# Full wwPDB EM Validation Report ⓘ

Oct 28, 2026 – 05:36 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 9SJ3 / pdb_00009sj3 |
| EMDB ID | : | EMD-54936 |
| Title | : | Structure of a circMbl 48S translation initiation complex in the AUG recognition state |
| Authors | : | Zuber, P.K.; Li, X.; Du, Y.; Gordiyenko, Y.; Haddad, T.F.M.; Ramakrishnan, V. |
| Deposited on | : | 2025-08-29 |
| Resolution | : | 4.00 Å(reported) |
| Based on initial models | : | 1YFG, 6ZMW |

This is a Full wwPDB EM Validation 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.

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

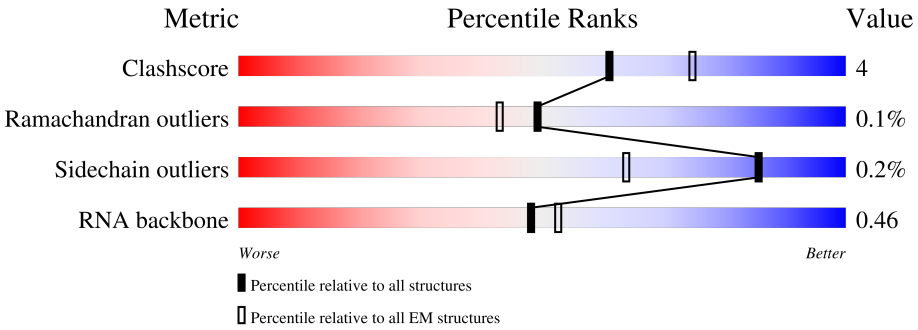
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.2 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.51 |

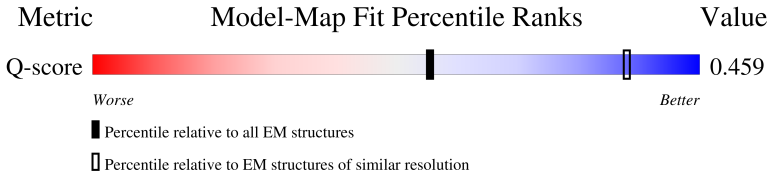
# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 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) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| RNA backbone | 8273 | 3508 | - |
| Q-score | - | 25397 | 7587 ( 3.50 - 4.50 ) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1382 | 39% 45% 8% 47% |
| 2 | B | 445 | 84% 76% 10% 14% |
| 3 | D | 315 | 44% 77% 11% 12% |

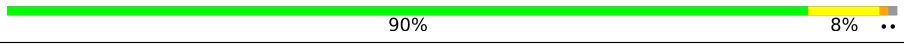
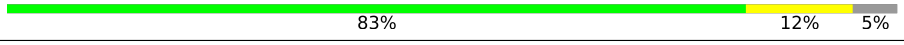
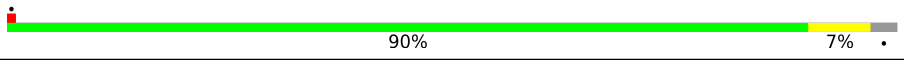
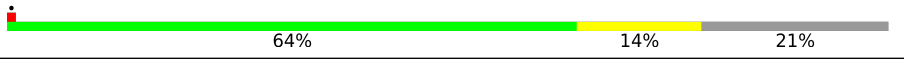
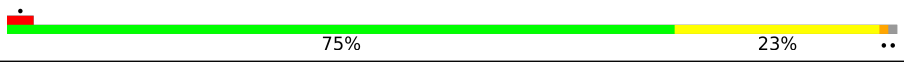
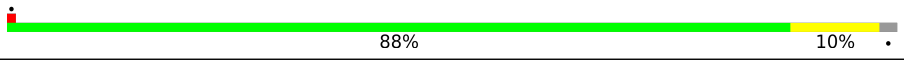
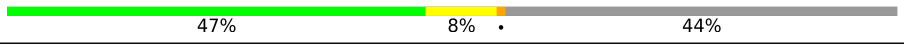
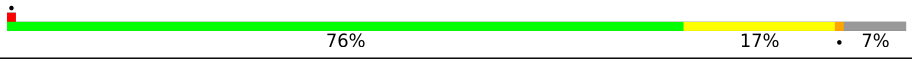
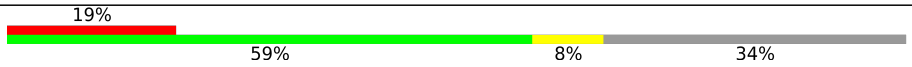
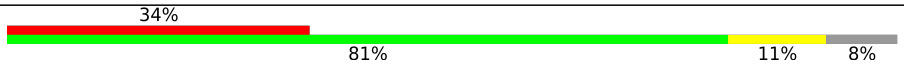
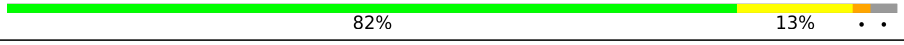
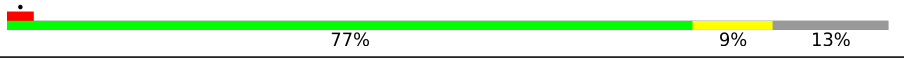
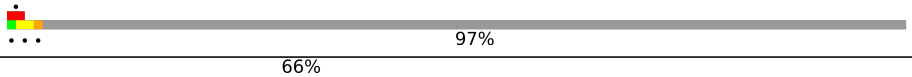
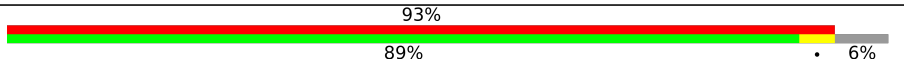
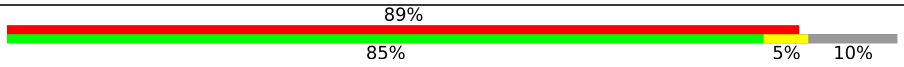
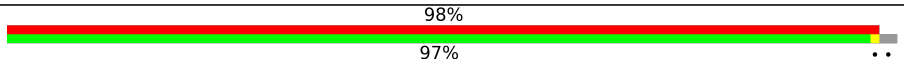
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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | E | 472 | 98% 85% 13% |
| 5 | F | 325 | 100% 97% |
| 6 | G | 147 | 26% 56% 10% 34% |
| 7 | H | 116 | 67% 60% 13% 27% |
| 8 | I | 814 | 71% 63% 8% 29% |
| 9 | J | 913 | 45% 60% 10% 29% |
| 10 | L | 194 | 76% 15% 8% |
| 11 | M | 84 | 74% 21% |
| 12 | N | 83 | 90% 7% |
| 13 | O | 293 | 68% 7% 25% |
| 14 | P | 264 | 67% 12% 20% |
| 15 | Q | 295 | 62% 11% 28% |
| 16 | R | 115 | 80% 6% 14% |
| 17 | S | 249 | 79% 14% 8% |
| 18 | T | 151 | 75% 13% 12% |
| 19 | V | 151 | 95% 5% |
| 20 | W | 1869 | 59% 26% 5% 8% |
| 21 | X | 158 | 81% 9% 10% |
| 22 | Y | 263 | 90% 7% |
| 23 | Z | 194 | 82% 9% 9% |
| 24 | y | 75 | 24% 55% 32% 11% |
| 25 | 7 | 320 | 22% 21% 76% |
| 26 | 9 | 25 | 8% 80% 16% |
| 27 | a | 143 | 90% 8% |
| 28 | b | 59 | 14% 90% 7% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | c | 130 |   |
| 30 | d | 208 |   |
| 31 | e | 133 |   |
| 32 | f | 204 |   |
| 33 | g | 146 |   |
| 34 | h | 243 |   |
| 35 | i | 165 |   |
| 36 | j | 145 |   |
| 37 | k | 317 |   |
| 38 | l | 145 |   |
| 39 | m | 125 |   |
| 40 | n | 152 |   |
| 41 | o | 56 |   |
| 42 | p | 80 |   |
| 43 | q | 132 |   |
| 44 | s | 69 |   |
| 45 | v | 135 |   |
| 46 | w | 119 |   |
| 47 | z | 774 |   |
| 48 | x | 548 |   |
| 49 | 6 | 374 |   |
| 50 | 4 | 357 |   |
| 51 | 8 | 352 |   |
| 52 | 3 | 218 |   |
| 53 | 5 | 564 |   |

# 2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 114857 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 Eukaryotic translation initiation factor 3 subunit A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 733 | 5504 | 3452 | 1005 | 1024 | 23 | 0 | 0 |

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 384 | 2635 | 1657 | 477 | 489 | 12 | 0 | 0 |

- Molecule 3 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | D | 278 | 2234 | 1410 | 390 | 421 | 13 | 0 | 0 |

- Molecule 4 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | E | 464 | 3540 | 2245 | 620 | 658 | 17 | 0 | 0 |

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit I.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 5 | F | 325 | 1598 | 947 | 325 | 326 | 0 | 0 |

- Molecule 6 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | G | 97 | 789 | 492 | 147 | 146 | 4 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | -2 | GLY | - | expression tag | UNP P47813 |
| G | -1 | ALA | - | expression tag | UNP P47813 |
| G | 0 | HIS | - | expression tag | UNP P47813 |

- Molecule 7 is a protein called Eukaryotic translation initiation factor 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | H | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 691 | 438 | 125 | 126 | 2 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| H | -2 | GLY | - | expression tag | UNP P41567 |
| H | -1 | ALA | - | expression tag | UNP P41567 |
| H | 0 | HIS | - | expression tag | UNP P41567 |

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | I | 575 | Total | C | N | O | S | 0 | 0 |
| | | | 4569 | 2935 | 788 | 828 | 18 | | |

- Molecule 9 is a protein called Eukaryotic translation initiation factor 3 subunit C.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | J | 645 | Total | C | N | O | S | 0 | 0 |
| | | | 4940 | 3096 | 888 | 923 | 33 | | |

- Molecule 10 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | L | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1439 | 923 | 262 | 253 | 1 | | |

- Molecule 11 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | M | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 631 | 397 | 116 | 111 | 7 | | |

- Molecule 12 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | N | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 636 | 393 | 117 | 121 | 5 | | |

- Molecule 13 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | O | 220 | Total | C | N | O | S | 0 | 0 |
| | | | 1707 | 1104 | 292 | 301 | 10 | | |

- Molecule 14 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | P | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1715 | 1088 | 307 | 306 | 14 | | |

- Molecule 15 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | Q | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1686 | 1072 | 295 | 311 | 8 | | |

- Molecule 16 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | R | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 792 | 492 | 165 | 130 | 5 | | |

- Molecule 17 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | S | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1862 | 1164 | 371 | 320 | 7 | | |

- Molecule 18 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | T | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 998 | 610 | 196 | 186 | 6 | | |

- Molecule 19 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | V | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1208 | 773 | 229 | 205 | 1 | | |

- Molecule 20 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | W | 1717 | Total | C | N | O | P | 0 | 0 |
| | | | 36695 | 16405 | 6575 | 11998 | 1717 | | |

- Molecule 21 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | X | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1166 | 743 | 218 | 199 | 6 | | |

- Molecule 22 is a protein called Small ribosomal subunit protein eS4, X isoform.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | Y | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2041 | 1305 | 379 | 349 | 8 | | |

- Molecule 23 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | Z | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1477 | 941 | 295 | 239 | 2 | | |

- Molecule 24 is a RNA chain called tRNAi-Met.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | y | 75 | Total | C | N | O | P | 0 | 0 |
| | | | 1639 | 734 | 298 | 531 | 76 | | |

- Molecule 25 is a protein called Eukaryotic translation initiation factor 3 subunit G.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 25 | 7 | 77 | Total | C | N | O | 0 | 0 |
| | | | 616 | 389 | 111 | 116 | | |

- Molecule 26 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | 9 | 24 | Total | C | N | O | S | 0 | 0 |
| | | | 230 | 139 | 62 | 26 | 3 | | |

- Molecule 27 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | a | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1087 | 687 | 215 | 182 | 3 | | |

- Molecule 28 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | b | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 452 | 279 | 99 | 73 | 1 | | |

- Molecule 29 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | c | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1034 | 659 | 193 | 176 | 6 | | |

- Molecule 30 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | d | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1628 | 1021 | 322 | 280 | 5 | | |

- Molecule 31 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | e | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 1015 | 642 | 199 | 169 | 5 | | |

- Molecule 32 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | f | 184 | Total | C | N | O | S | 0 | 0 |
| | | | 1461 | 914 | 276 | 264 | 7 | | |

- Molecule 33 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | g | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1124 | 715 | 212 | 194 | 3 | | |

- Molecule 34 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | h | 225 | Total | C | N | O | S | 0 | 0 |
| | | | 1752 | 1117 | 315 | 313 | 7 | | |

- Molecule 35 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | i | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 834 | 544 | 149 | 135 | 6 | | |

- Molecule 36 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | j | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 946 | 602 | 175 | 162 | 7 | | |

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | k | 313 | Total | C | N | O | S | 0 | 0 |
| | | | 2436 | 1535 | 424 | 465 | 12 | | |

- Molecule 38 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | l | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1105 | 692 | 213 | 197 | 3 | | |

- Molecule 39 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | m | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 559 | 360 | 102 | 96 | 1 | | |

- Molecule 40 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | n | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1176 | 737 | 239 | 199 | 1 | | |

- Molecule 41 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | o | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 459 | 286 | 94 | 74 | 5 | | |

- Molecule 42 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | p | 53 | Total | C | N | O | S | 0 | 0 |
| | | | 435 | 276 | 82 | 70 | 7 | | |

- Molecule 43 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | q | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 950 | 596 | 168 | 177 | 9 | | |

- Molecule 44 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | s | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 498 | 302 | 101 | 93 | 2 | | |

- Molecule 45 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | v | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1064 | 668 | 198 | 194 | 4 | | |

- Molecule 46 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | w | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 817 | 511 | 155 | 147 | 4 | | |

- Molecule 47 is a RNA chain called circMbl-FLAG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | z | 27 | Total | C | N | O | P | 0 | 0 |
| | | | 575 | 258 | 106 | 184 | 27 | | |

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit D.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | x | 440 | Total | C | N | O | S | 0 | 0 |
| | | | 2920 | 1798 | 539 | 574 | 9 | | |

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit M.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | 6 | 350 | Total | C | N | O | S | 0 | 0 |
| | | | 1917 | 1159 | 376 | 380 | 2 | | |

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit F.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 50 | 4 | 257 | Total | C | N | O | 0 | 0 |
| | | | 1272 | 757 | 257 | 258 | | |

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit H.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 51 | 8 | 317 | Total | C | N | O | 0 | 0 |
| | | | 1571 | 936 | 317 | 318 | | |

- Molecule 52 is a protein called Eukaryotic translation initiation factor 3 subunit K.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 52 | 3 | 213 | Total | C | N | O | 0 | 0 |
| | | | 1057 | 631 | 213 | 213 | | |

- Molecule 53 is a protein called Eukaryotic translation initiation factor 3 subunit L.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 53 | 5 | 319 | Total | C | N | O | 0 | 0 |
| | | | 1581 | 943 | 319 | 319 | | |

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 54 | R | 1 | Total Zn<br>1 1 | 0 |
| 54 | o | 1 | Total Zn<br>1 1 | 0 |
| 54 | p | 1 | Total Zn<br>1 1 | 0 |

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 55 | S | 1 | Total Mg<br>1 1 | 0 |
| 55 | T | 1 | Total Mg<br>1 1 | 0 |
| 55 | W | 85 | Total Mg<br>85 85 | 0 |
| 55 | f | 1 | Total Mg<br>1 1 | 0 |

- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 56 | W | 3 | Total K<br>3 3 | 0 |

