 0.63 | 1/3870 (0.0%) | 0.75 | 1/5252 (0.0%) |
| 11 | K | 1.32 | 15/981 (1.5%) | 0.69 | 5/1317 (0.4%) |
| 12 | L | 0.70 | 4/2914 (0.1%) | 0.86 | 14/3929 (0.4%) |
| 13 | y | 0.96 | 5/707 (0.7%) | 0.77 | 6/953 (0.6%) |
| 14 | M | 0.53 | 0/791 | 0.80 | 0/1058 |
| 15 | N | 0.88 | 1/1210 (0.1%) | 1.00 | 3/1622 (0.2%) |
| 16 | O | 0.80 | 2/2324 (0.1%) | 0.92 | 5/3135 (0.2%) |
| 17 | P | 0.86 | 1/841 (0.1%) | 1.05 | 2/1117 (0.2%) |
| 18 | R | 0.78 | 4/1976 (0.2%) | 1.03 | 10/2651 (0.4%) |
| 19 | S | 0.59 | 0/1268 | 0.80 | 1/1714 (0.1%) |
| 20 | T | 1.05 | 1/2526 (0.0%) | 1.11 | 4/3443 (0.1%) |
| 21 | Q | 0.20 | 0/5279 | 0.40 | 0/6583 |
| 22 | U | 1.03 | 0/196 | 1.09 | 1/265 (0.4%) |
| 23 | V | 0.55 | 0/3453 | 0.76 | 4/4640 (0.1%) |
| 24 | W | 0.57 | 1/2336 (0.0%) | 0.73 | 3/3027 (0.1%) |
| 25 | X | 0.46 | 0/486 | 0.54 | 0/658 |
| 26 | Y | 0.65 | 2/1450 (0.1%) | 0.88 | 9/1975 (0.5%) |
| 27 | Z | 0.50 | 0/2528 | 0.99 | 3/3139 (0.1%) |
| 28 | q | 1.07 | 4/929 (0.4%) | 0.70 | 3/1260 (0.2%) |
| 28 | r | 1.08 | 4/912 (0.4%) | 0.71 | 3/1239 (0.2%) |
| 28 | s | 1.91 | 4/1497 (0.3%) | 0.83 | 4/1866 (0.2%) |
| 28 | t | 1.06 | 2/480 (0.4%) | 0.57 | 0/650 |
| 29 | u | 0.38 | 0/3175 | 0.65 | 0/4286 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 30 | v | 0.38 | 0/1225 | 0.60 | 0/1648 |
| 31 | w | 0.36 | 0/748 | 0.71 | 3/1012 (0.3%) |
| 32 | x | 0.43 | 0/221 | 0.66 | 0/296 |
| 33 | a | 0.46 | 0/616 | 0.66 | 0/830 |
| 33 | h | 0.46 | 0/627 | 0.68 | 0/842 |
| 34 | b | 0.52 | 0/685 | 0.82 | 0/913 |
| 34 | i | 0.53 | 0/700 | 0.82 | 0/933 |
| 35 | c | 0.56 | 0/649 | 0.78 | 0/877 |
| 35 | j | 0.56 | 0/657 | 0.77 | 0/888 |
| 36 | d | 0.69 | 0/778 | 0.86 | 0/1045 |
| 36 | k | 0.69 | 0/696 | 0.86 | 0/935 |
| 37 | f | 0.82 | 0/588 | 0.84 | 0/795 |
| 37 | m | 0.82 | 0/588 | 0.84 | 0/795 |
| 38 | e | 0.62 | 0/660 | 0.83 | 0/886 |
| 38 | l | 0.61 | 0/660 | 0.83 | 0/886 |
| 39 | g | 0.53 | 0/576 | 0.78 | 0/771 |
| 39 | n | 0.53 | 0/539 | 0.80 | 0/718 |
| 40 | o | 0.59 | 0/1294 | 1.63 | 18/1754 (1.0%) |
| 41 | p | 0.56 | 0/774 | 1.35 | 6/1035 (0.6%) |
| 42 | 1 | 0.34 | 0/970 | 0.60 | 0/1209 |
| 43 | 2 | 0.54 | 0/1649 | 0.64 | 0/2035 |
| 44 | 3 | 0.68 | 0/682 | 0.89 | 3/849 (0.4%) |
| 45 | 4 | 0.35 | 0/184 | 0.70 | 0/255 |
| All | All | 0.76 | 119/105947 (0.1%) | 0.91 | 329/142775 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 6 |
| 3 | C | 0 | 3 |
| 4 | D | 0 | 1 |
| 10 | J | 0 | 1 |
| 12 | L | 0 | 1 |
| 13 | y | 0 | 1 |
| 14 | M | 0 | 1 |
| 15 | N | 0 | 1 |
| 18 | R | 0 | 1 |
| 20 | T | 0 | 2 |
| 26 | Y | 0 | 3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 27 | Z | 0 | 29 |
| 28 | s | 0 | 4 |
| 36 | d | 0 | 1 |
| 36 | k | 0 | 1 |
| All | All | 0 | 56 |

The worst 5 of 119 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|--------|-------------|----------|
| 28 | s | 481[A] | VAL | N-CA | 48.51 | 2.43 | 1.46 |
| 28 | s | 481[B] | VAL | N-CA | 48.51 | 2.43 | 1.46 |
| 11 | K | 106 | CYS | CB-SG | -23.18 | 1.42 | 1.82 |
| 13 | y | 36 | CYS | CB-SG | -18.29 | 1.51 | 1.82 |
| 11 | K | 132 | CYS | CB-SG | -17.41 | 1.52 | 1.82 |

The worst 5 of 329 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|--------|-------------|----------|
| 28 | s | 481[A] | VAL | N-CA-C | -15.66 | 68.71 | 111.00 |
| 28 | s | 481[B] | VAL | N-CA-C | -15.66 | 68.71 | 111.00 |
| 40 | o | 55 | ARG | NE-CZ-NH1 | 15.07 | 127.83 | 120.30 |
| 1 | A | 642 | ARG | NE-CZ-NH2 | -14.47 | 113.06 | 120.30 |
| 40 | o | 55 | ARG | CD-NE-CZ | 13.79 | 142.90 | 123.60 |

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 166 | PHE | Peptide |
| 1 | A | 346 | ASP | Peptide |
| 1 | A | 408 | PRO | Peptide |
| 1 | A | 433 | GLU | Peptide |
| 1 | A | 642 | ARG | Sidechain |

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 2247/2335 (96%) | 2100 (94%) | 107 (5%) | 40 (2%) | 8 | 40 |
| 3 | C | 856/972 (88%) | 779 (91%) | 57 (7%) | 20 (2%) | 6 | 36 |
| 4 | D | 1900/2136 (89%) | 1799 (95%) | 96 (5%) | 5 (0%) | 41 | 75 |
| 5 | E | 297/357 (83%) | 272 (92%) | 16 (5%) | 9 (3%) | 4 | 31 |
| 9 | I | 493/855 (58%) | 475 (96%) | 10 (2%) | 8 (2%) | 9 | 43 |
| 10 | J | 530/848 (62%) | 483 (91%) | 30 (6%) | 17 (3%) | 4 | 30 |
| 11 | K | 144/225 (64%) | 134 (93%) | 6 (4%) | 4 (3%) | 5 | 32 |
| 12 | L | 401/802 (50%) | 375 (94%) | 19 (5%) | 7 (2%) | 9 | 42 |
| 13 | y | 106/307 (34%) | 98 (92%) | 8 (8%) | 0 | 100 | 100 |
| 14 | M | 89/243 (37%) | 80 (90%) | 3 (3%) | 6 (7%) | 1 | 17 |
| 15 | N | 141/144 (98%) | 126 (89%) | 12 (8%) | 3 (2%) | 7 | 38 |
| 16 | O | 279/420 (66%) | 247 (88%) | 26 (9%) | 6 (2%) | 6 | 37 |
| 17 | P | 92/229 (40%) | 82 (89%) | 9 (10%) | 1 (1%) | 14 | 50 |
| 18 | R | 235/536 (44%) | 207 (88%) | 14 (6%) | 14 (6%) | 1 | 19 |
| 19 | S | 157/166 (95%) | 144 (92%) | 10 (6%) | 3 (2%) | 8 | 39 |
| 20 | T | 311/514 (60%) | 282 (91%) | 17 (6%) | 12 (4%) | 3 | 26 |
| 21 | Q | 1304/1485 (88%) | 1279 (98%) | 25 (2%) | 0 | 100 | 100 |
| 22 | U | 24/2752 (1%) | 20 (83%) | 3 (12%) | 1 (4%) | 3 | 24 |
| 23 | V | 444/908 (49%) | 413 (93%) | 26 (6%) | 5 (1%) | 14 | 50 |
| 24 | W | 436/579 (75%) | 385 (88%) | 32 (7%) | 19 (4%) | 2 | 24 |
| 25 | X | 69/425 (16%) | 65 (94%) | 2 (3%) | 2 (3%) | 4 | 32 |
| 26 | Y | 202/323 (62%) | 182 (90%) | 6 (3%) | 14 (7%) | 1 | 16 |
| 27 | Z | 611/1227 (50%) | 517 (85%) | 61 (10%) | 33 (5%) | 2 | 21 |
| 28 | q | 130/504 (26%) | 119 (92%) | 7 (5%) | 4 (3%) | 4 | 31 |
| 28 | r | 129/504 (26%) | 118 (92%) | 9 (7%) | 2 (2%) | 9 | 43 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 28 | s | 369/504 (73%) | 352 (95%) | 16 (4%) | 1 (0%) | 41 | 75 |
| 28 | t | 65/504 (13%) | 64 (98%) | 0 | 1 (2%) | 10 | 44 |
| 29 | u | 388/411 (94%) | 376 (97%) | 9 (2%) | 3 (1%) | 19 | 58 |
| 30 | v | 142/148 (96%) | 138 (97%) | 4 (3%) | 0 | 100 | 100 |
| 31 | w | 89/174 (51%) | 87 (98%) | 1 (1%) | 1 (1%) | 14 | 50 |
| 32 | x | 23/703 (3%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 33 | a | 75/126 (60%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 33 | h | 76/126 (60%) | 75 (99%) | 1 (1%) | 0 | 100 | 100 |
| 34 | b | 81/229 (35%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 34 | i | 84/229 (37%) | 82 (98%) | 2 (2%) | 0 | 100 | 100 |
| 35 | c | 79/119 (66%) | 76 (96%) | 3 (4%) | 0 | 100 | 100 |
| 35 | j | 80/119 (67%) | 77 (96%) | 3 (4%) | 0 | 100 | 100 |
| 36 | d | 95/118 (80%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 36 | k | 81/118 (69%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 37 | f | 72/86 (84%) | 69 (96%) | 3 (4%) | 0 | 100 | 100 |
| 37 | m | 72/86 (84%) | 68 (94%) | 4 (6%) | 0 | 100 | 100 |
| 38 | e | 77/92 (84%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 38 | l | 77/92 (84%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 39 | g | 72/76 (95%) | 70 (97%) | 2 (3%) | 0 | 100 | 100 |
| 39 | n | 64/76 (84%) | 62 (97%) | 2 (3%) | 0 | 100 | 100 |
| 40 | o | 160/255 (63%) | 146 (91%) | 12 (8%) | 2 (1%) | 12 | 47 |
| 41 | p | 92/225 (41%) | 90 (98%) | 2 (2%) | 0 | 100 | 100 |
| 42 | 1 | 239/301 (79%) | 232 (97%) | 7 (3%) | 0 | 100 | 100 |
| 43 | 2 | 386/646 (60%) | 358 (93%) | 20 (5%) | 8 (2%) | 7 | 38 |
| 44 | 3 | 167/754 (22%) | 165 (99%) | 2 (1%) | 0 | 100 | 100 |
| 45 | 4 | 35/37 (95%) | 29 (83%) | 2 (6%) | 4 (11%) | 0 | 6 |
| All | All | 14867/26150 (57%) | 13893 (93%) | 719 (5%) | 255 (2%) | 13 | 42 |

5 of 255 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 82 | ARG |
| 1 | A | 92 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 167 | PRO |
| 1 | A | 188 | LEU |
| 1 | A | 331 | TRP |

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 |
|-----|-------|-----------------|------------|----------|-------------|
| 1 | A | 1778/2108 (84%) | 1648 (93%) | 130 (7%) | 14 41 |
| 3 | C | 760/866 (88%) | 694 (91%) | 66 (9%) | 10 35 |
| 5 | E | 256/300 (85%) | 244 (95%) | 12 (5%) | 26 53 |
| 10 | J | 241/751 (32%) | 222 (92%) | 19 (8%) | 12 39 |
| 11 | K | 54/196 (28%) | 49 (91%) | 5 (9%) | 9 32 |
| 12 | L | 193/709 (27%) | 156 (81%) | 37 (19%) | 1 9 |
| 13 | y | 33/256 (13%) | 30 (91%) | 3 (9%) | 9 33 |
| 14 | M | 85/209 (41%) | 64 (75%) | 21 (25%) | 0 4 |
| 15 | N | 130/130 (100%) | 125 (96%) | 5 (4%) | 33 59 |
| 16 | O | 253/361 (70%) | 248 (98%) | 5 (2%) | 55 73 |
| 17 | P | 90/203 (44%) | 78 (87%) | 12 (13%) | 4 21 |
| 18 | R | 210/457 (46%) | 156 (74%) | 54 (26%) | 0 4 |
| 19 | S | 129/134 (96%) | 118 (92%) | 11 (8%) | 10 37 |
| 20 | T | 269/441 (61%) | 252 (94%) | 17 (6%) | 18 46 |
| 22 | U | 21/2432 (1%) | 16 (76%) | 5 (24%) | 0 5 |
| 23 | V | 324/838 (39%) | 303 (94%) | 21 (6%) | 17 45 |
| 24 | W | 115/502 (23%) | 81 (70%) | 34 (30%) | 0 2 |
| 25 | X | 33/381 (9%) | 20 (61%) | 13 (39%) | 0 0 |
| 26 | Y | 114/289 (39%) | 87 (76%) | 27 (24%) | 1 5 |
| 28 | q | 78/435 (18%) | 69 (88%) | 9 (12%) | 5 24 |
| 28 | r | 76/435 (18%) | 66 (87%) | 10 (13%) | 4 21 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 28 | t | 40/435 (9%) | 37 (92%) | 3 (8%) | 13 | 40 |
| 29 | u | 344/361 (95%) | 339 (98%) | 5 (2%) | 65 | 79 |
| 30 | v | 132/134 (98%) | 131 (99%) | 1 (1%) | 81 | 88 |
| 31 | w | 76/143 (53%) | 75 (99%) | 1 (1%) | 69 | 81 |
| 32 | x | 23/581 (4%) | 23 (100%) | 0 | 100 | 100 |
| 33 | a | 68/101 (67%) | 68 (100%) | 0 | 100 | 100 |
| 33 | h | 68/101 (67%) | 68 (100%) | 0 | 100 | 100 |
| 34 | b | 76/167 (46%) | 74 (97%) | 2 (3%) | 46 | 67 |
| 34 | i | 77/167 (46%) | 75 (97%) | 2 (3%) | 46 | 67 |
| 35 | c | 76/101 (75%) | 74 (97%) | 2 (3%) | 46 | 67 |
| 35 | j | 77/101 (76%) | 75 (97%) | 2 (3%) | 46 | 67 |
| 36 | d | 88/110 (80%) | 86 (98%) | 2 (2%) | 50 | 70 |
| 36 | k | 80/110 (73%) | 78 (98%) | 2 (2%) | 47 | 68 |
| 37 | f | 63/74 (85%) | 62 (98%) | 1 (2%) | 62 | 78 |
| 37 | m | 63/74 (85%) | 62 (98%) | 1 (2%) | 62 | 78 |
| 38 | e | 74/84 (88%) | 74 (100%) | 0 | 100 | 100 |
| 38 | l | 74/84 (88%) | 74 (100%) | 0 | 100 | 100 |
| 39 | g | 62/66 (94%) | 61 (98%) | 1 (2%) | 62 | 78 |
| 39 | n | 59/66 (89%) | 58 (98%) | 1 (2%) | 60 | 78 |
| 40 | o | 138/218 (63%) | 134 (97%) | 4 (3%) | 42 | 64 |
| 41 | p | 82/195 (42%) | 79 (96%) | 3 (4%) | 34 | 59 |
| 45 | 4 | 1/1 (100%) | 1 (100%) | 0 | 100 | 100 |
| All | All | 7083/15907 (44%) | 6534 (92%) | 549 (8%) | 16 | 39 |

5 of 549 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | X | 29 | LYS |
| 26 | Y | 24 | LYS |
| 25 | X | 25 | LYS |
| 29 | u | 301 | ASN |
| 3 | C | 941 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | N | 107 | GLN |
| 35 | c | 64 | ASN |
| 18 | R | 215 | ASN |
| 34 | b | 76 | ASN |
| 34 | i | 76 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 2 | B | 82/117 (70%) | 17 (20%) | 6 (7%) |
| 6 | F | 96/107 (89%) | 43 (44%) | 17 (17%) |
| 7 | G | 85/275 (30%) | 50 (58%) | 8 (9%) |
| 8 | H | 132/188 (70%) | 26 (19%) | 4 (3%) |
| All | All | 395/687 (57%) | 136 (34%) | 35 (8%) |

5 of 136 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 12 | U |
| 2 | B | 13 | C |
| 2 | B | 19 | A |
| 2 | B | 20 | G |
| 2 | B | 21 | A |

5 of 35 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 23 | U |
| 7 | G | 146 | C |
| 8 | H | 156 | U |
| 6 | F | 35 | A |
| 6 | F | 34 | G |