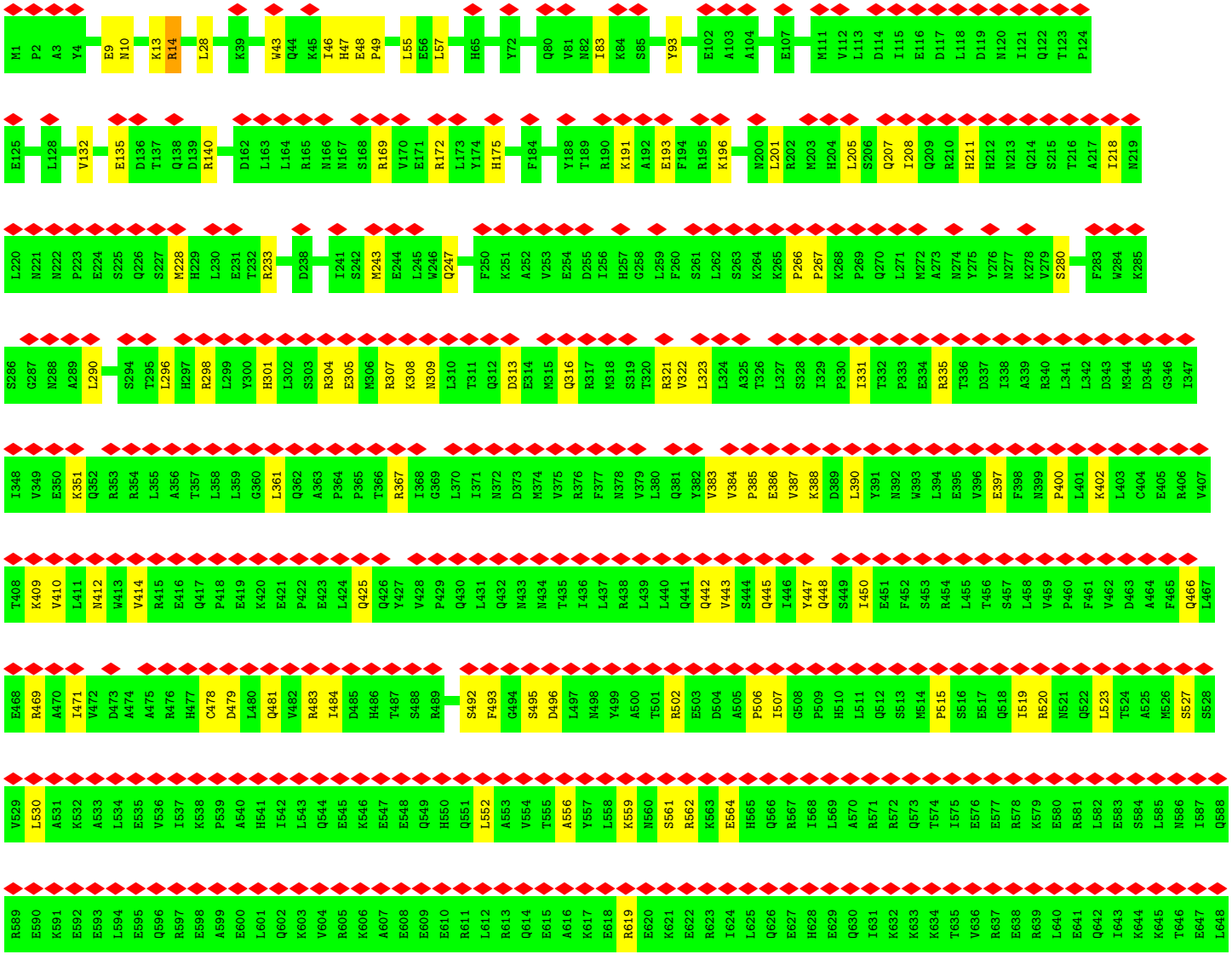
# 3 Residue-property plots (i)

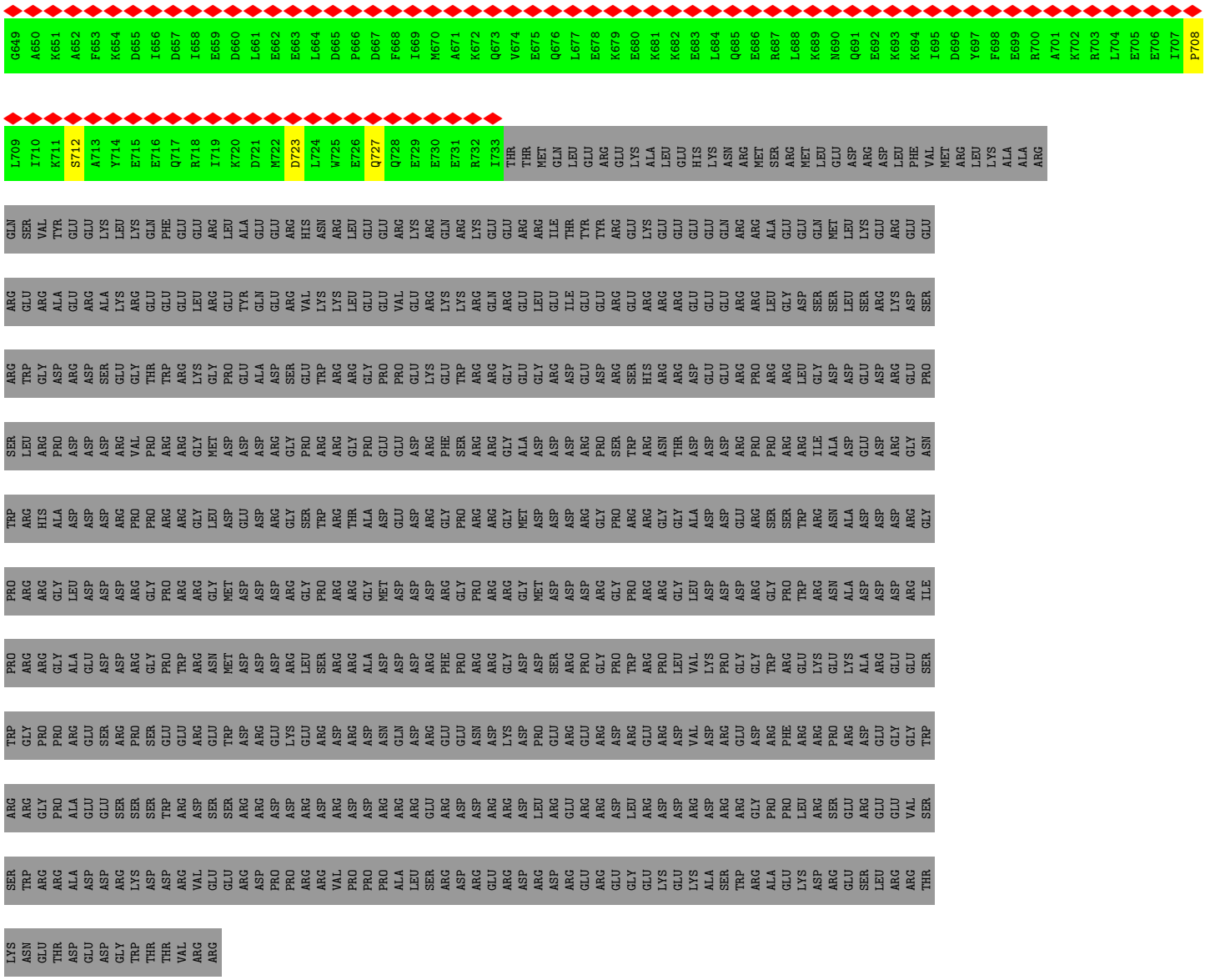
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Eukaryotic translation initiation factor 3 subunit A

Chain A:



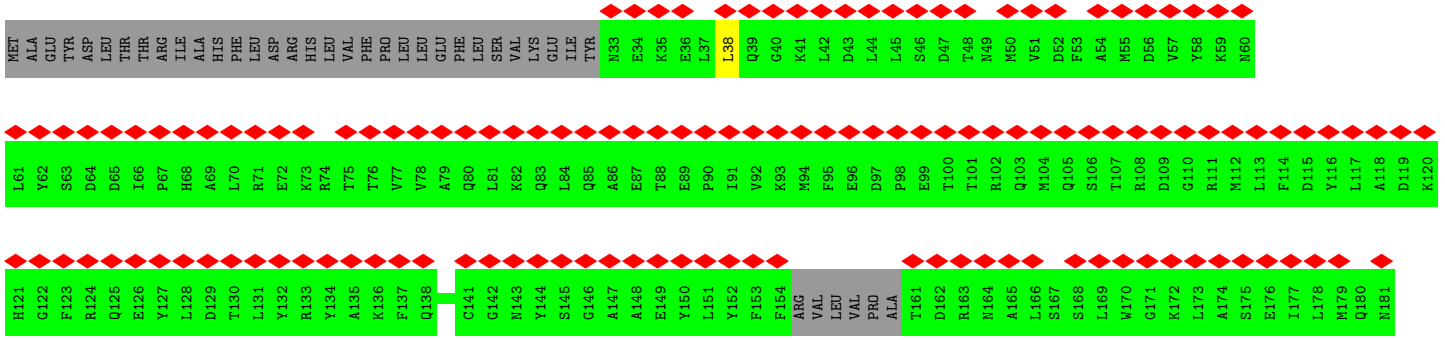



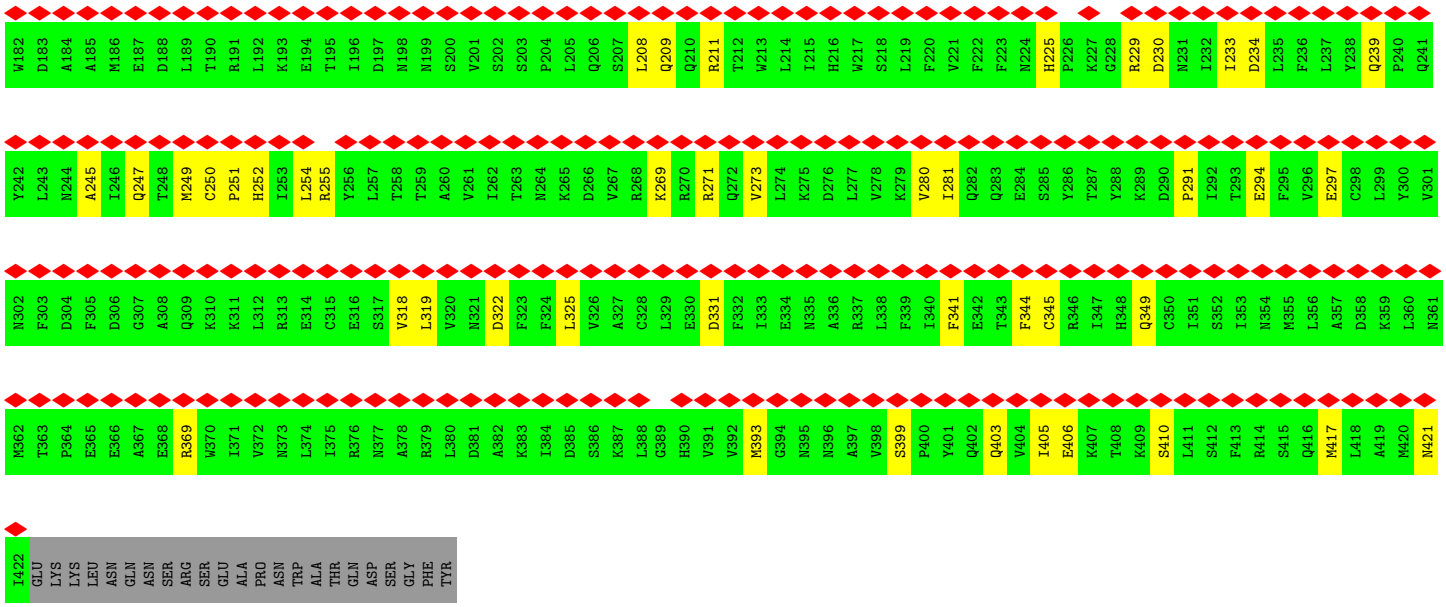



• Molecule 2: Eukaryotic translation initiation factor 3 subunit E

Chain B:



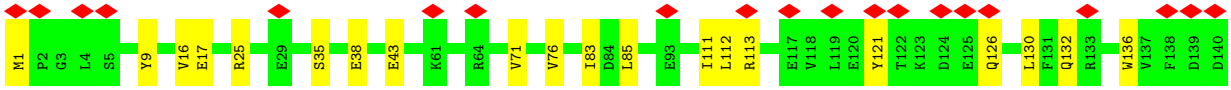






• Molecule 3: Eukaryotic translation initiation factor 2 subunit 1

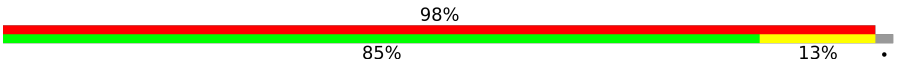
Chain D:

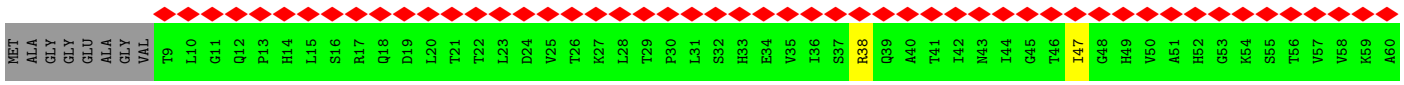


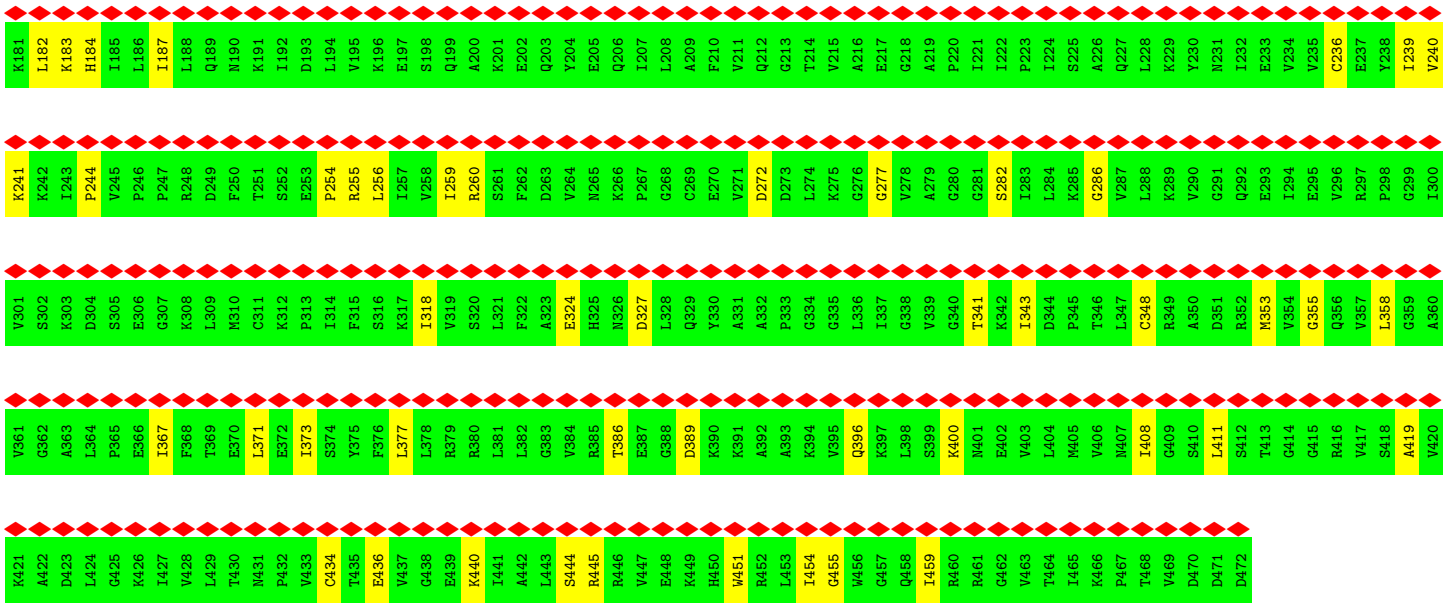




• Molecule 4: Eukaryotic translation initiation factor 2 subunit 3

Chain E:



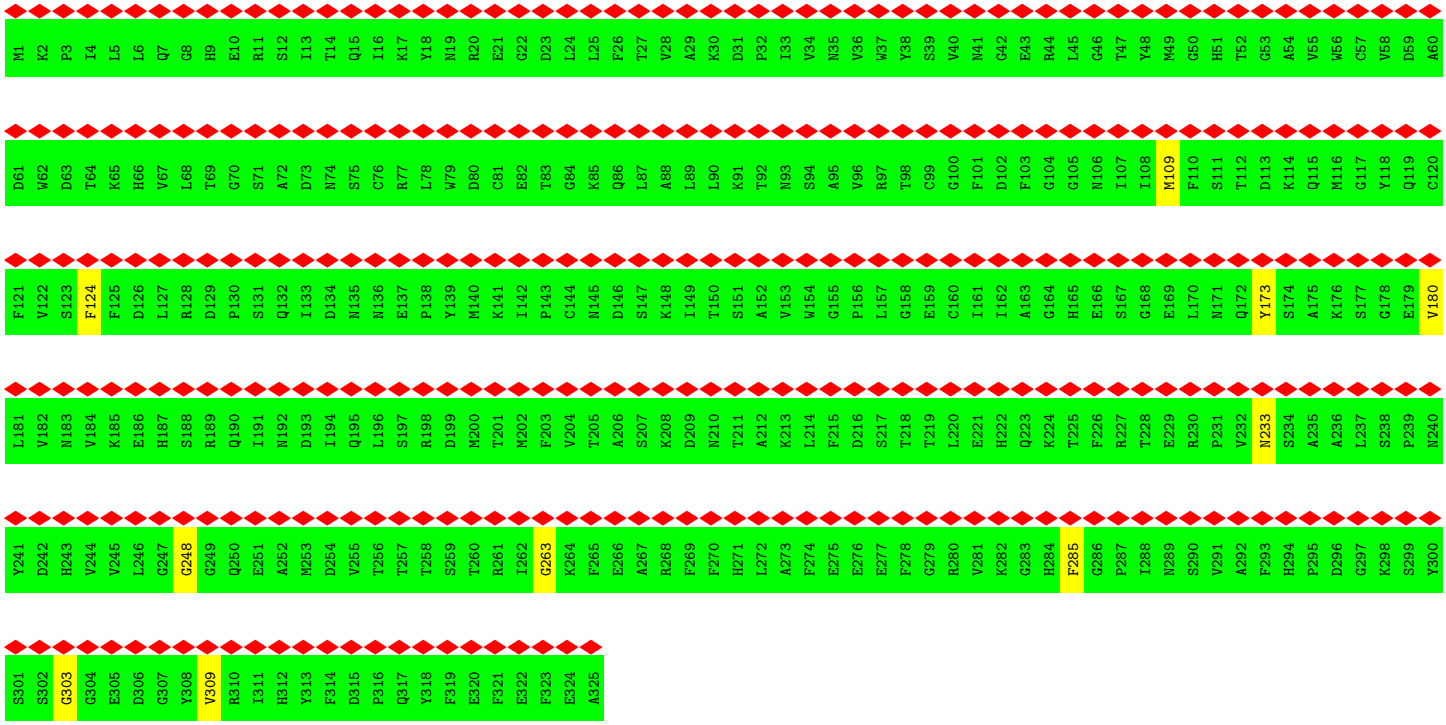






• Molecule 5: Eukaryotic translation initiation factor 3 subunit I

Chain F:

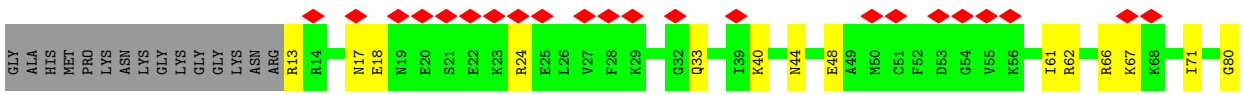


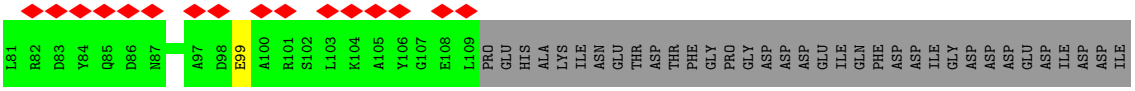




• Molecule 6: Eukaryotic translation initiation factor 1A, X-chromosomal

Chain G:

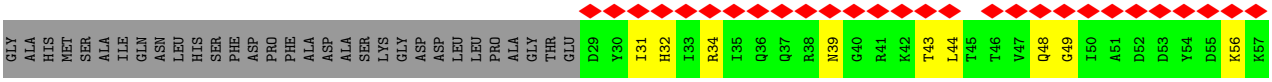


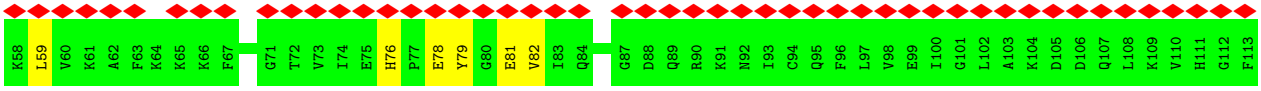






• Molecule 7: Eukaryotic translation initiation factor 1

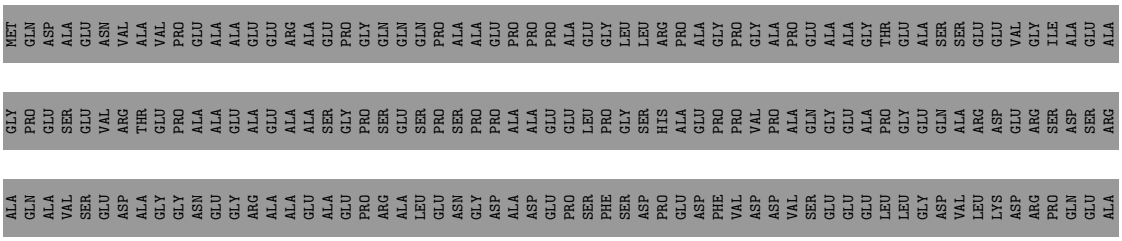


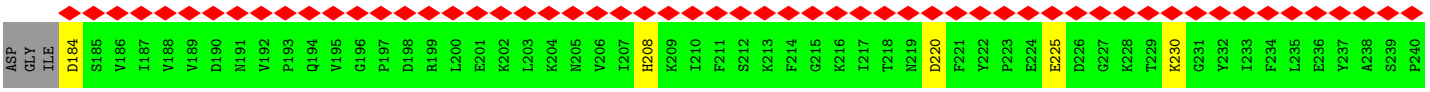



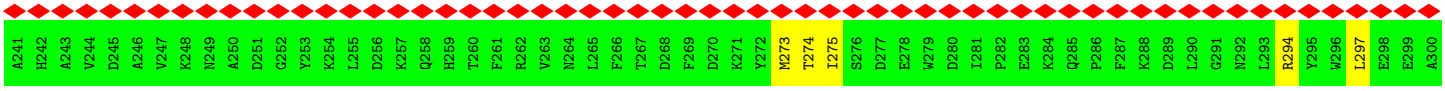



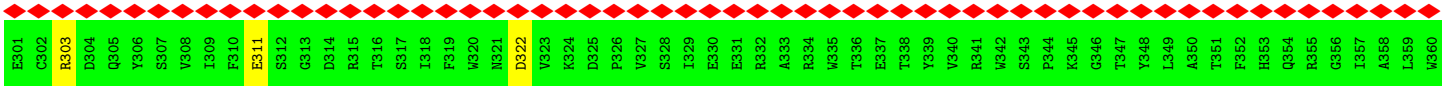

• Molecule 8: Eukaryotic translation initiation factor 3 subunit B

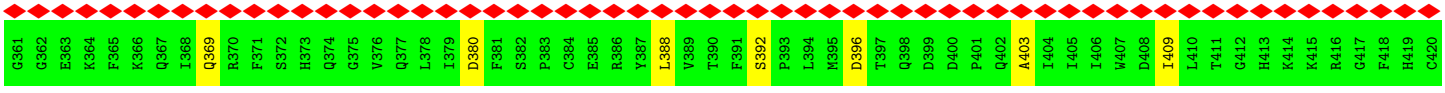


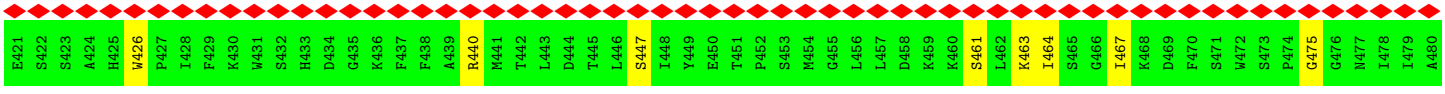



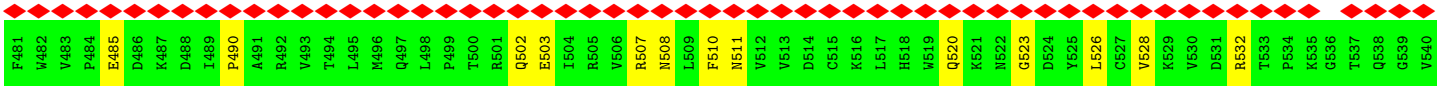



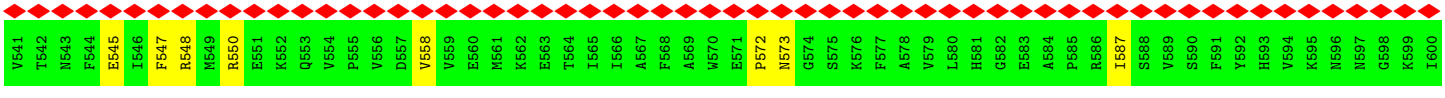



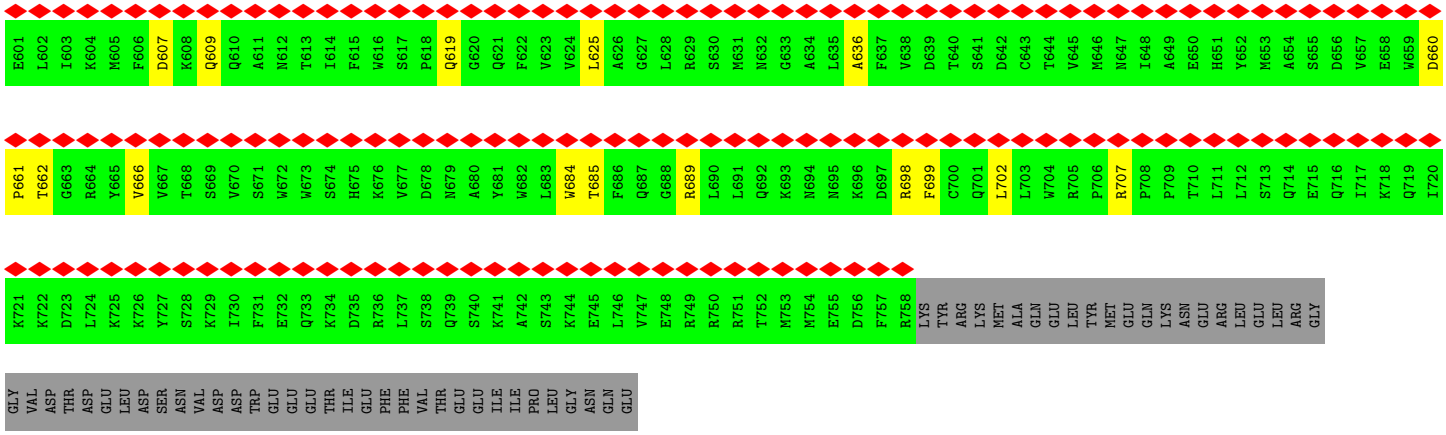



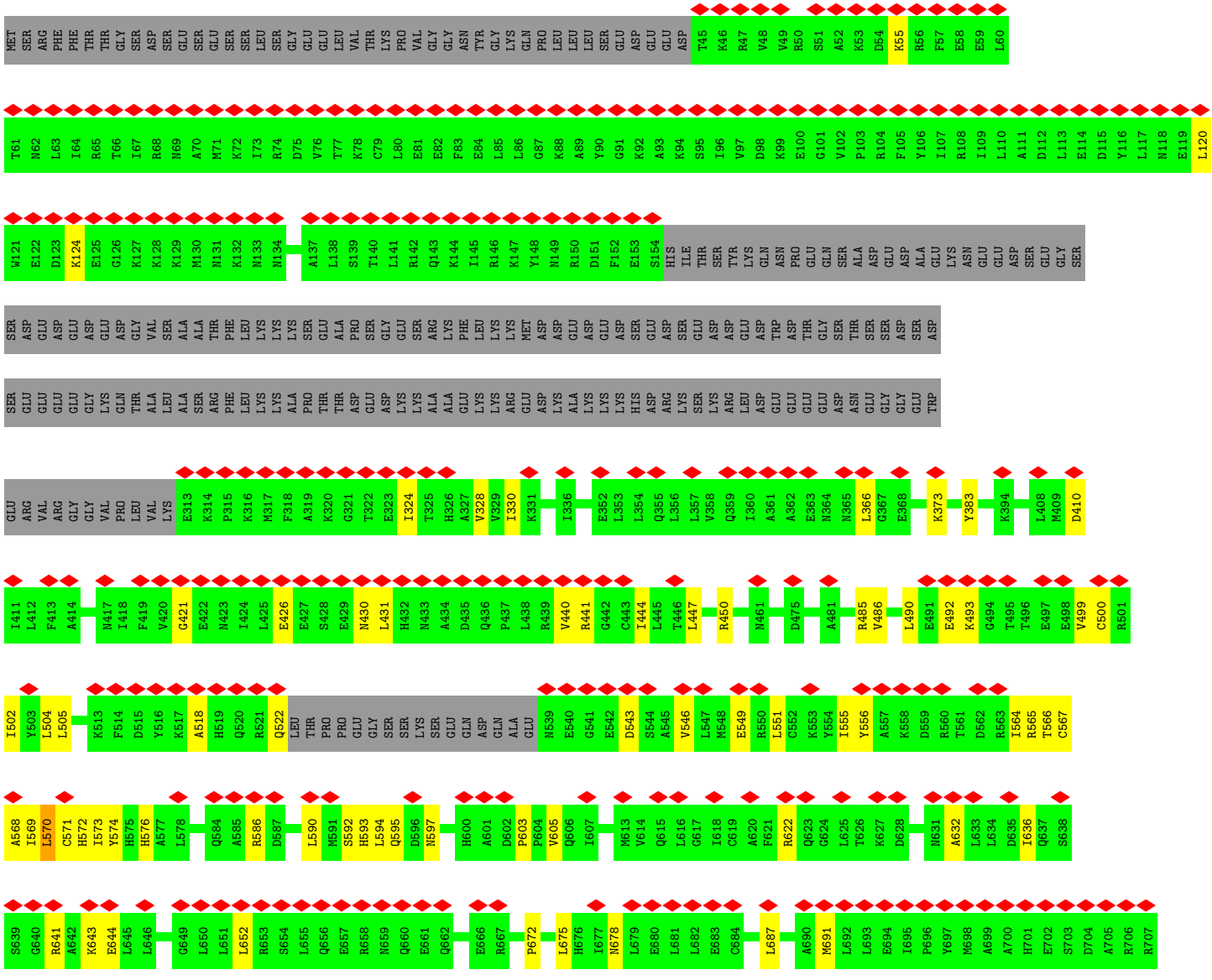



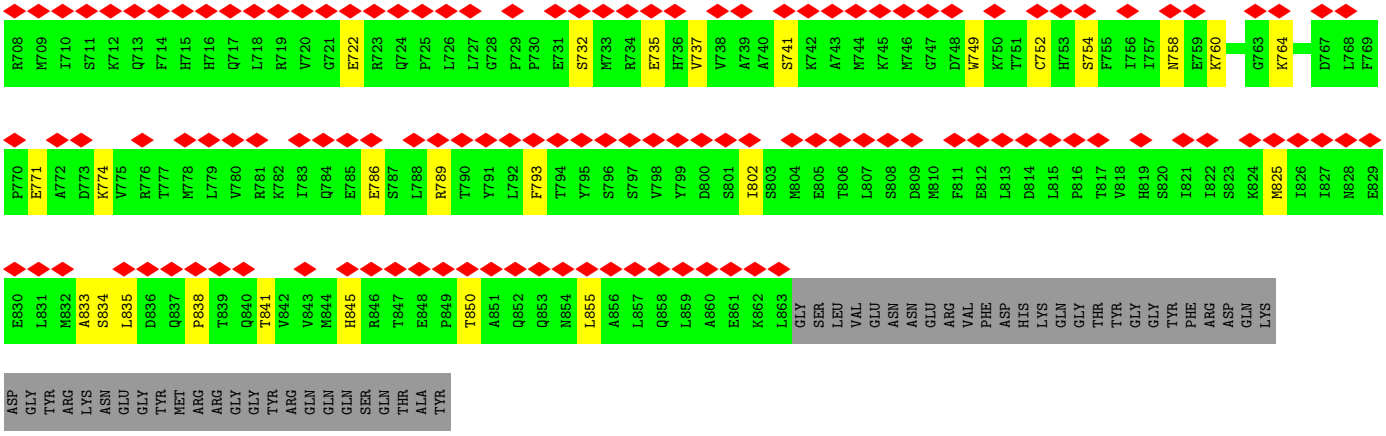



• Molecule 9: Eukaryotic translation initiation factor 3 subunit C

Chain J:



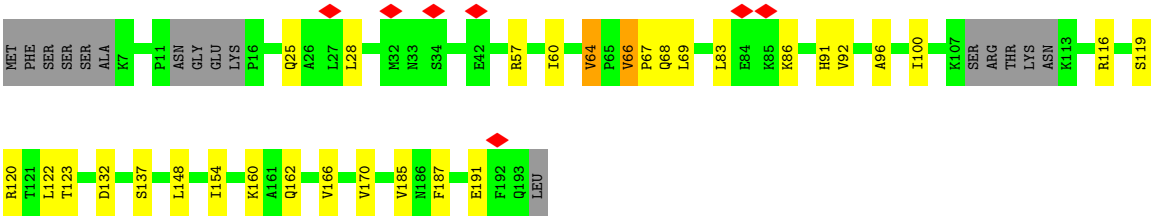






• Molecule 10: 40S ribosomal protein S7

Chain L:

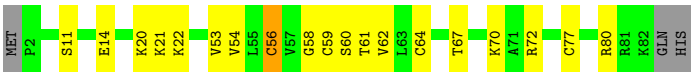



• Molecule 11: 40S ribosomal protein S27

Chain M:

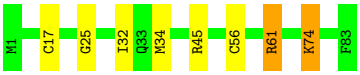



• Molecule 12: 40S ribosomal protein S21

Chain N:

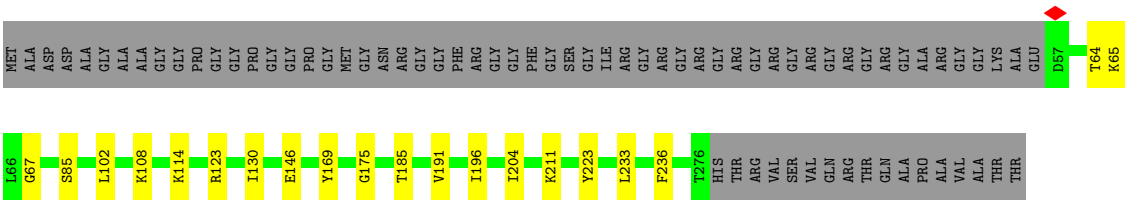



• Molecule 13: 40S ribosomal protein S2

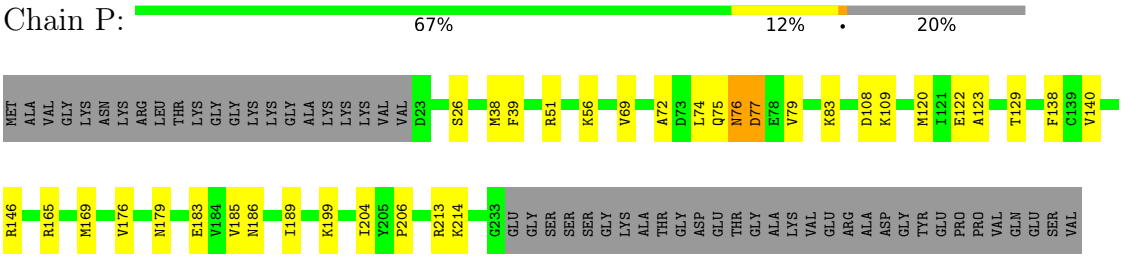
Chain O:



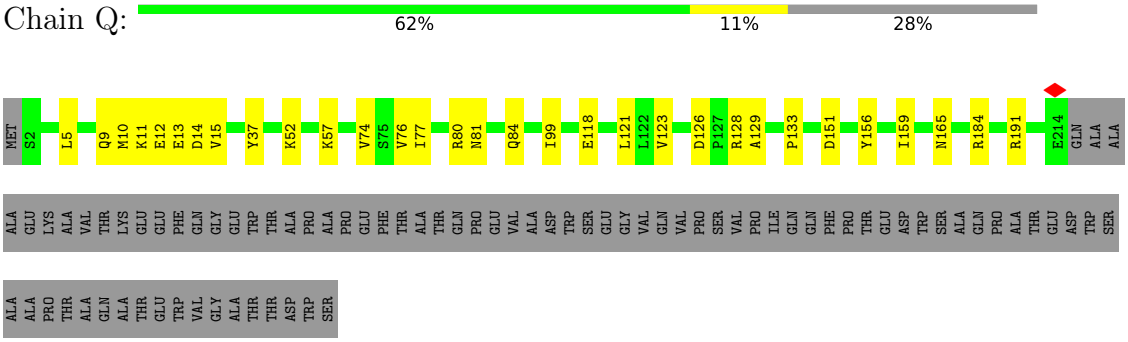

• Molecule 14: 40S ribosomal protein S3a

Chain P:



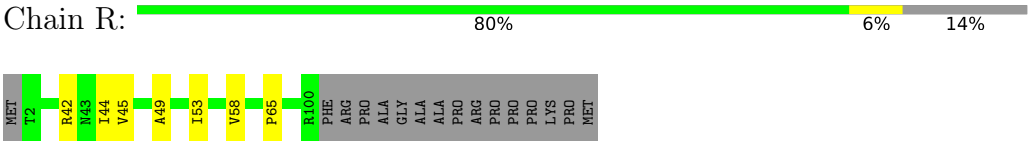

• Molecule 15: 40S ribosomal protein SA

Chain Q:



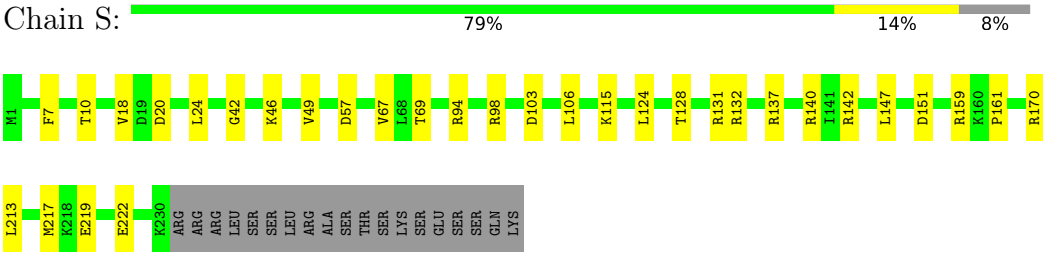

• Molecule 16: 40S ribosomal protein S26

Chain R:



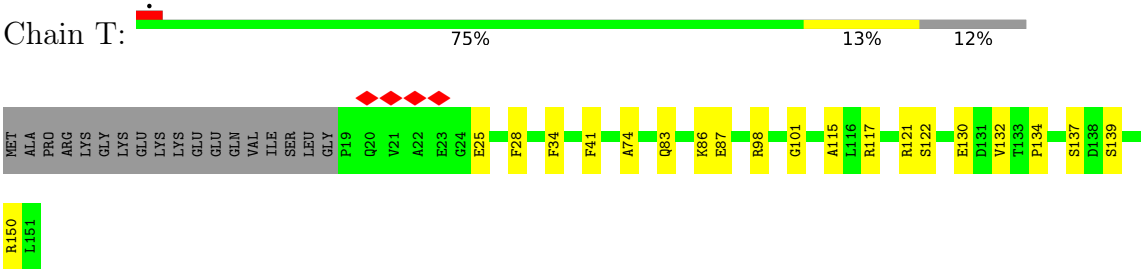

• Molecule 17: 40S ribosomal protein S6

Chain S:



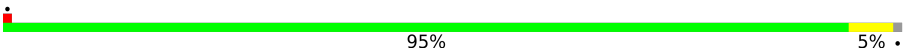

• Molecule 18: 40S ribosomal protein S14

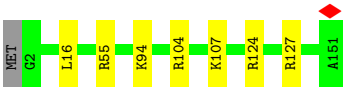
Chain T:




• Molecule 19: 40S ribosomal protein S13

Chain V:

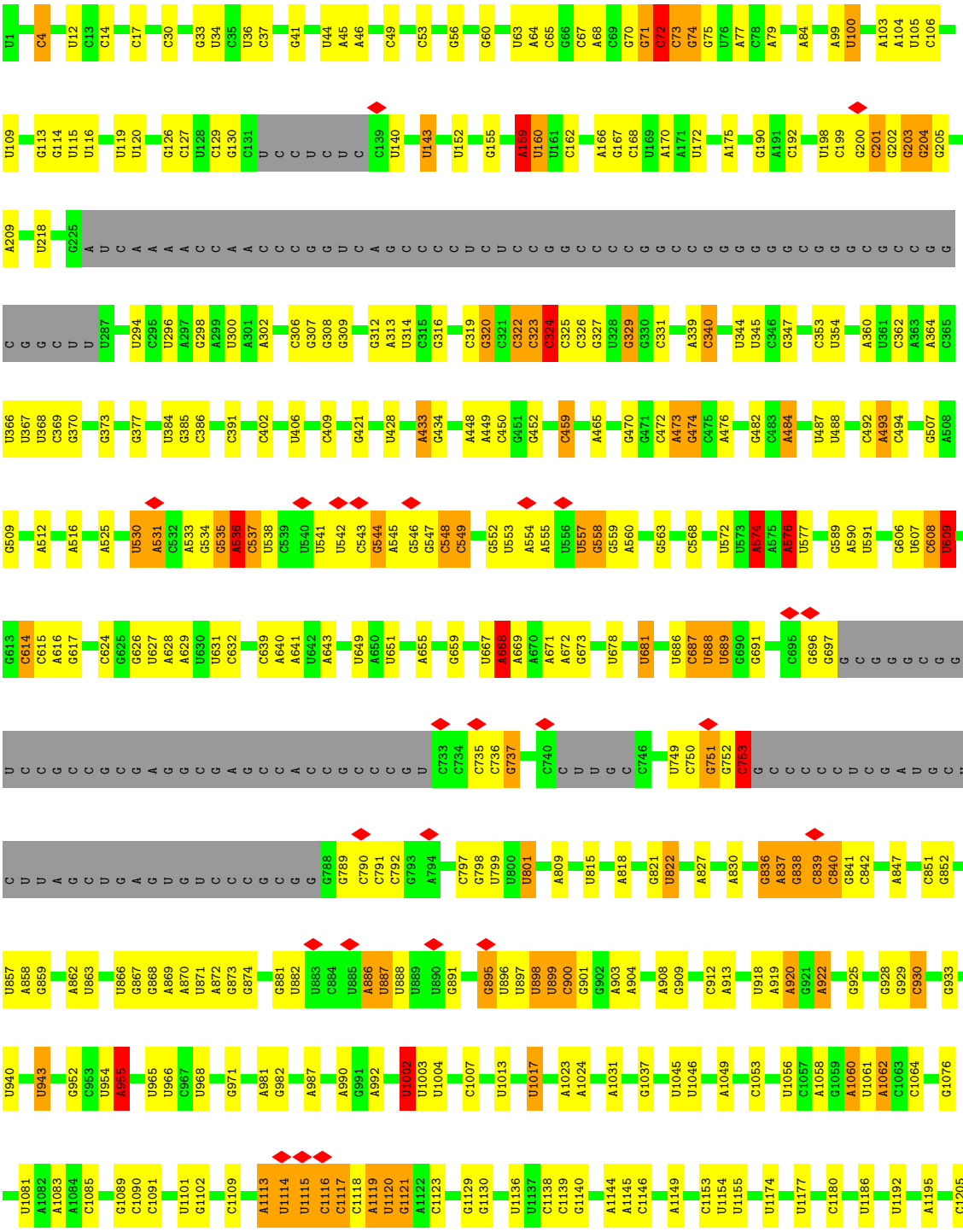


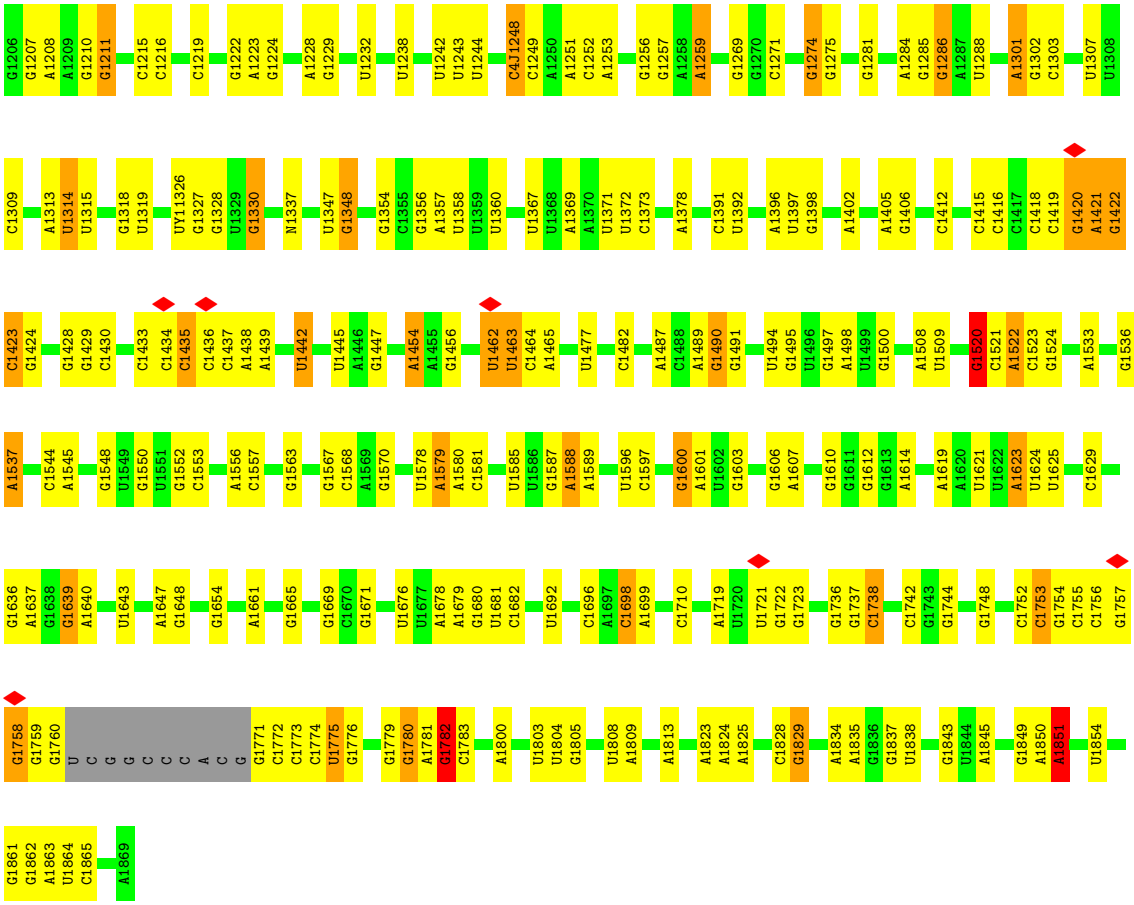




• Molecule 20: 18S rRNA

Chain W:





• Molecule 21: 40S ribosomal protein S11

Chain X:






• Molecule 22: Small ribosomal subunit protein eS4, X isoform

Chain Y:






• Molecule 23: 40S ribosomal protein S9

Chain Z:

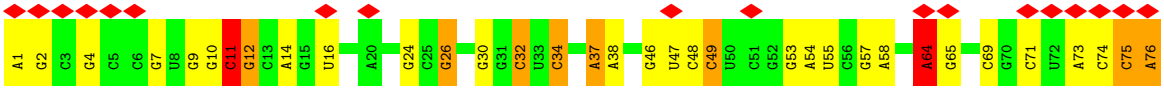





• Molecule 24: tRNAi-Met

Chain y:

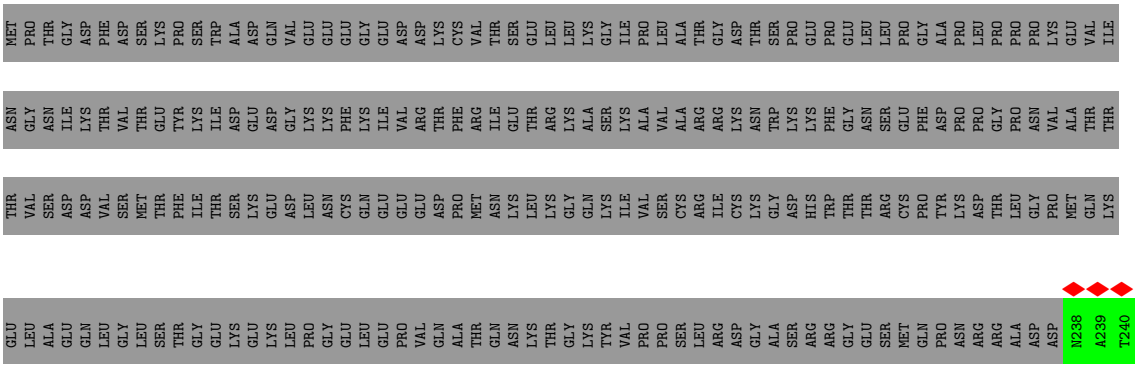



• Molecule 25: Eukaryotic translation initiation factor 3 subunit G

Chain 7:

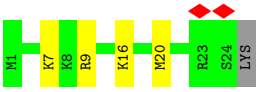



• Molecule 26: 60S ribosomal protein L41

Chain 9:

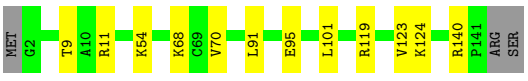



• Molecule 27: 40S ribosomal protein S23

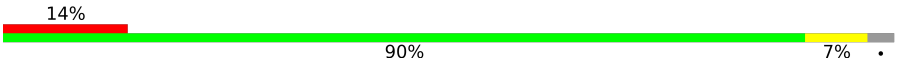
Chain a:

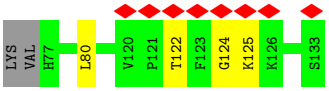



• Molecule 28: 40S ribosomal protein S30

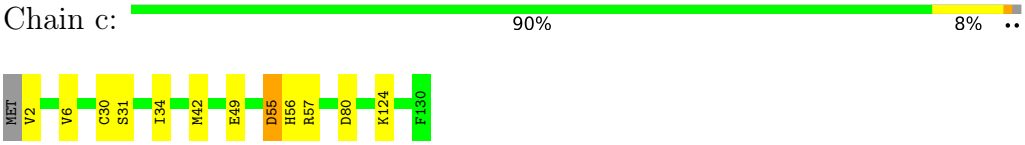
Chain b:



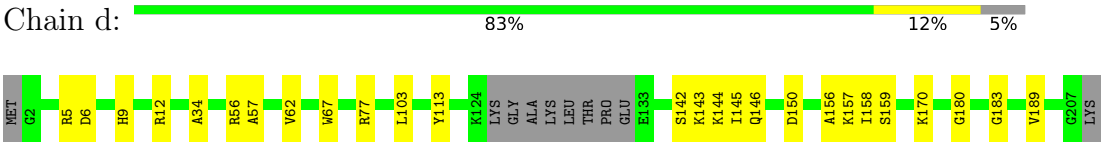
• Molecule 29: 40S ribosomal protein S15a

Chain c:



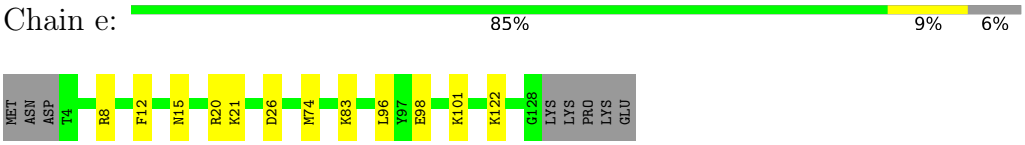

• Molecule 30: 40S ribosomal protein S8

Chain d:



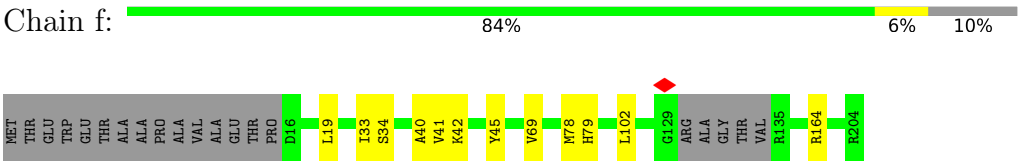

• Molecule 31: 40S ribosomal protein S24

Chain e:



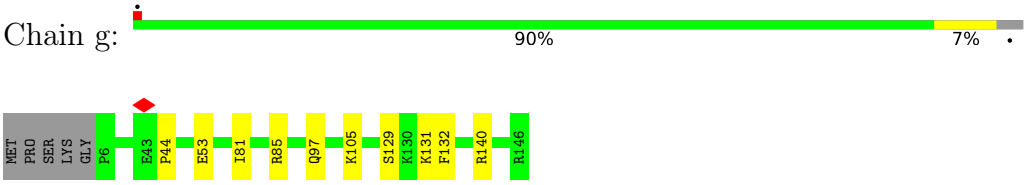

• Molecule 32: 40S ribosomal protein S5

Chain f:



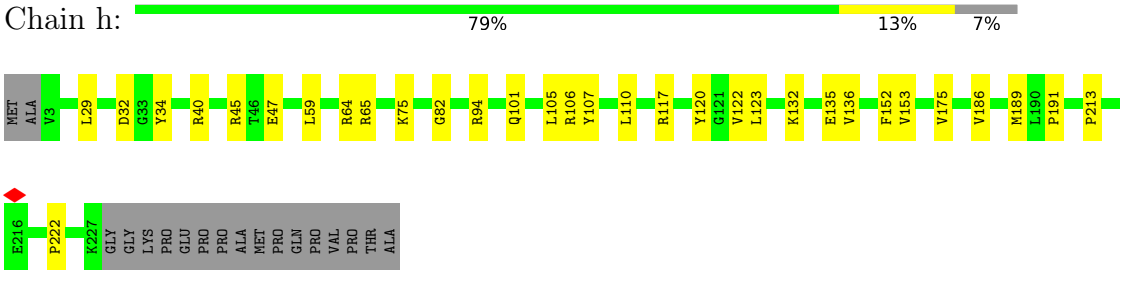

• Molecule 33: 40S ribosomal protein S16

Chain g:




• Molecule 34: 40S ribosomal protein S3

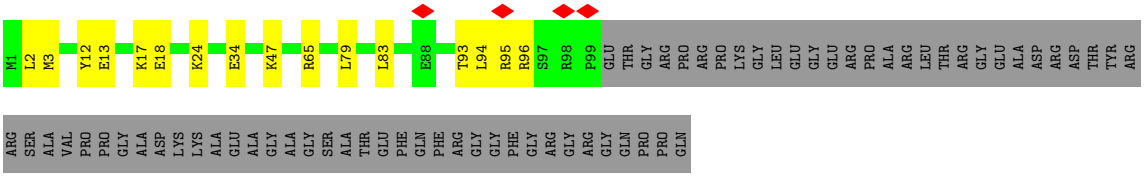
Chain h:




• Molecule 35: 40S ribosomal protein S10

Chain i:

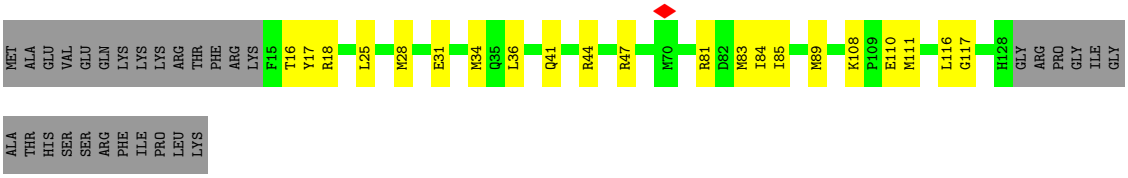





• Molecule 36: 40S ribosomal protein S15

Chain j:

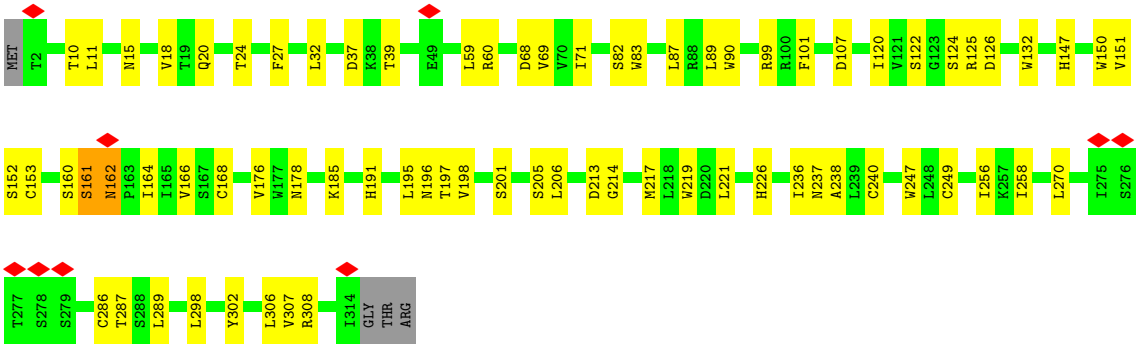



• Molecule 37: Receptor of activated protein C kinase 1

Chain k:

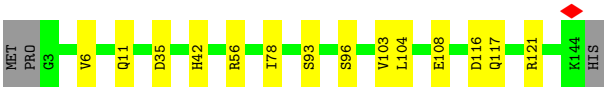



• Molecule 38: 40S ribosomal protein S19

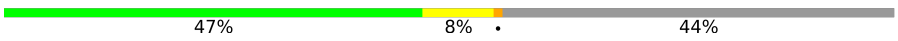
Chain l:

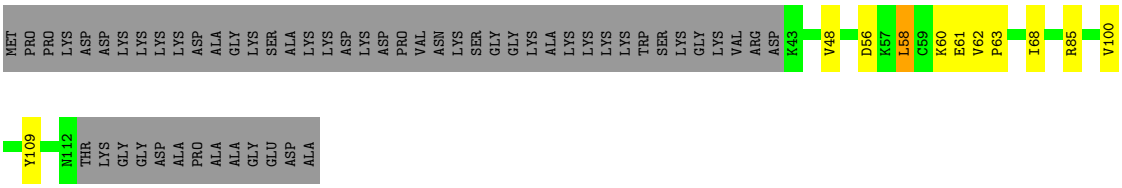



• Molecule 39: 40S ribosomal protein S25

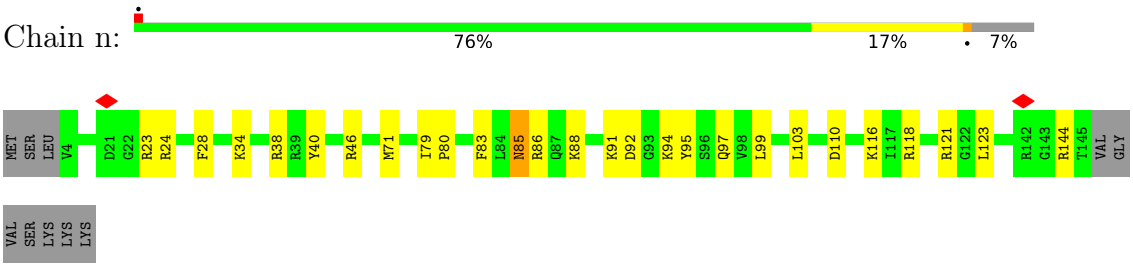
Chain m:



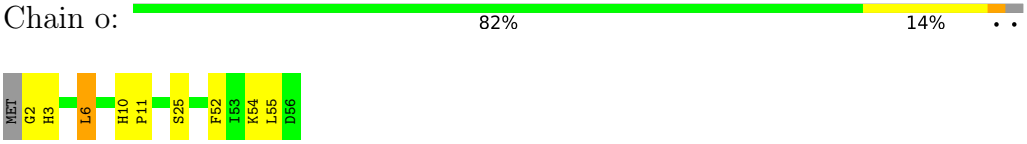

• Molecule 40: 40S ribosomal protein S18

Chain n:



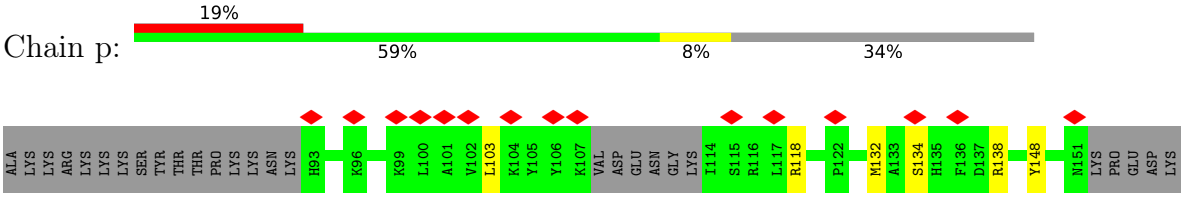

• Molecule 41: 40S ribosomal protein S29

Chain o:



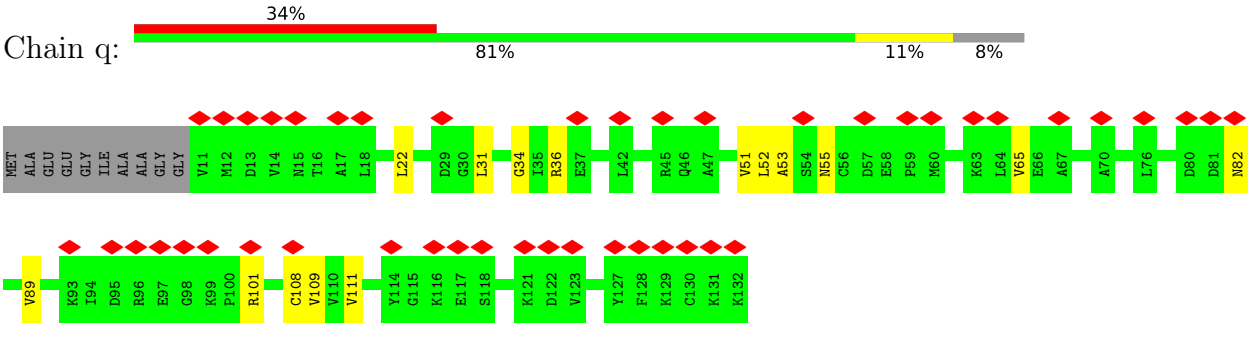

• Molecule 42: Ubiquitin-ribosomal protein eS31 fusion protein

Chain p:



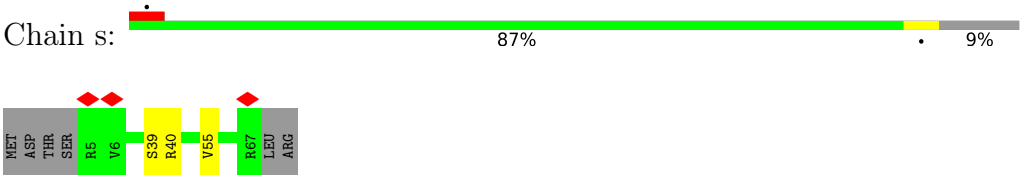

• Molecule 43: 40S ribosomal protein S12

Chain q:



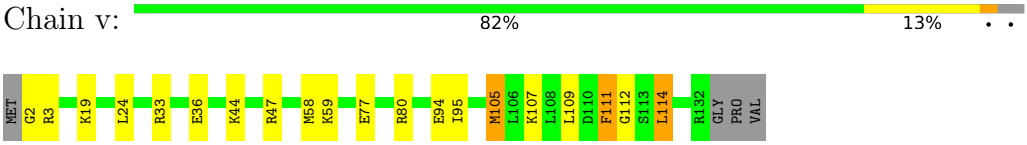

• Molecule 44: 40S ribosomal protein S28

Chain s:




• Molecule 45: 40S ribosomal protein S17

Chain v:




• Molecule 46: 40S ribosomal protein S20

Chain w:

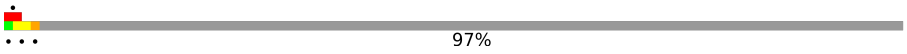


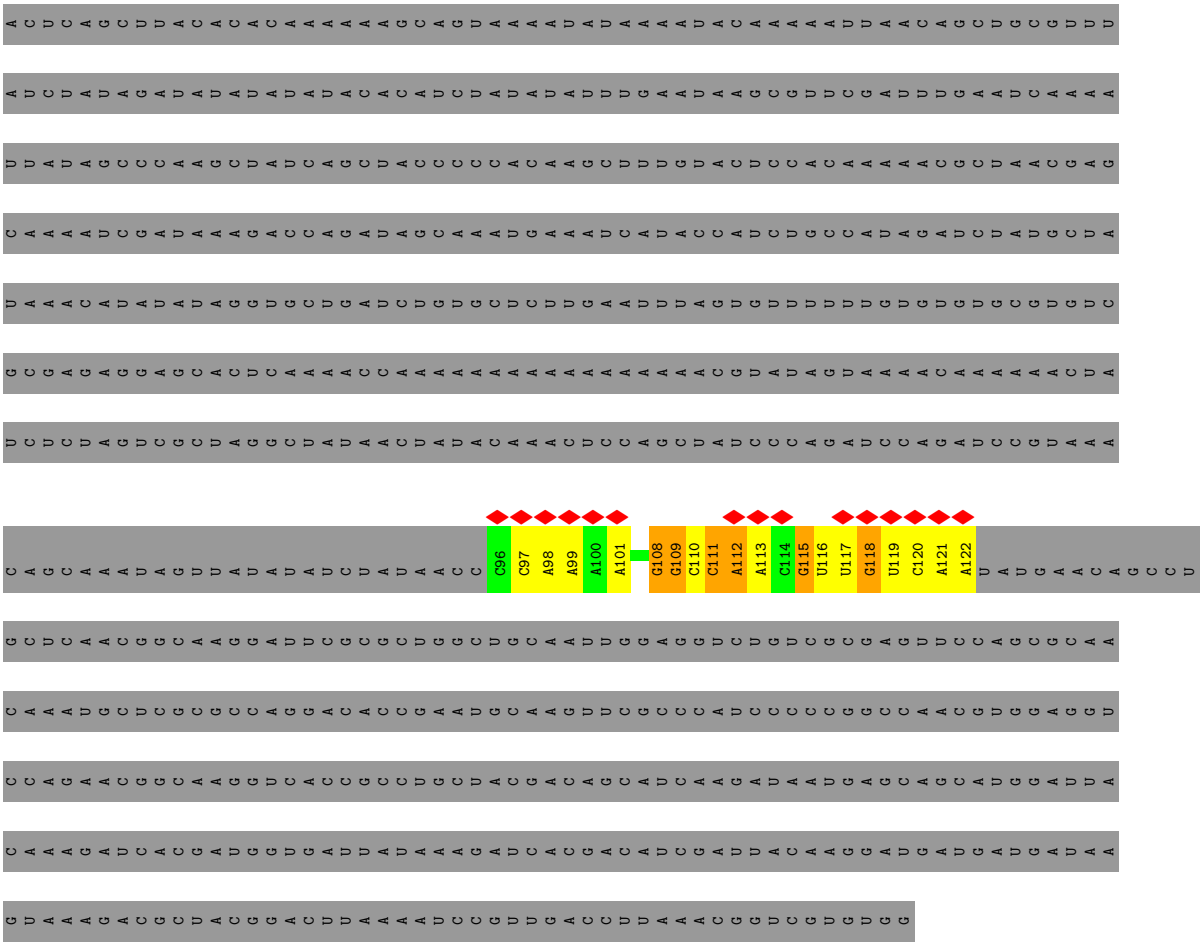




• Molecule 47: circMbl-FLAG

Chain z:

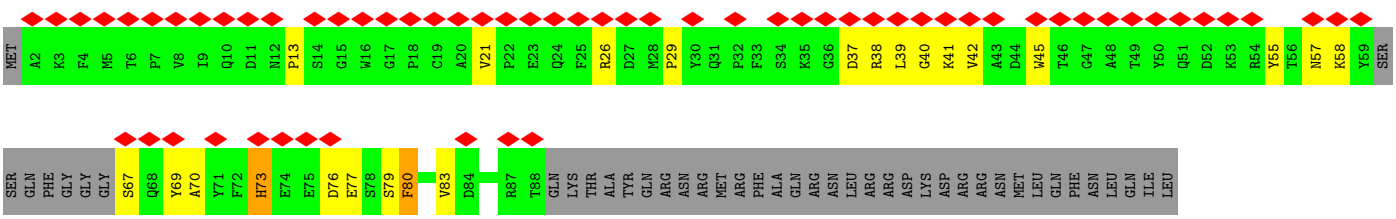


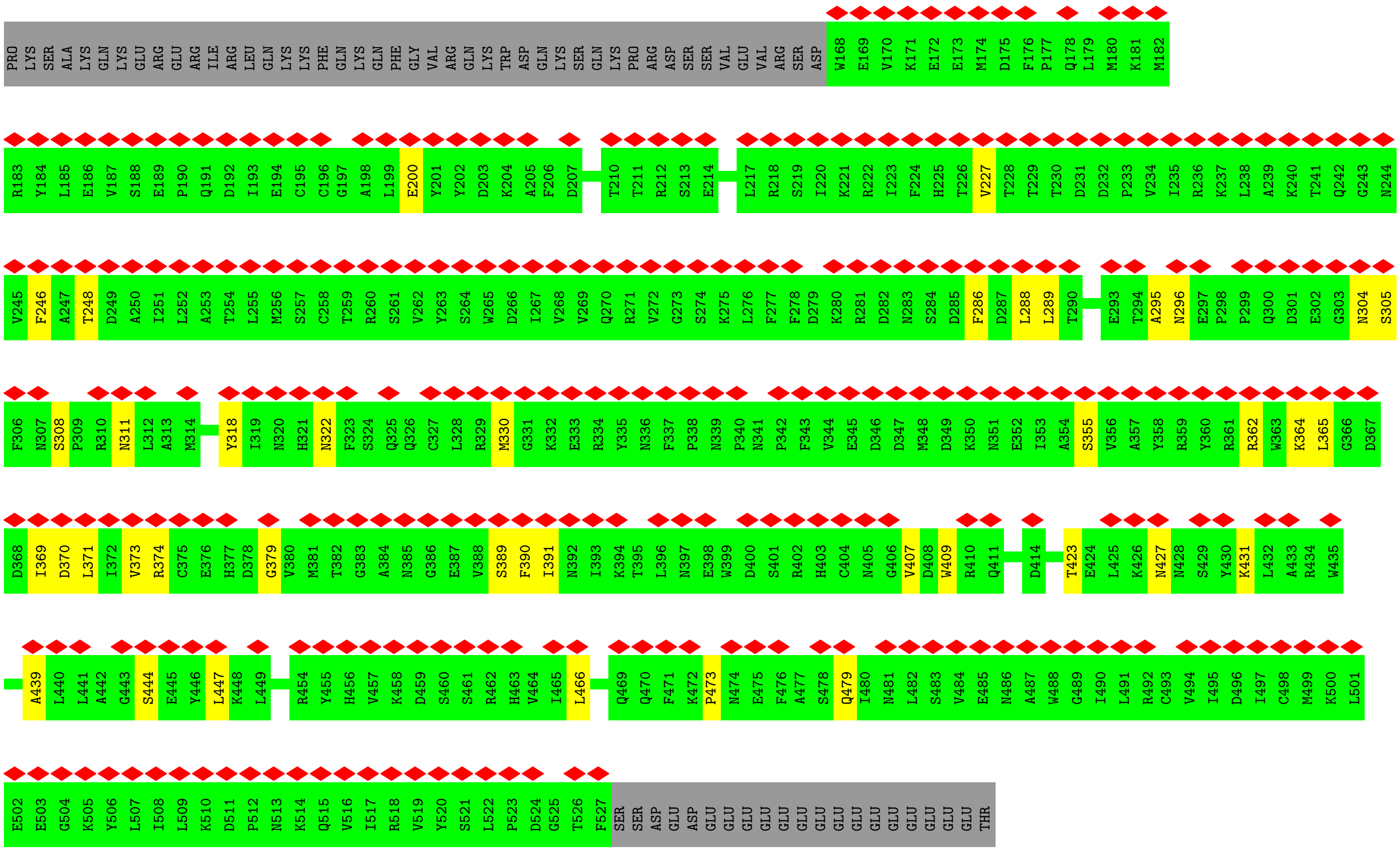




• Molecule 48: Eukaryotic translation initiation factor 3 subunit D

Chain x:

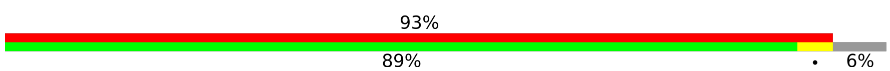


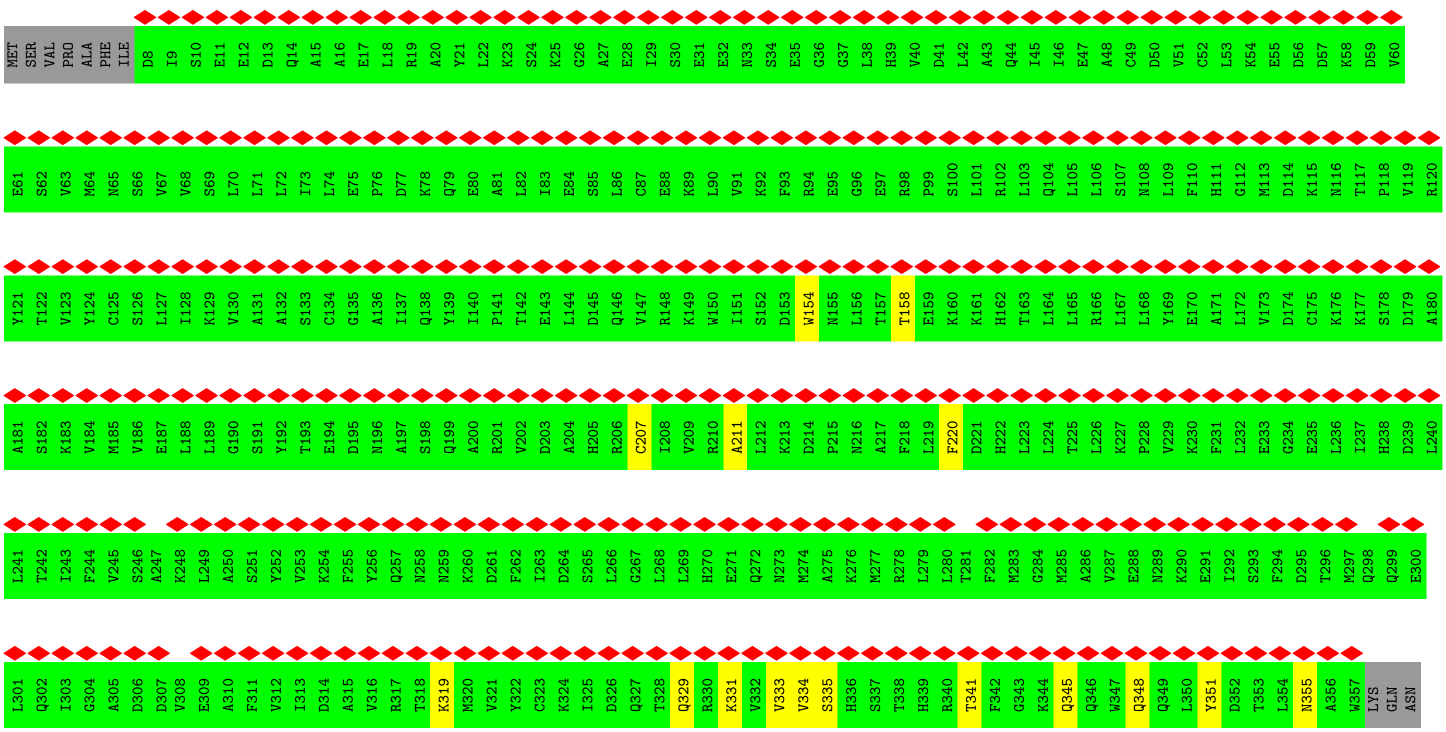






- Molecule 49: Eukaryotic translation initiation factor 3 subunit M

Chain 6:





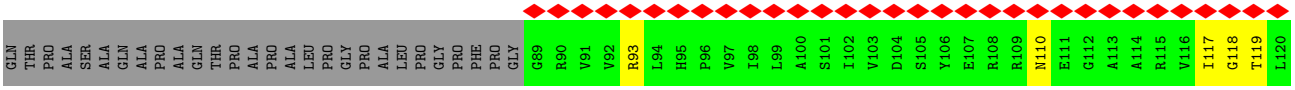

• Molecule 50: Eukaryotic translation initiation factor 3 subunit F

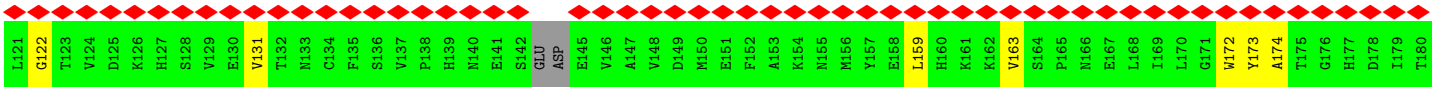
Chain 4:

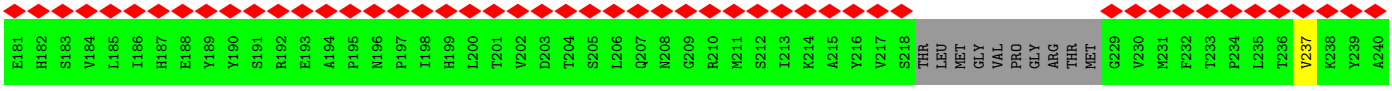


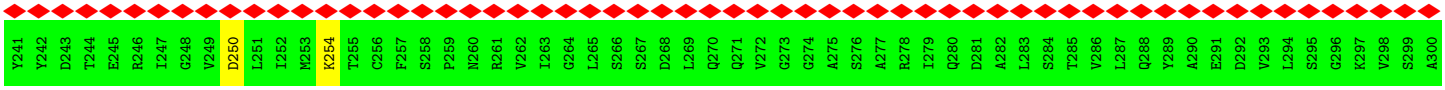


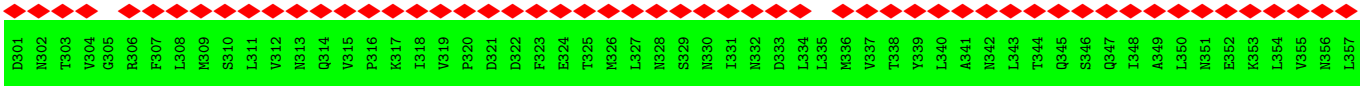




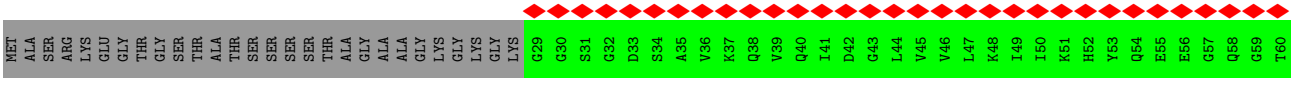



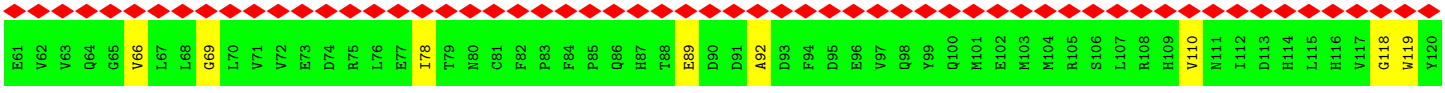



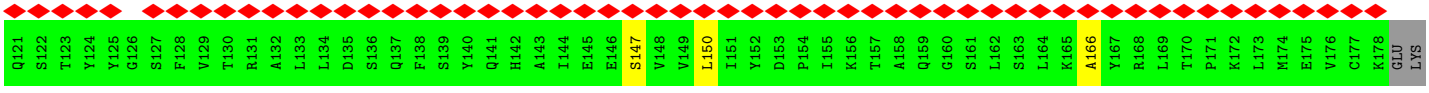

• Molecule 51: Eukaryotic translation initiation factor 3 subunit H

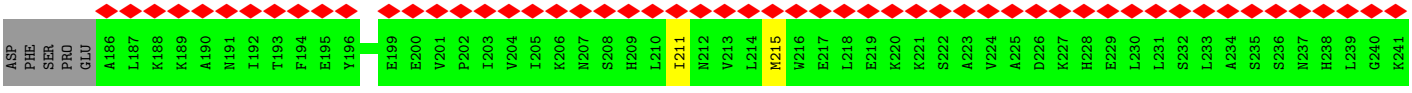
Chain 8:

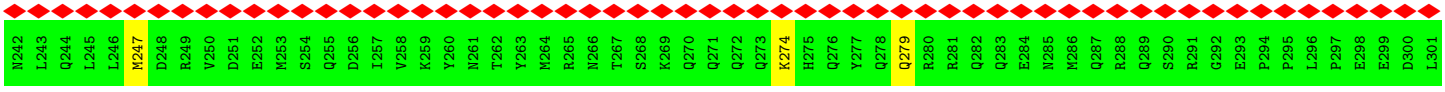


S302 K303 L304 F305 K306 P307 P308 Q309 P310 P311 A312 R313 M314 D315 S316 L317 L318 I319 A320 G321 Q322 I323 N324 T325 Y326 C327 Q328 N329 I330 K331 E332 F333 T334 A335 Q336 N337 L338 G339 K340 L341 F342 M343 A344 Q345 A346 L347 Q348 E349 Y350 N351 N352

• Molecule 52: Eukaryotic translation initiation factor 3 subunit K

Chain 3: 98% 97%

MET A2 M3 F4 E5 Q6 M7 R8 A9 N10 V11 G12 K13 L14 L15 K16 G17 I18 D19 R20 Y21 N22 P23 E24 N25 L26 A27 T28 L29 E30 R31 Y32 V33 E34 T35 Q36 A37 K38 E39 N40 A41 Y42 D43 L44 E45 A46 N47 L48 A49 V50 L51 K52 L53 Y54 Q55 F56 N57 P58 A59 F60

F61 Q62 T63 T64 V65 T66 A67 Q68 I69 L70 L71 K72 A73 L74 T75 N76 L77 P78 H79 T80 D81 F82 T83 L84 C85 K86 C87 M88 I89 D90 Q91 A92 H93 Q94 E95 E96 R97 P98 I99 R100 Q101 I102 L103 Y104 L105 G106 D107 L108 L109 E110 T111 C112 H113 F114 Q115 A116 F117 W118 Q119 A120

L121 D122 E123 N124 M125 D126 L127 L128 E129 G130 I131 T132 G133 F134 E135 D136 S137 V138 R139 K140 F141 I142 C143 H144 V145 V146 G147 I148 T149 Y150 Q151 H152 I153 D154 R155 W156 L157 L158 A159 E160 M161 L162 G163 D164 L165 S166 D167 S168 Q169 L170 K171 V172 W173 M174 S175 K176 Y177 G178 W179 S180

A181 D182 E183 SER GLY Q186 I187 F188 I189 C190 S191 Q192 E193 E194 S195 I196 K197 P198 K199 N200 I201 V202 E203 K204 I205 D206 F207 D208 S209 V210 S211 S212 I213 M214 A215 S216 SER GLN

• Molecule 53: Eukaryotic translation initiation factor 3 subunit L

Chain 5: 56% 55% 43%

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

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

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

GLN TRP L183 W184 D185 I186 I187 D188 E189 F190 I191 Y192 Q193 F194 Q195 S196 F197 S198 Q199 Y200 R201 C202 K203 T204 A205 K206 K207 S208 E209 E210 E211 I212 D213 F214 L215 R216 S217 N218 P219 K220 I221 W222 N223 V224 H225 S226 V227 L228 N229 V230 L231 H232 S233 L234 V235 D236 K237 S238 N239 I240

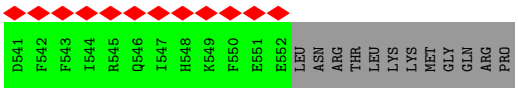
N241 R242 Q243 L244 E245 V246 Y247 T248 S249 G250 G251 D252 P253 E254 S255 V256 A257 G258 E259 Y260 G261 R262 H263 S264 L265 Y266 K267 M268 L269 G270 Y271 F272 S273 L274 V275 G276 L277 L278 R279 L280 H281 S282 L283 L284 G285 D286 Y287 Y288 Q289 A290 I291 K292 V293 L294 E295 N296 I297 E298 L299 N300

K301 K302 S303 M304 TYR SER ARG VAL PRO GLU C311 Q312 V313 T314 T315 Y316 Y317 Y318 V319 G320 F321 A322 Y323 L324 M325 M326 R327 R328 Y329 Q330 D331 A332 I333 R334 V335 F336 A337 N338 I339 L340 L341 Y342 I343 GLN ARG THR LYS SER MET PHE GLN ARG THR THR TYR LYS Y357 E358 M359 I360

N361 K362 Q363 N364 E365 Q366 M367 H368 A369 L370 L371 A372 I373 A374 L375 THR MET TYR PRO MET ARG I382 D383 E384 S385 I386 H387 L388 Q389 L390 R391 E392 K393 Y394 G395 D396 K397 M398 L399 R400 M401 Q402 K403 G404 D405 P406 Q407 V408 Y409 E410 E411 L412 F413 S414 Y415 S416 C417 PRO LYS PHE

LEU SER PRO VAL VAL PRO ASN TYR ASP ASN VAL HIS PRO ASN TYR H436 K437 E438 P439 F440 L441 Q442 Q443 L444 K445 V446 F447 S448 D449 E450 V451 Q452 Q453 Q454 A455 Q456 L457 S458 T459 I460 R461 S462 F463 L464 K465 L466 Y467 T468 T469 M470 P471 V472 A473 K474 L475 A476 G477 F478 L479 D480


L481 THR GLU GLN GLU PHE ARG ILE GLN L490 L491 V492 F493 K494 H495 K496 M497 K498 N499 L500 V501 W502 T503 S504 G505 I506 S507 A508 L509 D510 G511 E512 F513 Q514 S515 A516 S517 E518 V519 D520 F521 Y522 I523 D524 K525 D526 M527 I528 H529 I530 A531 D532 T533 K534 V535 A536 R537 R538 Y539 G540


D541 F542 F543 I544 R545 Q546 I547 H548 K549 F550 E551 E552 LEU ASN ARG THR LEU LYS LYS MET GLY GLN ARG PRO

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 21721 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 40.0 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 2800 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.048 | Depositor |
| Minimum map value | -0.014 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.001 | Depositor |
| Recommended contour level | 0.0045 | Depositor |
| Map size (Å) | 494.4, 494.4, 494.4 | wwPDB |
| Map dimensions | 600, 600, 600 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.824, 0.824, 0.824 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: T6A, OMC, M2G, MG, 5MC, PSU, 1MG, A2M, UY1, MA6, H2U, 1MA, OMG, 2MG, OMU, 4AC, ZN, 5MU, K, RIA, 7MG, G7M, C4J, 6MZ, JMH

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 | 0.25 | 0/5593 | 0.59 | 0/7599 |
| 2 | B | 0.23 | 0/2672 | 0.55 | 0/3647 |
| 3 | D | 0.24 | 0/2267 | 0.57 | 0/3056 |
| 4 | E | 0.22 | 0/3598 | 0.54 | 0/4868 |
| 5 | F | 0.11 | 0/1597 | 0.30 | 0/2216 |
| 6 | G | 0.26 | 0/797 | 0.65 | 0/1061 |
| 7 | H | 0.29 | 0/701 | 0.73 | 0/936 |
| 8 | I | 0.21 | 0/4696 | 0.49 | 0/6379 |
| 9 | J | 0.28 | 0/5018 | 0.60 | 0/6791 |
| 10 | L | 0.40 | 0/1460 | 0.69 | 3/1953 (0.2%) |
| 11 | M | 0.58 | 0/644 | 0.84 | 0/864 |
| 12 | N | 0.48 | 0/643 | 0.72 | 1/860 (0.1%) |
| 13 | O | 0.42 | 0/1743 | 0.52 | 0/2354 |
| 14 | P | 0.41 | 0/1742 | 0.63 | 2/2330 (0.1%) |
| 15 | Q | 0.44 | 0/1723 | 0.68 | 0/2341 |
| 16 | R | 0.43 | 0/805 | 0.57 | 0/1079 |
| 17 | S | 0.30 | 0/1885 | 0.53 | 0/2510 |
| 18 | T | 0.54 | 0/1011 | 0.81 | 1/1355 (0.1%) |
| 19 | V | 0.38 | 0/1232 | 0.45 | 0/1656 |
| 20 | W | 0.93 | 3/38778 (0.0%) | 1.00 | 76/60434 (0.1%) |
| 21 | X | 0.43 | 0/1186 | 0.47 | 0/1585 |
| 22 | Y | 0.45 | 0/2083 | 0.60 | 2/2805 (0.1%) |
| 23 | Z | 0.40 | 0/1502 | 0.57 | 0/2008 |
| 24 | y | 0.61 | 2/1531 (0.1%) | 1.01 | 5/2384 (0.2%) |
| 25 | 7 | 0.26 | 0/628 | 0.61 | 0/846 |
| 26 | 9 | 0.45 | 0/231 | 0.72 | 0/294 |
| 27 | a | 0.44 | 0/1105 | 0.54 | 0/1476 |
| 28 | b | 0.46 | 0/458 | 0.73 | 1/602 (0.2%) |
| 29 | c | 0.54 | 0/1051 | 0.85 | 4/1406 (0.3%) |
| 30 | d | 0.44 | 0/1655 | 0.65 | 0/2205 |
| 31 | e | 0.35 | 0/1032 | 0.48 | 0/1371 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 32 | f | 0.39 | 0/1481 | 0.58 | 0/1988 |
| 33 | g | 0.38 | 0/1142 | 0.59 | 0/1528 |
| 34 | h | 0.35 | 0/1780 | 0.51 | 0/2397 |
| 35 | i | 0.42 | 0/859 | 0.68 | 0/1159 |
| 36 | j | 0.31 | 0/964 | 0.54 | 0/1289 |
| 37 | k | 0.35 | 0/2493 | 0.59 | 0/3394 |
| 38 | l | 0.38 | 0/1123 | 0.58 | 0/1504 |
| 39 | m | 0.43 | 0/565 | 0.67 | 0/759 |
| 40 | n | 0.36 | 0/1194 | 0.68 | 1/1599 (0.1%) |
| 41 | o | 0.47 | 0/470 | 0.73 | 1/623 (0.2%) |
| 42 | p | 0.23 | 0/444 | 0.59 | 0/588 |
| 43 | q | 0.32 | 0/960 | 0.73 | 0/1286 |
| 44 | s | 0.40 | 0/500 | 0.55 | 0/669 |
| 45 | v | 0.44 | 0/1078 | 0.81 | 1/1447 (0.1%) |
| 46 | w | 0.36 | 0/827 | 0.56 | 0/1110 |
| 47 | z | 0.71 | 0/643 | 0.99 | 1/999 (0.1%) |
| 48 | x | 0.29 | 0/2963 | 0.58 | 1/4050 (0.0%) |
| 49 | 6 | 0.17 | 0/1926 | 0.47 | 0/2669 |
| 50 | 4 | 0.12 | 0/1269 | 0.33 | 0/1762 |
| 51 | 8 | 0.14 | 0/1569 | 0.42 | 0/2183 |
| 52 | 3 | 0.11 | 0/1055 | 0.32 | 0/1469 |
| 53 | 5 | 0.12 | 0/1575 | 0.36 | 0/2187 |
| All | All | 0.60 | 5/117947 (0.0%) | 0.77 | 100/167930 (0.1%) |

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 | 1 |
| 18 | T | 0 | 1 |
| 22 | Y | 0 | 1 |
| All | All | 0 | 3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | W | 159 | A2M | O3'-P | 5.31 | 1.61 | 1.56 |
| 20 | W | 576 | A2M | O3'-P | 5.26 | 1.61 | 1.56 |
| 20 | W | 512 | A2M | O3'-P | 5.17 | 1.61 | 1.56 |
| 24 | y | 64 | RIA | O3'-P | 5.03 | 1.61 | 1.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | y | 76 | A | N9-C4 | 5.02 | 1.40 | 1.37 |