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 18 | SEP | R | 224 | 18 | 8,9,10 | 0.81 | 0 | 8,12,14 | 1.14 | 0 |
| 18 | SEP | R | 232 | 18 | 8,9,10 | 0.73 | 0 | 8,12,14 | 1.38 | 1 (12%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 18 | SEP | R | 224 | 18 | - | 3/5/8/10 | - |
| 18 | SEP | R | 232 | 18 | - | 2/5/8/10 | - |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 18 | R | 232 | SEP | OG-CB-CA | -2.55 | 105.67 | 108.14 |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 18 | R | 224 | SEP | CB-OG-P-O1P |
| 18 | R | 224 | SEP | CB-OG-P-O2P |
| 18 | R | 224 | SEP | CB-OG-P-O3P |
| 18 | R | 232 | SEP | N-CA-CB-OG |
| 18 | R | 232 | SEP | CA-CB-OG-P |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 14 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 46 | IHP | A | 3000 | - | 36,36,36 | 1.01 | 2 (5%) | 54,60,60 | 1.62 | 12 (22%) |
| 49 | ADP | D | 2202 | - | 24,29,29 | 0.95 | 1 (4%) | 29,45,45 | 1.47 | 4 (13%) |
| 51 | ATP | u | 702 | 48 | 26,33,33 | 0.92 | 0 | 31,52,52 | 1.54 | 5 (16%) |
| 49 | ADP | D | 2201 | - | 24,29,29 | 0.97 | 1 (4%) | 29,45,45 | 1.34 | 4 (13%) |
| 47 | GTP | C | 1500 | 48 | 26,34,34 | 1.17 | 1 (3%) | 32,54,54 | 1.81 | 8 (25%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 46 | IHP | A | 3000 | - | - | 6/30/54/54 | 0/1/1/1 |
| 49 | ADP | D | 2202 | - | - | 2/12/32/32 | 0/3/3/3 |
| 51 | ATP | u | 702 | 48 | - | 0/18/38/38 | 0/3/3/3 |
| 49 | ADP | D | 2201 | - | - | 8/12/32/32 | 0/3/3/3 |
| 47 | GTP | C | 1500 | 48 | - | 7/18/38/38 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 47 | C | 1500 | GTP | C6-N1 | -3.48 | 1.32 | 1.37 |
| 46 | A | 3000 | IHP | P5-O45 | -2.84 | 1.43 | 1.54 |
| 46 | A | 3000 | IHP | P2-O12 | 2.65 | 1.64 | 1.59 |
| 49 | D | 2201 | ADP | C5-C4 | 2.52 | 1.47 | 1.40 |
| 49 | D | 2202 | ADP | C5-C4 | 2.31 | 1.47 | 1.40 |

The worst 5 of 33 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 51 | u | 702 | ATP | PB-O3B-PG | -4.33 | 117.98 | 132.83 |
| 46 | A | 3000 | IHP | O45-P5-O35 | 4.09 | 123.25 | 107.64 |
| 51 | u | 702 | ATP | N3-C2-N1 | -4.08 | 122.30 | 128.68 |
| 49 | D | 2202 | ADP | PA-O3A-PB | -4.02 | 119.02 | 132.83 |
| 46 | A | 3000 | IHP | O35-P5-O15 | -3.97 | 88.20 | 105.99 |

There are no chirality outliers.

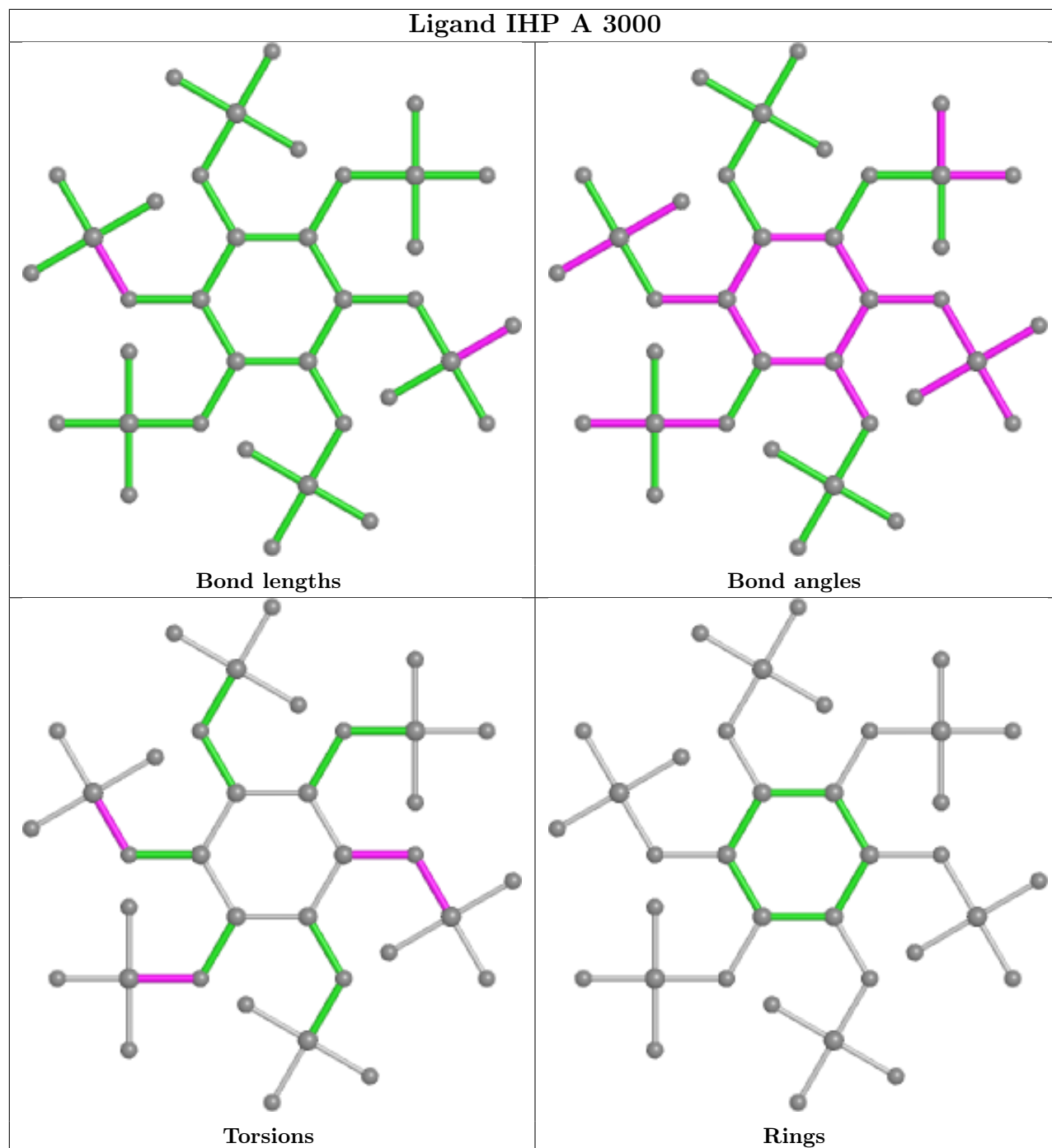
5 of 23 torsion outliers are listed below:

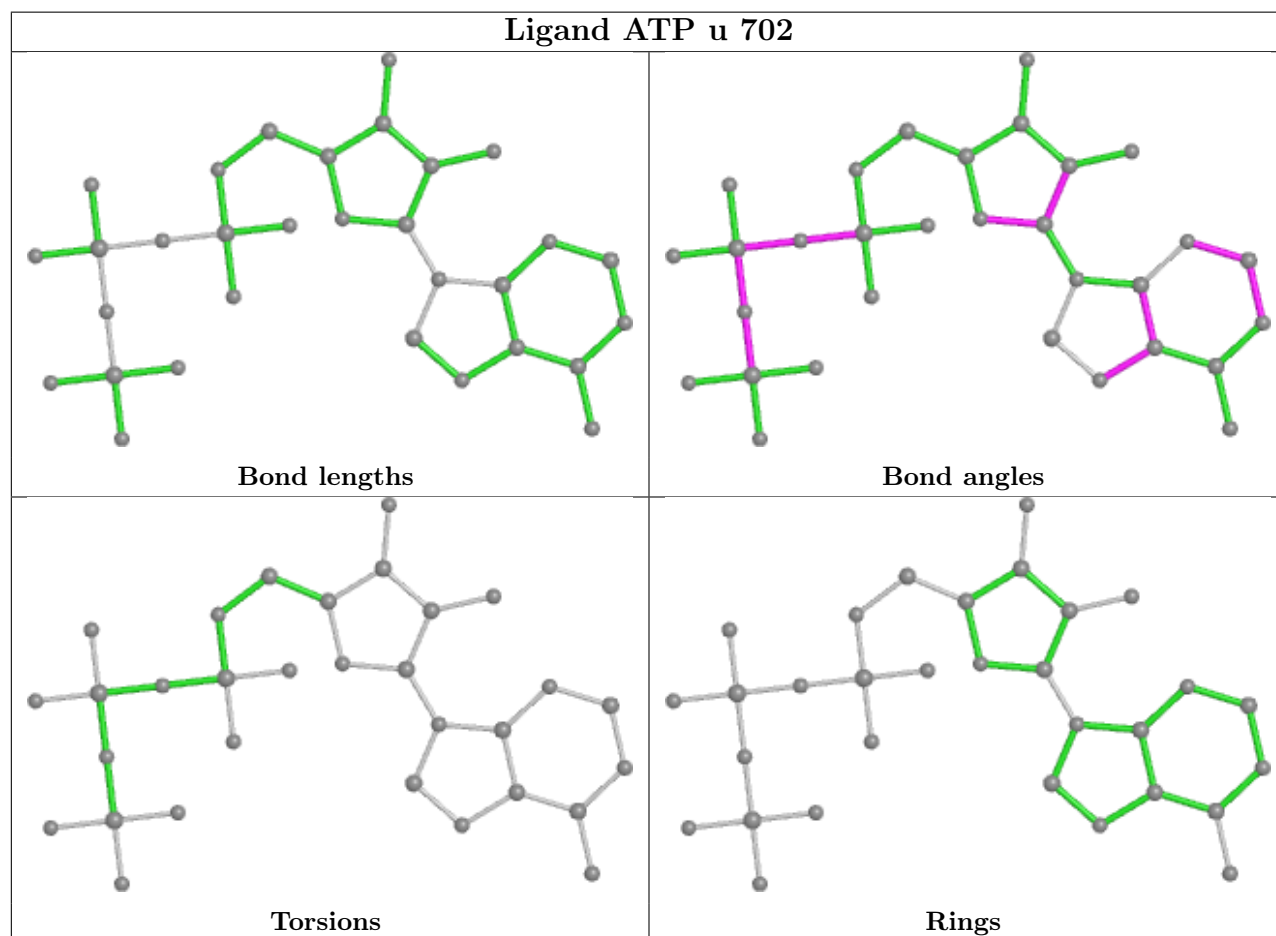
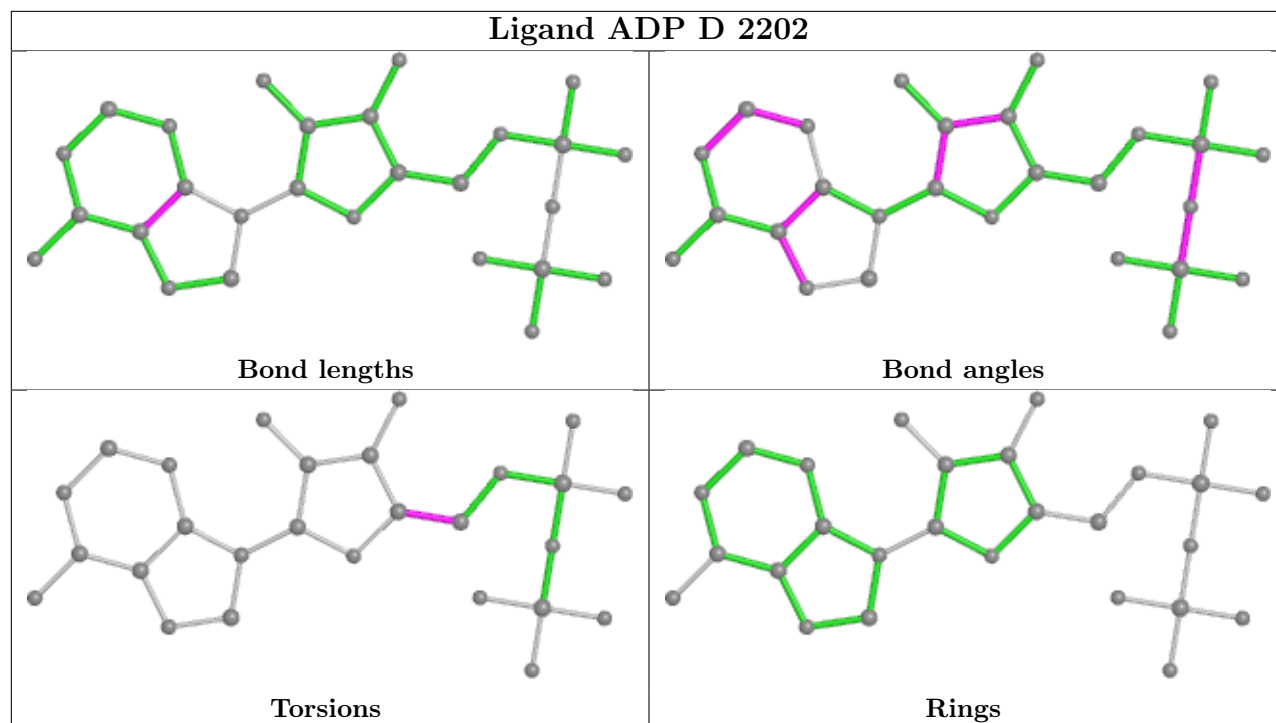
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 46 | A | 3000 | IHP | C4-C5-O15-P5 |
| 46 | A | 3000 | IHP | C6-C5-O15-P5 |
| 47 | C | 1500 | GTP | PB-O3B-PG-O3G |
| 47 | C | 1500 | GTP | C5'-O5'-PA-O3A |
| 47 | C | 1500 | GTP | C5'-O5'-PA-O1A |

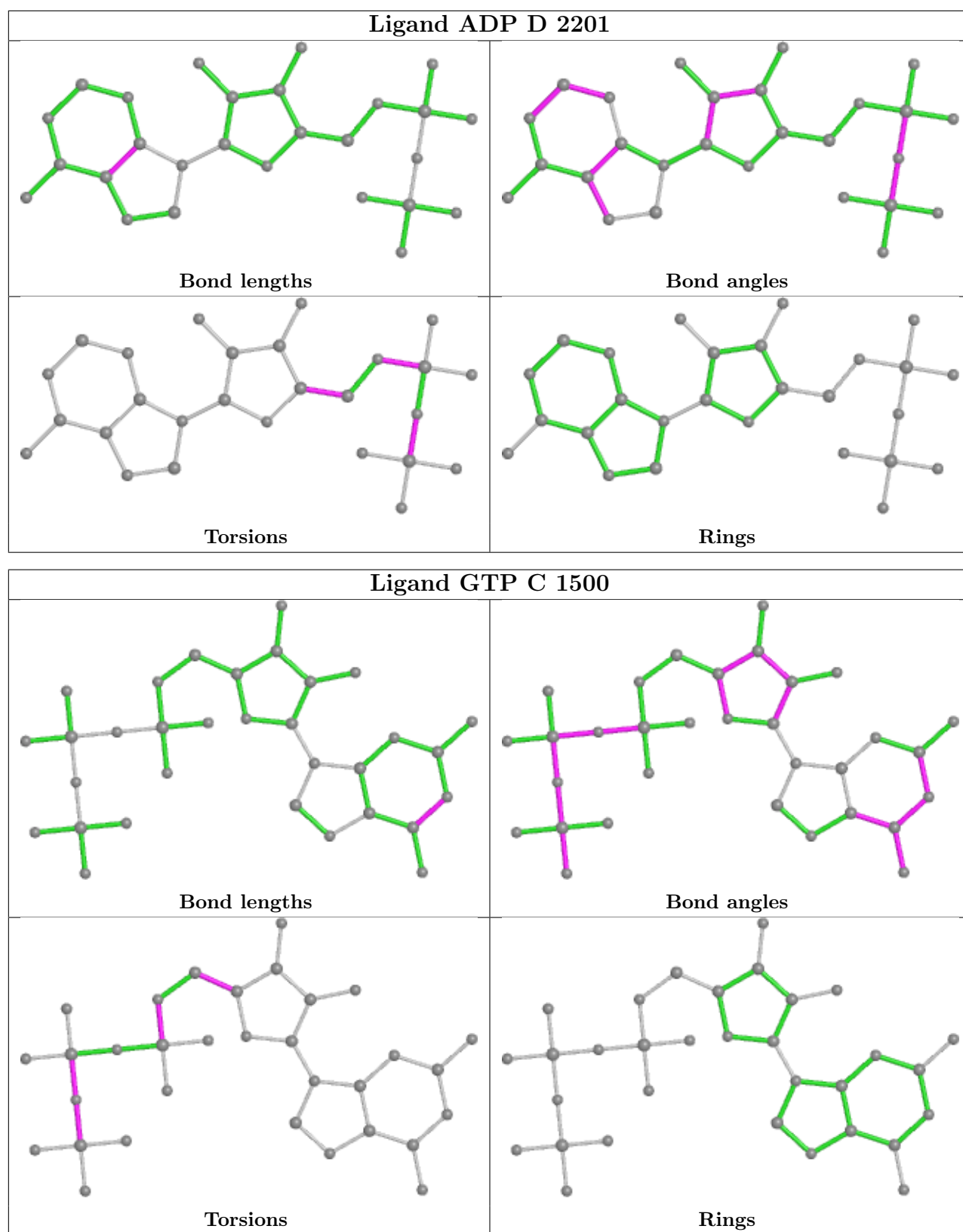
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

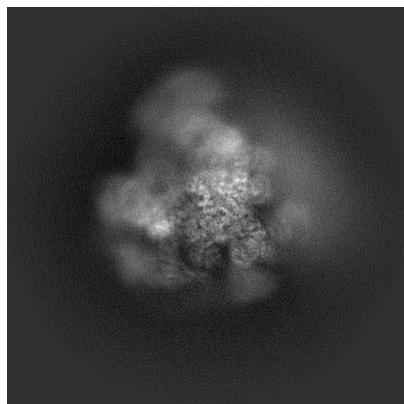
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6864. These allow visual inspection of the internal detail of the map and identification of artifacts.

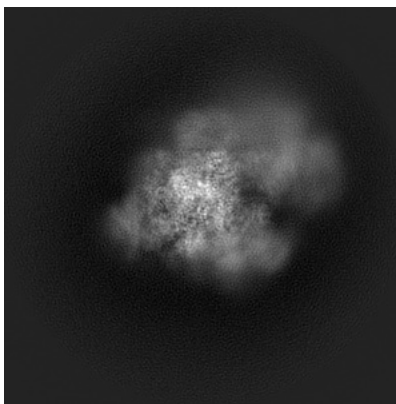
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

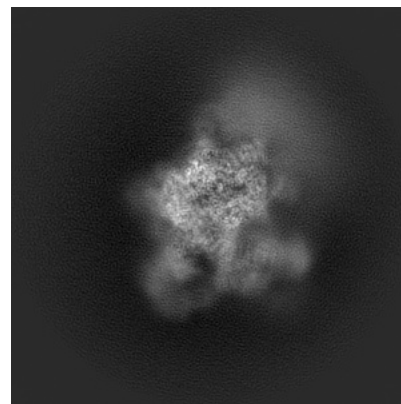
6.1.1 Primary map



X

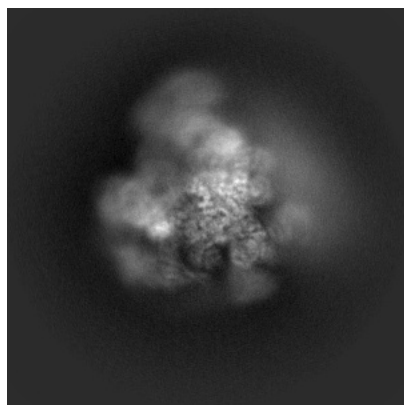


Y

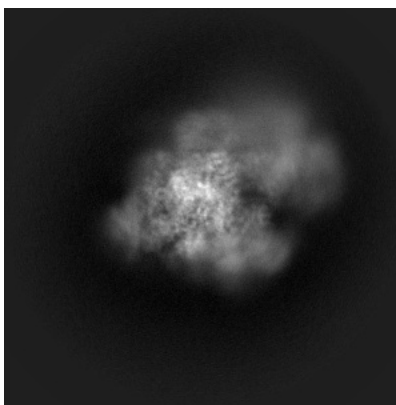


Z

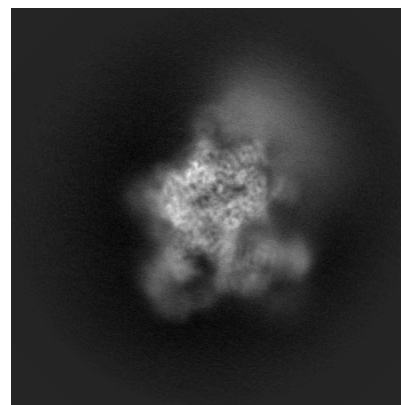
6.1.2 Raw map



X



Y

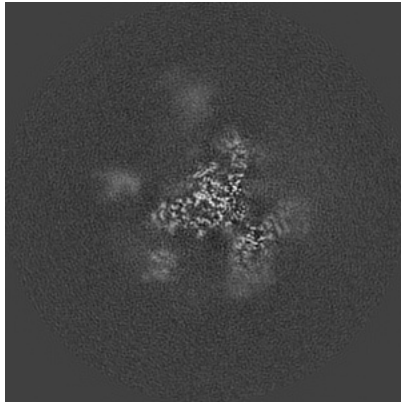


Z

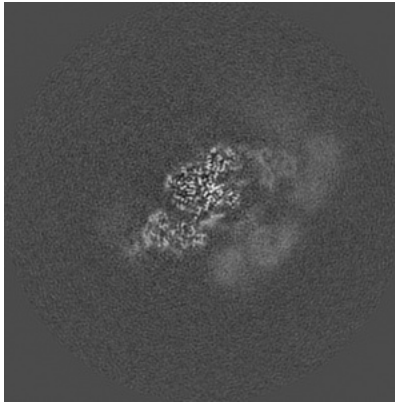
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

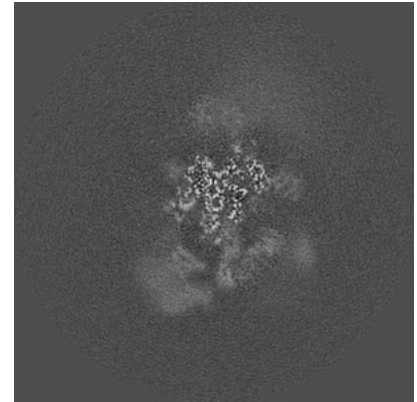
6.2.1 Primary map



X Index: 200

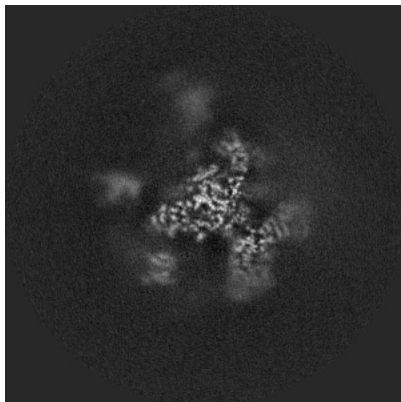


Y Index: 200

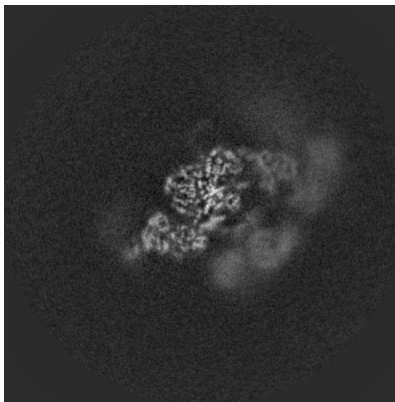


Z Index: 200

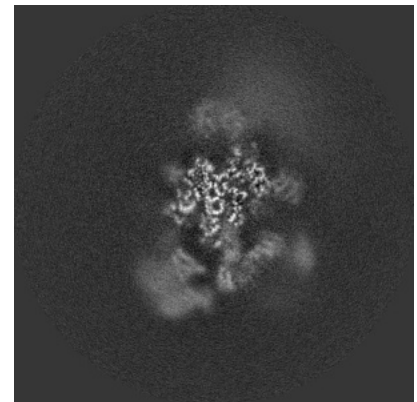
6.2.2 Raw map



X Index: 200



Y Index: 200

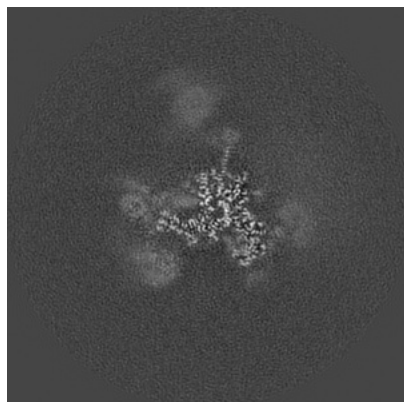


Z Index: 200

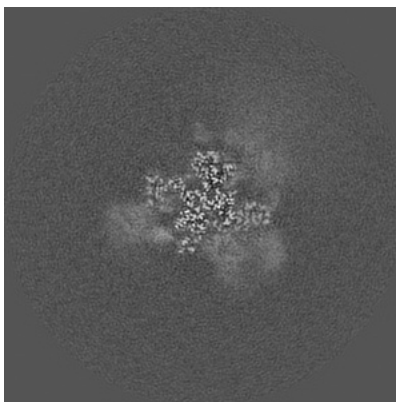
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

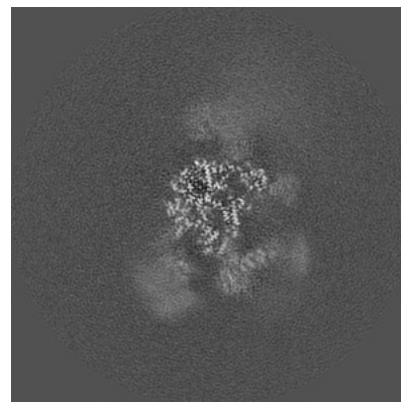
6.3.1 Primary map



X Index: 210

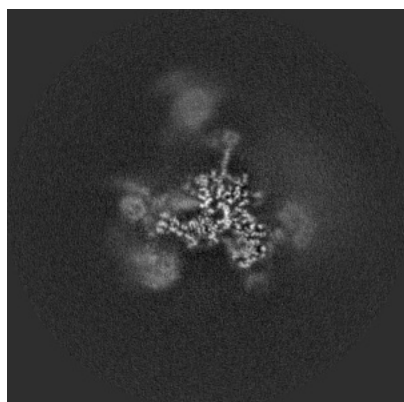


Y Index: 229

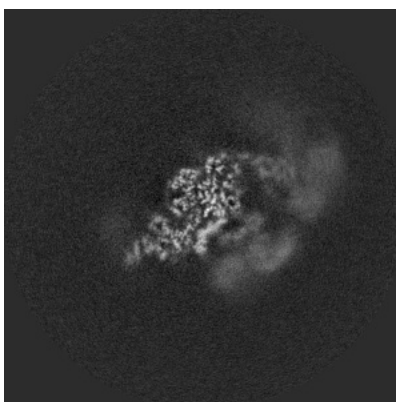


Z Index: 194

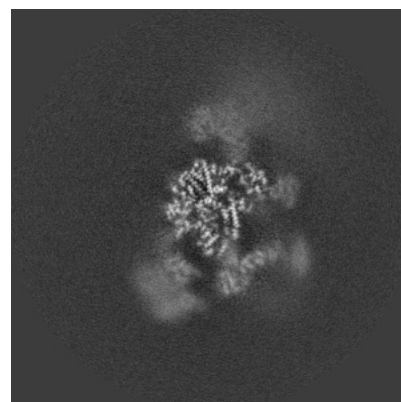
6.3.2 Raw map



X Index: 210



Y Index: 197



Z Index: 195

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

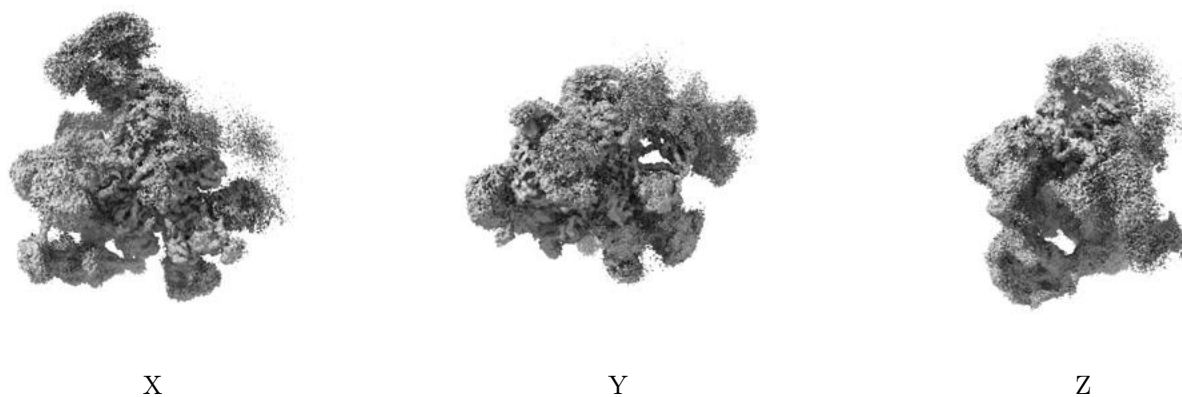
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.029. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

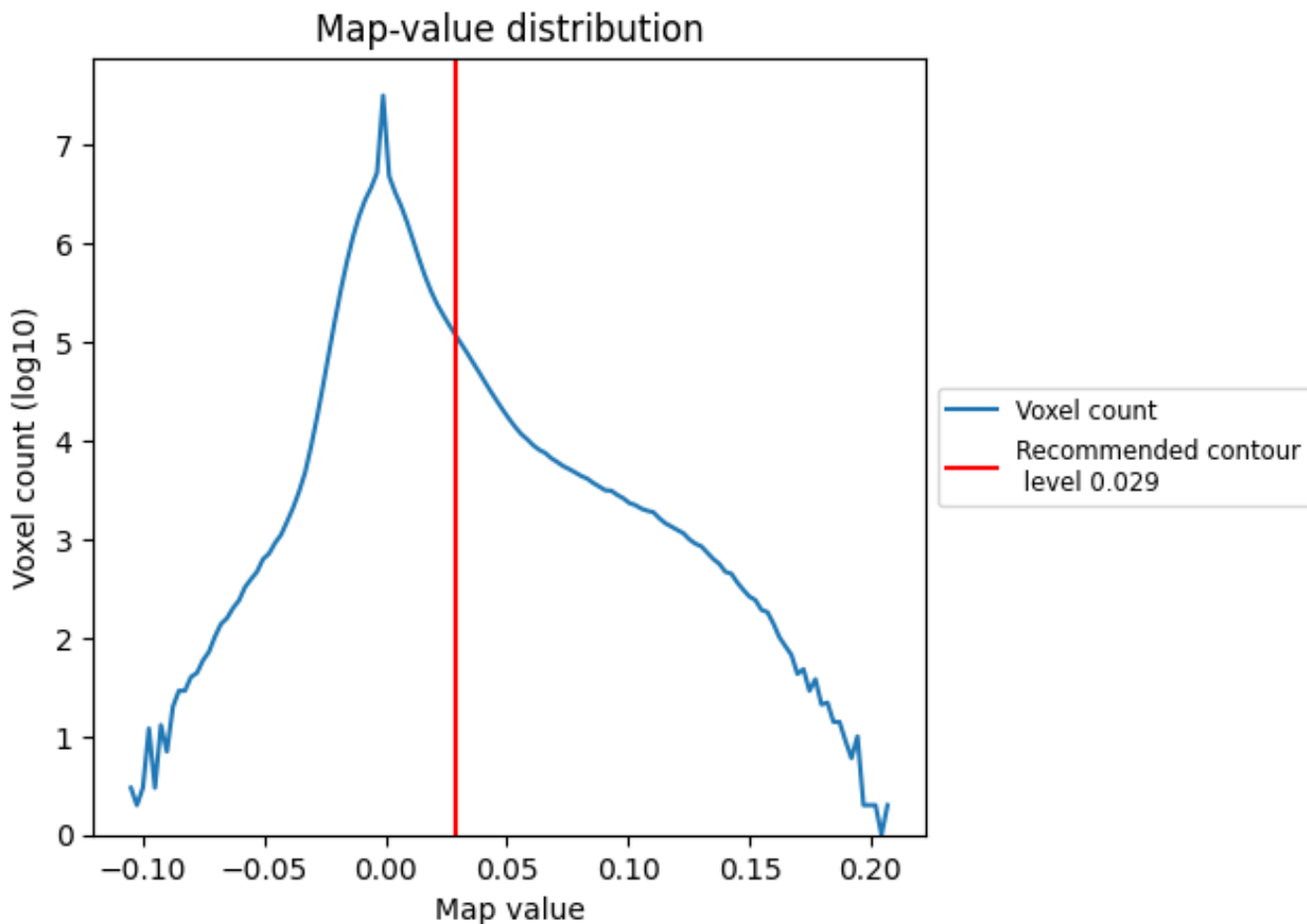
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

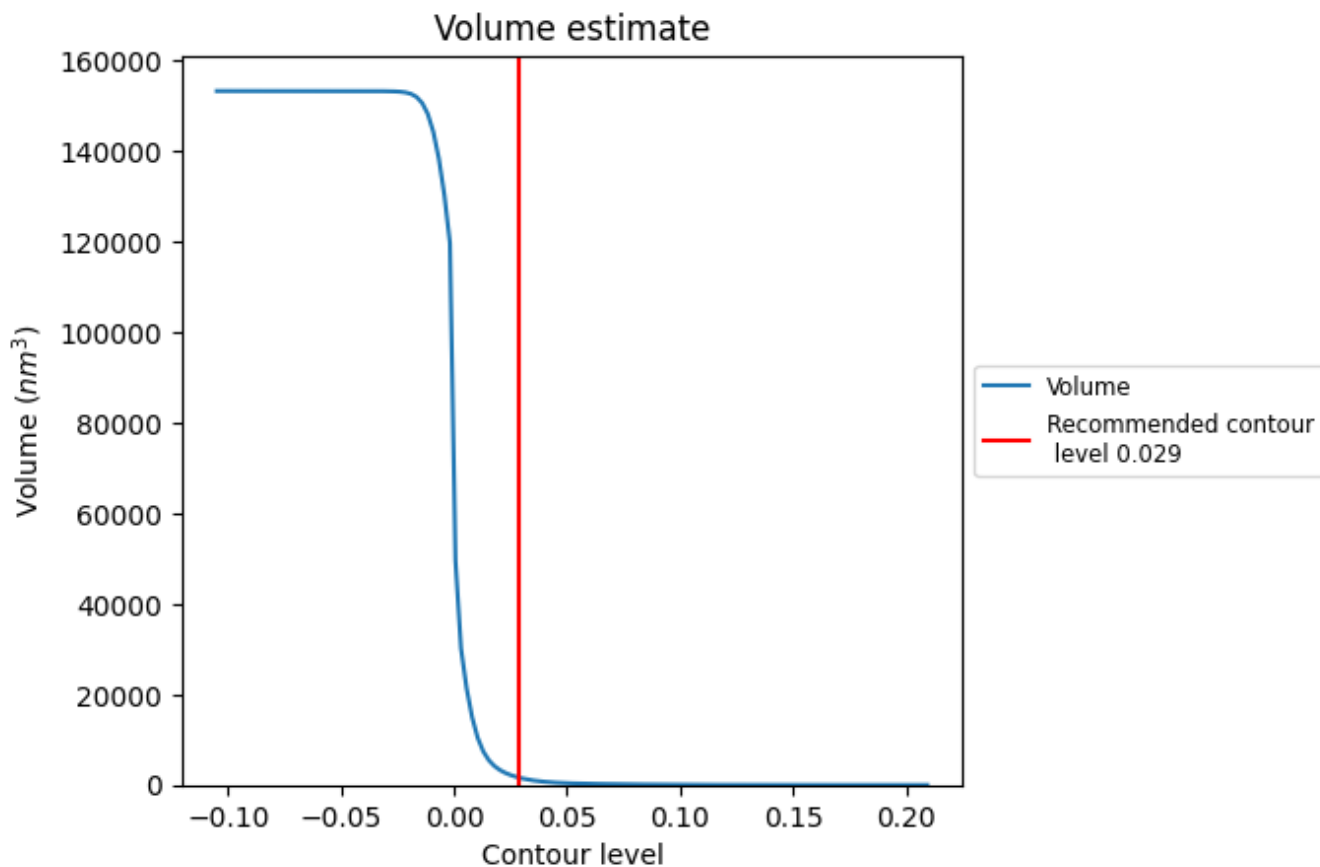
This section contains the results of statistical analysis of the map.

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.

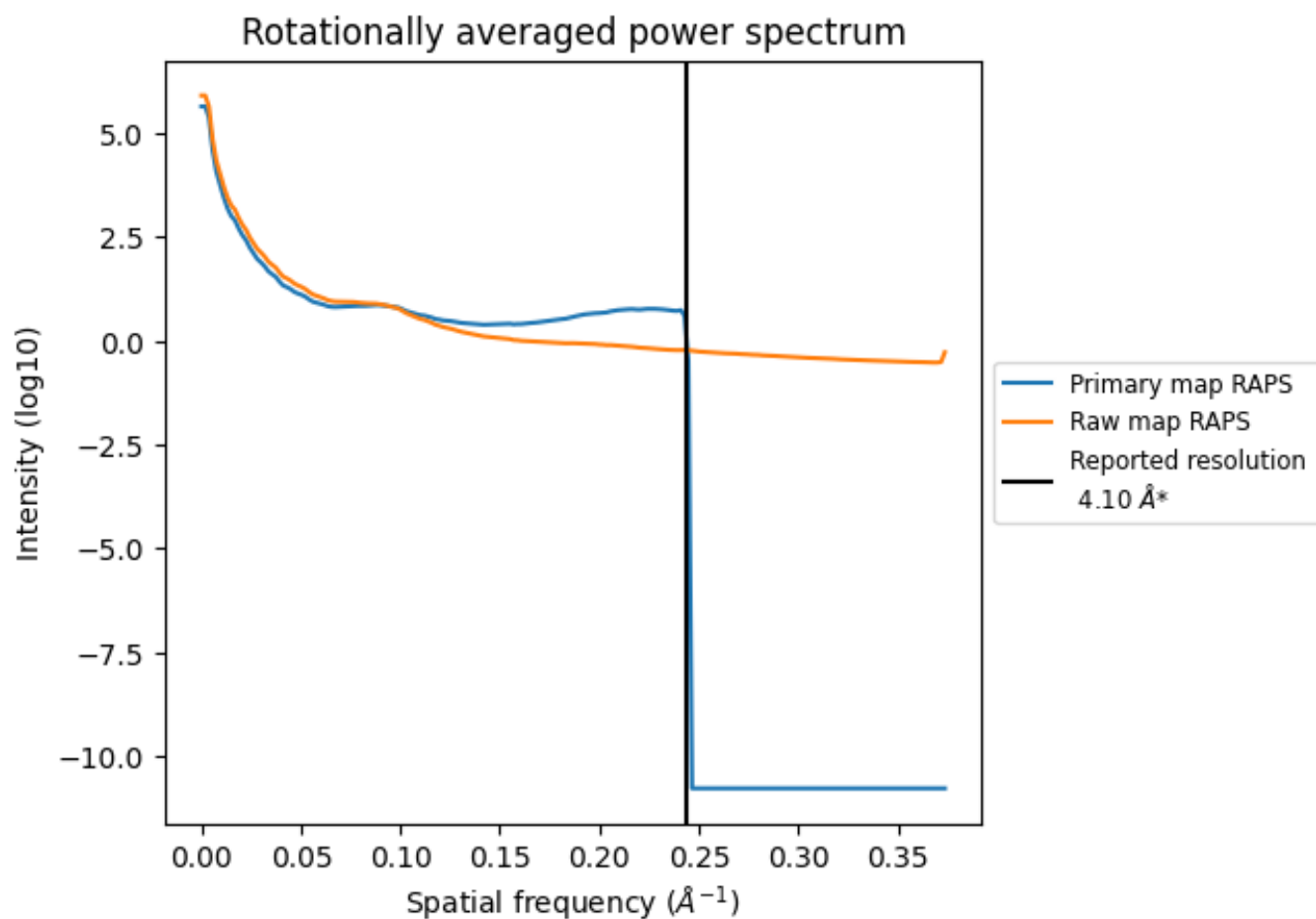
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1595 nm³; this corresponds to an approximate mass of 1441 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](#)

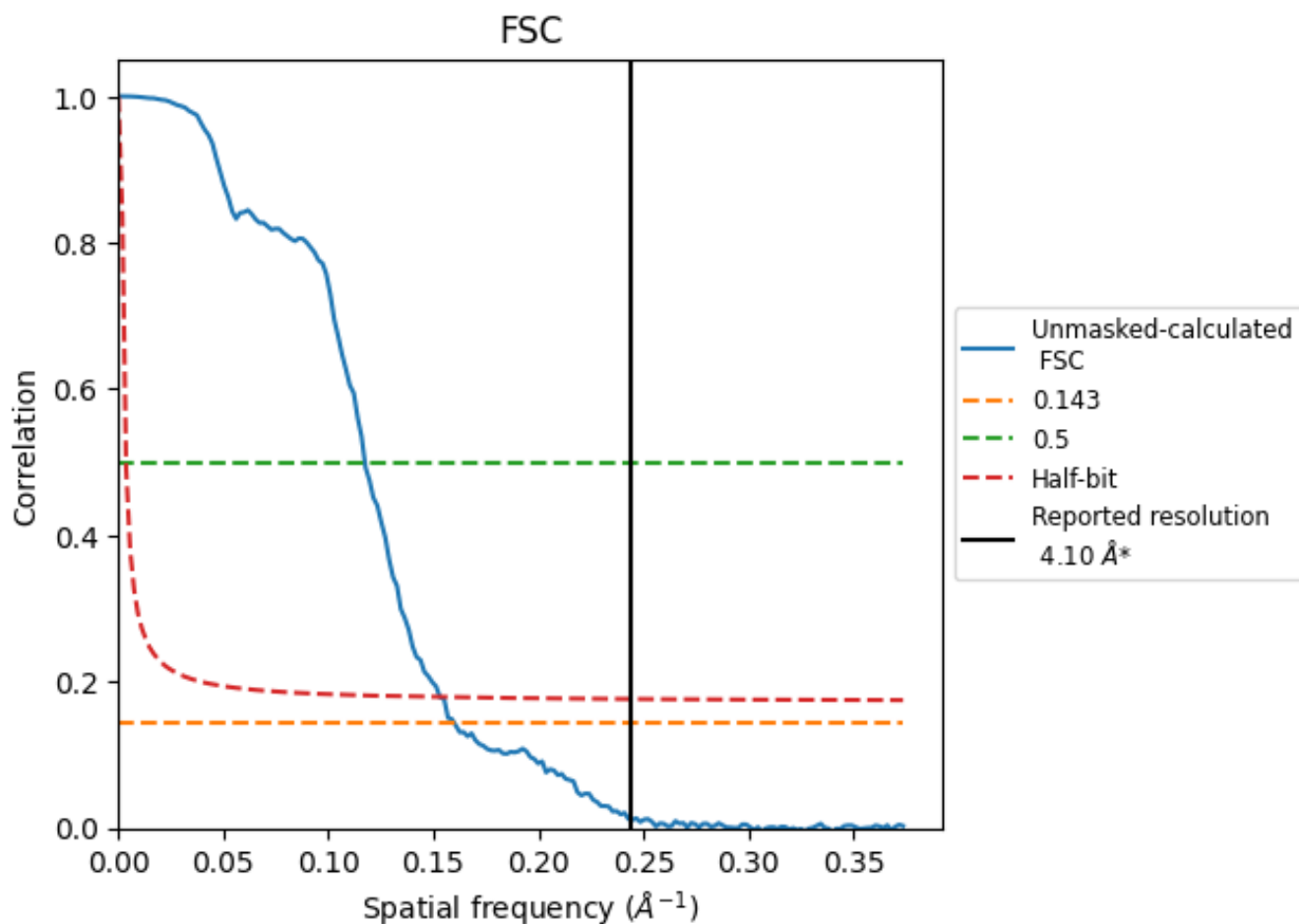


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

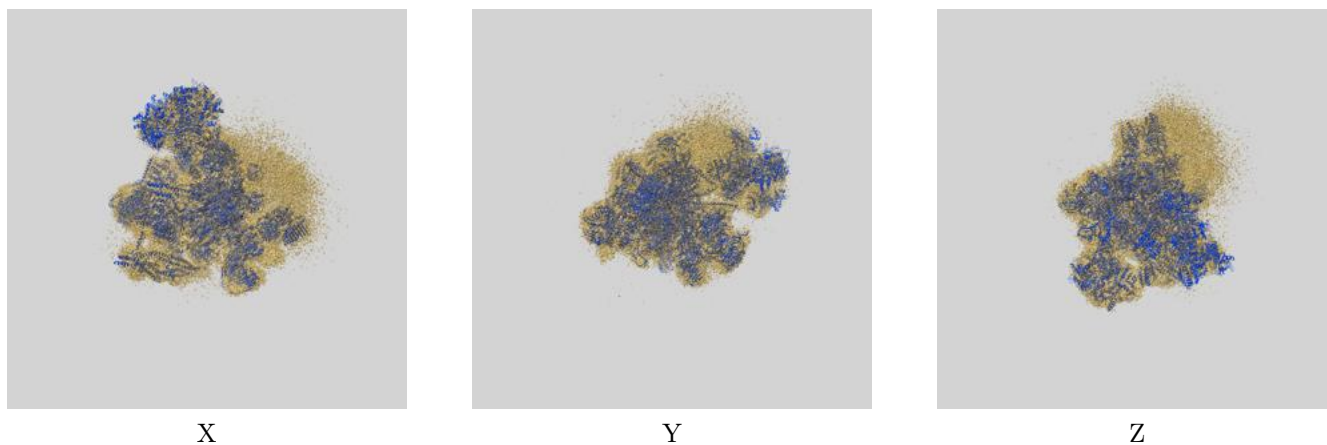
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.10 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 6.25 | 8.52 | 6.53 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.25 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

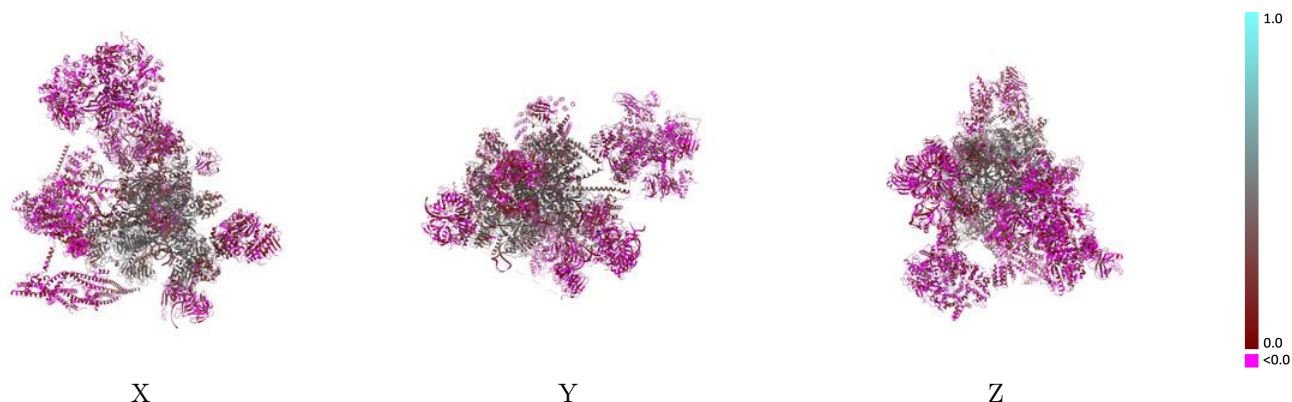
This section contains information regarding the fit between EMDB map EMD-6864 and PDB model 5YZG. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



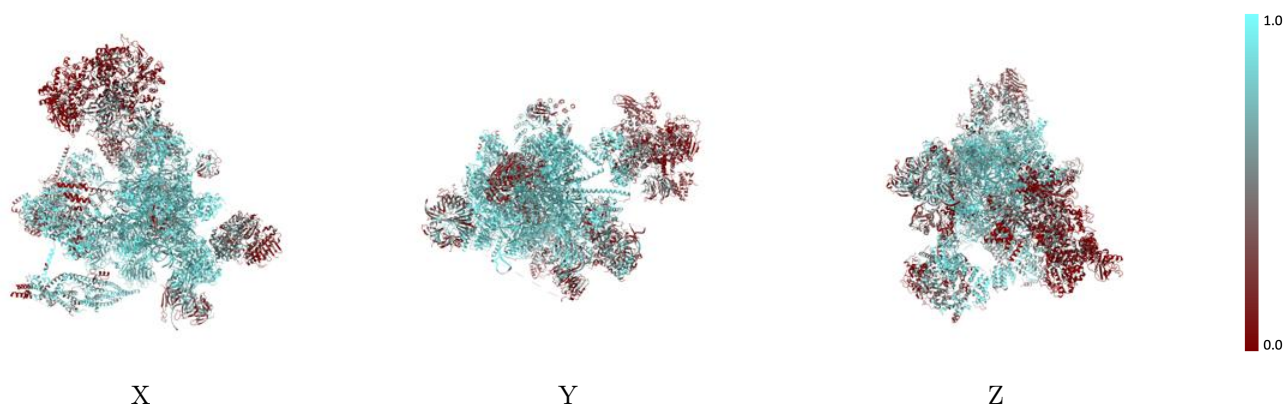
The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



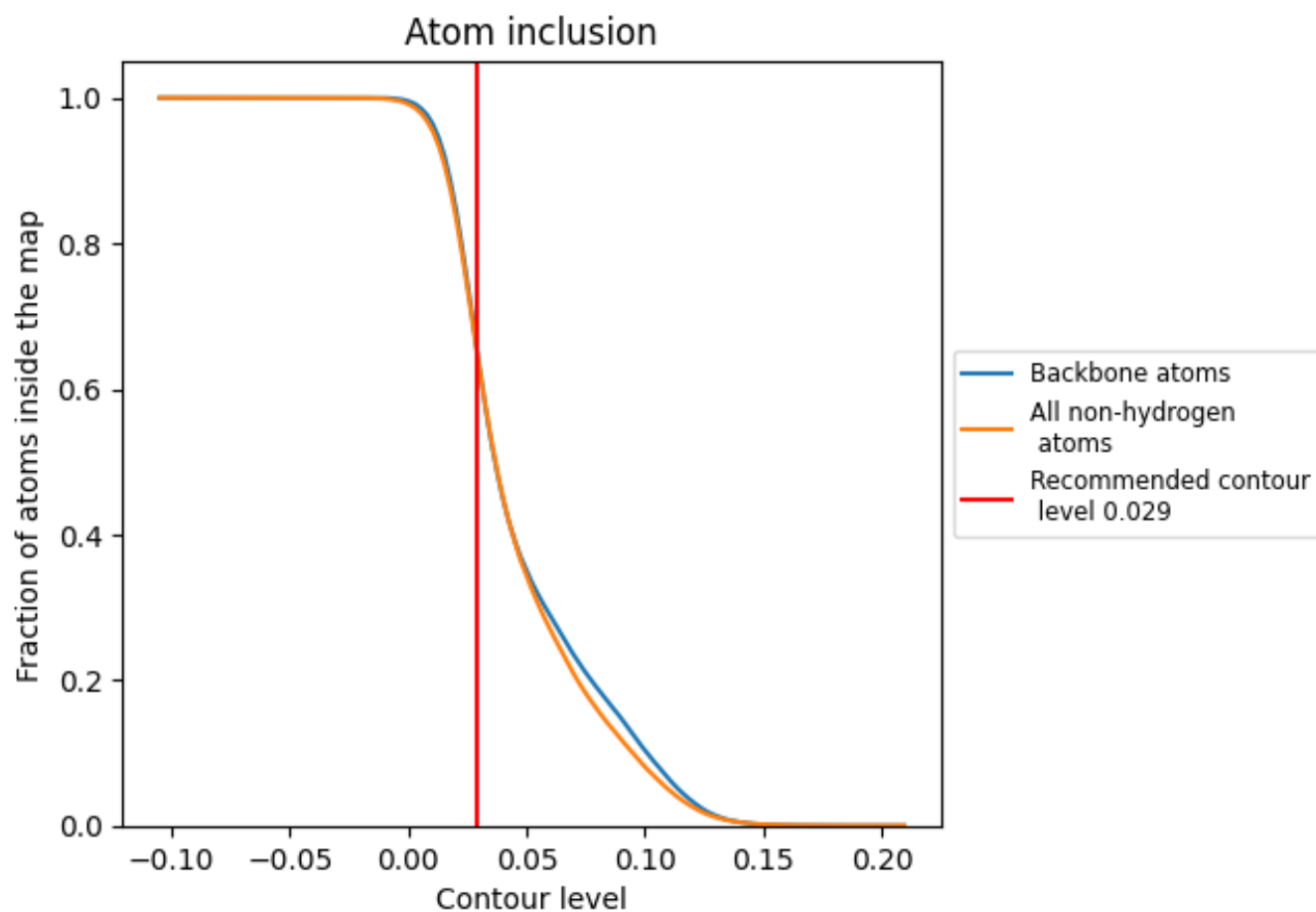
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.029).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary











































The table lists the average atom inclusion at the recommended contour level (0.029) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.6506 |  0.2050 |
| 1 |  0.7202 |  0.1430 |
| 2 |  0.4002 |  0.0390 |
| 3 |  0.4678 |  0.1560 |
| 4 |  0.8696 |  0.3750 |
| A |  0.8373 |  0.3780 |
| B |  0.8518 |  0.2730 |
| C |  0.8681 |  0.3820 |
| D |  0.1458 |  0.0280 |
| E |  0.8899 |  0.3500 |
| F |  0.8649 |  0.2960 |
| G |  0.8507 |  0.2700 |
| H |  0.6307 |  0.0890 |
| I |  0.7740 |  0.0680 |
| J |  0.7230 |  0.2200 |
| K |  0.7125 |  0.0690 |
| L |  0.7545 |  0.2330 |
| M |  0.6960 |  0.2110 |
| N |  0.8733 |  0.4120 |
| O |  0.8471 |  0.3230 |
| P |  0.8098 |  0.3700 |
| Q |  0.4888 |  0.0330 |
| R |  0.8266 |  0.3610 |
| S |  0.8434 |  0.3040 |
| T |  0.9239 |  0.4440 |
| U |  0.9358 |  0.4430 |
| V |  0.6770 |  0.2120 |
| W |  0.7043 |  0.1780 |
| X |  0.8270 |  0.3130 |
| Y |  0.8358 |  0.3570 |
| Z |  0.6213 |  0.1250 |
| a |  0.3926 |  0.0090 |
| b |  0.3742 |  0.0240 |
| c |  0.4241 |  0.0370 |
| d |  0.4005 |  0.0410 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| e |  0.5362 |  0.0140 |
| f |  0.4081 |  0.0310 |
| g |  0.4813 |  0.0080 |
| h |  0.5263 |  0.0240 |
| i |  0.4030 |  -0.0170 |
| j |  0.4984 |  0.0360 |
| k |  0.4199 |  0.0330 |
| l |  0.4906 |  -0.0020 |
| m |  0.5671 |  0.0230 |
| n |  0.5657 |  0.0530 |
| o |  0.1711 |  0.0460 |
| p |  0.3105 |  -0.0180 |
| q |  0.4197 |  0.0250 |
| r |  0.6584 |  0.0370 |
| s |  0.4311 |  0.0090 |
| t |  0.5923 |  0.0430 |
| u |  0.4448 |  0.0850 |
| v |  0.1648 |  0.0720 |
| w |  0.1538 |  0.0230 |
| x |  0.0861 |  0.0040 |
| y |  0.7299 |  0.1960 |