All (100) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | c | 55 | ASP | N-CA-C | -7.76 | 98.46 | 110.17 |
| 22 | Y | 30 | ARG | N-CA-CB | 7.32 | 119.47 | 110.17 |
| 18 | T | 139 | SER | N-CA-C | 7.30 | 122.15 | 108.65 |
| 20 | W | 1782 | G | P-O3'-C3' | 7.06 | 128.17 | 119.70 |
| 40 | n | 85 | ASN | CB-CA-C | -6.71 | 98.43 | 110.70 |
| 20 | W | 574 | A | O5'-C5'-C4' | 6.45 | 114.56 | 109.40 |
| 41 | o | 6 | LEU | N-CA-C | -6.43 | 106.07 | 114.04 |
| 45 | v | 111 | PHE | N-CA-C | -6.33 | 105.84 | 112.93 |
| 20 | W | 1520 | G | C2'-C3'-O3' | -6.23 | 103.73 | 113.70 |
| 20 | W | 955 | A | O5'-C5'-C4' | 6.02 | 114.22 | 109.40 |
| 47 | z | 108 | G | P-O3'-C3' | 5.99 | 126.89 | 119.70 |
| 20 | W | 402 | C | C6-N1-C2 | -5.96 | 117.92 | 120.30 |
| 20 | W | 1271 | C | N1-C2-O2 | 5.96 | 122.47 | 118.90 |
| 20 | W | 459 | C | C6-N1-C2 | -5.95 | 117.92 | 120.30 |
| 20 | W | 1216 | C | N1-C2-O2 | 5.94 | 122.47 | 118.90 |
| 10 | L | 162 | GLN | CA-CB-CG | 5.93 | 125.97 | 114.10 |
| 20 | W | 1435 | C | O5'-C5'-C4' | 5.89 | 114.11 | 109.40 |
| 20 | W | 106 | C | C6-N1-C2 | -5.88 | 117.95 | 120.30 |
| 20 | W | 324 | C | N1-C2-O2 | 5.86 | 122.42 | 118.90 |
| 20 | W | 391 | C | C6-N1-C2 | -5.86 | 117.95 | 120.30 |
| 20 | W | 536 | A | P-O3'-C3' | 5.67 | 126.51 | 119.70 |
| 20 | W | 402 | C | C5-C6-N1 | 5.67 | 123.83 | 121.00 |
| 24 | y | 34 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 24 | y | 34 | C | C6-N1-C2 | -5.62 | 118.05 | 120.30 |
| 20 | W | 632 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 20 | W | 1149 | A | C2-N3-C4 | 5.57 | 113.39 | 110.60 |
| 14 | P | 176 | VAL | CA-C-N | 5.55 | 132.15 | 121.54 |
| 14 | P | 176 | VAL | C-N-CA | 5.55 | 132.15 | 121.54 |
| 20 | W | 1130 | G | O5'-C5'-C4' | 5.55 | 113.84 | 109.40 |
| 20 | W | 1696 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |
| 20 | W | 632 | C | C5-C6-N1 | 5.49 | 123.75 | 121.00 |
| 20 | W | 1259 | A | C2-N3-C4 | 5.48 | 113.34 | 110.60 |
| 20 | W | 1420 | G | P-O3'-C3' | 5.48 | 126.27 | 119.70 |
| 20 | W | 577 | U | O5'-C5'-C4' | 5.47 | 113.78 | 109.40 |
| 20 | W | 1314 | U | C2-N1-C1' | 5.46 | 124.25 | 117.70 |
| 20 | W | 632 | C | C2-N1-C1' | 5.45 | 124.80 | 118.80 |
| 20 | W | 1002 | U | N1-C2-O2 | 5.43 | 126.60 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | W | 1146 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 20 | W | 1149 | A | N1-C6-N6 | -5.42 | 115.35 | 118.60 |
| 20 | W | 473 | A | O5'-C5'-C4' | 5.42 | 113.73 | 109.40 |
| 20 | W | 1123 | C | N1-C2-O2 | 5.41 | 122.15 | 118.90 |
| 20 | W | 30 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 20 | W | 1600 | G | C4-N9-C1' | 5.41 | 133.53 | 126.50 |
| 29 | c | 56 | HIS | N-CA-C | -5.39 | 107.25 | 112.97 |
| 20 | W | 322 | C | N1-C2-O2 | 5.39 | 122.13 | 118.90 |
| 20 | W | 1064 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 10 | L | 66 | VAL | N-CA-CB | 5.36 | 114.63 | 110.45 |
| 20 | W | 14 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 20 | W | 72 | C | C3'-C2'-C1' | -5.34 | 97.56 | 101.30 |
| 20 | W | 1123 | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 20 | W | 1271 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 20 | W | 1544 | C | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 20 | W | 12 | U | N3-C2-O2 | -5.31 | 118.48 | 122.20 |
| 20 | W | 1623 | A | O4'-C1'-N9 | 5.30 | 112.21 | 108.50 |
| 20 | W | 1002 | U | N3-C2-O2 | -5.23 | 118.54 | 122.20 |
| 20 | W | 402 | C | C2-N3-C4 | 5.22 | 122.51 | 119.90 |
| 20 | W | 49 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 20 | W | 1500 | G | C5-C6-O6 | -5.20 | 125.48 | 128.60 |
| 20 | W | 1330 | G | C3'-C2'-C1' | -5.19 | 97.34 | 101.50 |
| 20 | W | 1373 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |
| 20 | W | 1286 | G | O5'-C5'-C4' | 5.18 | 113.55 | 109.40 |
| 20 | W | 1002 | U | C2-N1-C1' | 5.17 | 123.91 | 117.70 |
| 20 | W | 753 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 29 | c | 55 | ASP | CA-C-N | -5.15 | 114.27 | 122.66 |
| 29 | c | 55 | ASP | C-N-CA | -5.15 | 114.27 | 122.66 |
| 20 | W | 4 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 20 | W | 1205 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 28 | b | 124 | GLY | CA-C-O | -5.14 | 117.61 | 122.39 |
| 20 | W | 1130 | G | O4'-C1'-N9 | 5.13 | 112.09 | 108.50 |
| 24 | y | 11 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 20 | W | 340 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 48 | x | 77 | GLU | N-CA-C | -5.12 | 106.78 | 112.57 |
| 20 | W | 49 | C | N3-C2-O2 | -5.12 | 118.32 | 121.90 |
| 24 | y | 32 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 12 | N | 61 | ARG | CA-CB-CG | 5.10 | 124.31 | 114.10 |
| 20 | W | 120 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 20 | W | 474 | G | C4-N9-C1' | 5.09 | 133.12 | 126.50 |
| 20 | W | 14 | C | N3-C2-O2 | -5.08 | 118.34 | 121.90 |
| 20 | W | 1348 | G | N3-C4-C5 | -5.08 | 126.06 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | W | 1412 | C | C5-C6-N1 | 5.08 | 123.54 | 121.00 |
| 20 | W | 1738 | C | C5-C6-N1 | 5.08 | 123.54 | 121.00 |
| 22 | Y | 30 | ARG | CB-CA-C | -5.08 | 104.24 | 110.08 |
| 20 | W | 37 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 20 | W | 106 | C | C5-C6-N1 | 5.08 | 123.54 | 121.00 |
| 20 | W | 433 | A | C2'-C3'-O3' | 5.08 | 121.82 | 113.70 |
| 10 | L | 64 | VAL | N-CA-CB | -5.07 | 104.12 | 111.21 |
| 24 | y | 76 | A | C4-N9-C1' | 5.06 | 135.41 | 126.30 |
| 20 | W | 37 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 20 | W | 459 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 20 | W | 1696 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 20 | W | 1696 | C | N3-C2-O2 | -5.05 | 118.37 | 121.90 |
| 20 | W | 1090 | C | C6-N1-C2 | -5.04 | 118.28 | 120.30 |
| 20 | W | 1676 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 20 | W | 842 | C | N1-C2-O2 | 5.04 | 121.92 | 118.90 |
| 20 | W | 353 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 20 | W | 459 | C | C5-C6-N1 | 5.03 | 123.51 | 121.00 |
| 20 | W | 433 | A | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 20 | W | 1060 | A | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 20 | W | 1259 | A | C4-N9-C1' | 5.02 | 135.34 | 126.30 |
| 20 | W | 1271 | C | N3-C2-O2 | -5.01 | 118.39 | 121.90 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 14 | ARG | Sidechain |
| 18 | T | 137 | SER | Peptide |
| 22 | Y | 30 | ARG | Sidechain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 5504 | 0 | 5117 | 69 | 0 |
| 2 | B | 2635 | 0 | 2207 | 27 | 0 |
| 3 | D | 2234 | 0 | 2288 | 22 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | E | 3540 | 0 | 3690 | 37 | 0 |
| 5 | F | 1598 | 0 | 723 | 5 | 0 |
| 6 | G | 789 | 0 | 806 | 10 | 0 |
| 7 | H | 691 | 0 | 706 | 13 | 0 |
| 8 | I | 4569 | 0 | 4317 | 38 | 0 |
| 9 | J | 4940 | 0 | 4682 | 67 | 0 |
| 10 | L | 1439 | 0 | 1533 | 17 | 0 |
| 11 | M | 631 | 0 | 655 | 14 | 0 |
| 12 | N | 636 | 0 | 637 | 6 | 0 |
| 13 | O | 1707 | 0 | 1794 | 13 | 0 |
| 14 | P | 1715 | 0 | 1785 | 27 | 0 |
| 15 | Q | 1686 | 0 | 1688 | 22 | 0 |
| 16 | R | 792 | 0 | 841 | 5 | 0 |
| 17 | S | 1862 | 0 | 2018 | 23 | 0 |
| 18 | T | 998 | 0 | 1021 | 13 | 0 |
| 19 | V | 1208 | 0 | 1294 | 8 | 0 |
| 20 | W | 36695 | 0 | 18566 | 204 | 0 |
| 21 | X | 1166 | 0 | 1233 | 9 | 0 |
| 22 | Y | 2041 | 0 | 2143 | 11 | 0 |
| 23 | Z | 1477 | 0 | 1589 | 12 | 0 |
| 24 | y | 1639 | 0 | 850 | 21 | 0 |
| 25 | 7 | 616 | 0 | 600 | 6 | 0 |
| 26 | 9 | 230 | 0 | 276 | 3 | 0 |
| 27 | a | 1087 | 0 | 1154 | 11 | 0 |
| 28 | b | 452 | 0 | 494 | 1 | 0 |
| 29 | c | 1034 | 0 | 1080 | 7 | 0 |
| 30 | d | 1628 | 0 | 1706 | 16 | 0 |
| 31 | e | 1015 | 0 | 1086 | 7 | 0 |
| 32 | f | 1461 | 0 | 1511 | 9 | 0 |
| 33 | g | 1124 | 0 | 1193 | 5 | 0 |
| 34 | h | 1752 | 0 | 1848 | 22 | 0 |
| 35 | i | 834 | 0 | 861 | 14 | 0 |
| 36 | j | 946 | 0 | 988 | 16 | 0 |
| 37 | k | 2436 | 0 | 2391 | 45 | 0 |
| 38 | l | 1105 | 0 | 1138 | 10 | 0 |
| 39 | m | 559 | 0 | 616 | 8 | 0 |
| 40 | n | 1176 | 0 | 1233 | 20 | 0 |
| 41 | o | 459 | 0 | 448 | 8 | 0 |
| 42 | p | 435 | 0 | 434 | 5 | 0 |
| 43 | q | 950 | 0 | 985 | 9 | 0 |
| 44 | s | 498 | 0 | 525 | 4 | 0 |
| 45 | v | 1064 | 0 | 1118 | 17 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 46 | w | 817 | 0 | 882 | 7 | 0 |
| 47 | z | 575 | 0 | 293 | 7 | 0 |
| 48 | x | 2920 | 0 | 2231 | 42 | 0 |
| 49 | 6 | 1917 | 0 | 1096 | 8 | 0 |
| 50 | 4 | 1272 | 0 | 564 | 8 | 0 |
| 51 | 8 | 1571 | 0 | 683 | 10 | 0 |
| 52 | 3 | 1057 | 0 | 475 | 1 | 0 |
| 53 | 5 | 1581 | 0 | 689 | 4 | 0 |
| 54 | R | 1 | 0 | 0 | 0 | 0 |
| 54 | o | 1 | 0 | 0 | 0 | 0 |
| 54 | p | 1 | 0 | 0 | 0 | 0 |
| 55 | S | 1 | 0 | 0 | 0 | 0 |
| 55 | T | 1 | 0 | 0 | 0 | 0 |
| 55 | W | 85 | 0 | 0 | 0 | 0 |
| 55 | f | 1 | 0 | 0 | 0 | 0 |
| 56 | W | 3 | 0 | 0 | 0 | 0 |
| All | All | 114857 | 0 | 90781 | 873 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (873) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:M:72:ARG:HH12 | 20:W:1120:U:H1' | 1.39 | 0.86 |
| 20:W:928:G:H1 | 20:W:1013:U:H3 | 1.23 | 0.86 |
| 20:W:1301:A:HO2' | 41:o:2:GLY:N | 1.74 | 0.85 |
| 20:W:925:G:H1 | 20:W:1017:U:H3 | 1.36 | 0.73 |
| 11:M:72:ARG:NH1 | 20:W:1120:U:H1' | 2.03 | 0.73 |
| 11:M:80:ARG:HD3 | 48:x:79:SER:HB2 | 1.71 | 0.73 |
| 14:P:69:VAL:HG13 | 14:P:74:LEU:HD11 | 1.71 | 0.72 |
| 8:I:661:PRO:HG2 | 8:I:707:ARG:H | 1.54 | 0.72 |
| 20:W:1421:A:OP1 | 20:W:1422:G:H5" | 1.90 | 0.72 |
| 20:W:1462:U:H6 | 20:W:1462:U:H5' | 1.55 | 0.71 |
| 34:h:106:ARG:HG2 | 34:h:175:VAL:HG22 | 1.73 | 0.71 |
| 20:W:940:U:H3 | 20:W:1002:U:H3 | 1.39 | 0.70 |
| 24:y:37:T6A:N1 | 24:y:37:T6A:N11 | 2.34 | 0.70 |
| 20:W:1222:G:H5" | 32:f:78:MET:HE1 | 1.72 | 0.69 |
| 45:v:107:LYS:HA | 45:v:112:GLY:HA3 | 1.73 | 0.69 |
| 48:x:79:SER:O | 48:x:80:PHE:C | 2.35 | 0.69 |
| 9:J:421:GLY:HA2 | 9:J:441:ARG:H | 1.58 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:10:ASN:OD1 | 14:P:77:ASP:HA | 1.92 | 0.68 |
| 20:W:1603:G:H4' | 40:n:38:ARG:HH21 | 1.59 | 0.68 |
| 33:g:97:GLN:HB3 | 33:g:105:LYS:HG3 | 1.76 | 0.68 |
| 20:W:1588:A:H2' | 20:W:1589:A:C8 | 2.28 | 0.68 |
| 9:J:672:PRO:HD2 | 9:J:675:LEU:HD12 | 1.76 | 0.67 |
| 17:S:170:ARG:NH2 | 20:W:71:G:N7 | 2.42 | 0.67 |
| 22:Y:87:MET:HE3 | 22:Y:123:LEU:HB2 | 1.74 | 0.67 |
| 20:W:1116:C:H2' | 20:W:1117:C:C5 | 2.30 | 0.67 |
| 48:x:73:HIS:CD2 | 48:x:76:ASP:HA | 2.28 | 0.67 |
| 4:E:353:MET:HE1 | 24:y:74:C:H5' | 1.75 | 0.67 |
| 16:R:42:ARG:HH12 | 47:z:98:A:H1' | 1.61 | 0.66 |
| 18:T:121:ARG:HH11 | 44:s:40:ARG:HH11 | 1.44 | 0.66 |
| 42:p:118:ARG:HH21 | 42:p:134:SER:H | 1.44 | 0.66 |
| 37:k:87:LEU:HB2 | 37:k:101:PHE:HB2 | 1.76 | 0.66 |
| 20:W:1091:C:HO2' | 29:c:2:VAL:N | 1.93 | 0.66 |
| 20:W:73:C:H5" | 20:W:74:G:H5' | 1.77 | 0.66 |
| 2:B:209:GLN:HG3 | 48:x:21:VAL:HG23 | 1.78 | 0.66 |
| 36:j:18:ARG:NH1 | 40:n:88:LYS:HD2 | 2.11 | 0.65 |
| 1:A:483:ARG:HB2 | 1:A:492:SER:HB3 | 1.78 | 0.65 |
| 9:J:586:ARG:HG3 | 48:x:39:LEU:HD21 | 1.78 | 0.65 |
| 39:m:68:ILE:HB | 39:m:109:TYR:HB2 | 1.78 | 0.65 |
| 40:n:85:ASN:CG | 40:n:97:GLN:HE22 | 2.05 | 0.65 |
| 37:k:164:ILE:HG22 | 37:k:178:ASN:HA | 1.79 | 0.65 |
| 48:x:447:LEU:HB2 | 48:x:473:PRO:HG3 | 1.78 | 0.65 |
| 1:A:307:ARG:HD2 | 1:A:309:ASN:HB2 | 1.79 | 0.64 |
| 15:Q:74:VAL:HG12 | 15:Q:121:LEU:HB3 | 1.79 | 0.64 |
| 20:W:1422:G:H2' | 20:W:1423:C:H5" | 1.77 | 0.64 |
| 6:G:40:LYS:HB3 | 6:G:48:GLU:HB2 | 1.78 | 0.64 |
| 8:I:587:ILE:HG22 | 8:I:609:GLN:HE21 | 1.61 | 0.64 |
| 37:k:11:LEU:HB2 | 37:k:307:VAL:HB | 1.79 | 0.64 |
| 1:A:296:LEU:HB3 | 1:A:322:VAL:HG23 | 1.79 | 0.64 |
| 18:T:34:PHE:HB3 | 18:T:41:PHE:HB2 | 1.79 | 0.64 |
| 31:e:20:ARG:NH1 | 31:e:74:MET:SD | 2.71 | 0.64 |
| 1:A:351:LYS:NZ | 9:J:722:GLU:O | 2.31 | 0.63 |
| 45:v:44:LYS:HG3 | 45:v:47:ARG:HH21 | 1.64 | 0.63 |
| 4:E:38:ARG:NH2 | 4:E:327:ASP:O | 2.32 | 0.63 |
| 20:W:1753:C:OP1 | 20:W:1782:G:N2 | 2.33 | 0.62 |
| 33:g:129:SER:O | 33:g:131:LYS:NZ | 2.31 | 0.62 |
| 37:k:214:GLY:HA2 | 37:k:236:ILE:HG12 | 1.81 | 0.62 |
| 1:A:448:GLN:HA | 1:A:493:PHE:HB2 | 1.80 | 0.62 |
| 8:I:545:GLU:HG3 | 8:I:558:VAL:HG22 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:c:80:ASP:OD1 | 29:c:124:LYS:NZ | 2.29 | 0.62 |
| 16:R:44:ILE:HD12 | 16:R:65:PRO:HG2 | 1.82 | 0.62 |
| 4:E:259:ILE:HG22 | 4:E:260:ARG:HG2 | 1.81 | 0.62 |
| 20:W:72:C:H3' | 20:W:73:C:C2 | 2.34 | 0.62 |
| 20:W:981:A:H2' | 20:W:982:G:C8 | 2.35 | 0.62 |
| 19:V:124:ARG:NH2 | 20:W:1024:A:OP2 | 2.33 | 0.61 |
| 1:A:13:LYS:NZ | 14:P:76:ASN:HB3 | 2.14 | 0.61 |
| 13:O:204:ILE:O | 13:O:211:LYS:NZ | 2.33 | 0.61 |
| 14:P:76:ASN:HD22 | 14:P:77:ASP:H | 1.48 | 0.61 |
| 48:x:305:SER:H | 48:x:308:SER:HB3 | 1.65 | 0.61 |
| 20:W:818:A:OP1 | 23:Z:80:ARG:NH2 | 2.33 | 0.61 |
| 13:O:64:THR:HG23 | 13:O:67:GLY:H | 1.65 | 0.61 |
| 30:d:103:LEU:HD22 | 30:d:170:LYS:HB3 | 1.83 | 0.61 |
| 36:j:110:GLU:OE2 | 40:n:116:LYS:NZ | 2.34 | 0.61 |
| 4:E:396:GLN:O | 4:E:445:ARG:NH2 | 2.34 | 0.61 |
| 20:W:688:U:H4' | 20:W:689:U:O5' | 2.01 | 0.61 |
| 20:W:1115:U:H2' | 20:W:1118:C:N3 | 2.16 | 0.61 |
| 1:A:471:ILE:HD12 | 1:A:484:ILE:HG12 | 1.82 | 0.60 |
| 4:E:348:CYS:HB2 | 24:y:75:C:H1' | 1.83 | 0.60 |
| 20:W:1520:G:N3 | 20:W:1520:G:H2' | 2.15 | 0.60 |
| 4:E:445:ARG:HE | 4:E:454:ILE:HG21 | 1.65 | 0.60 |
| 4:E:377:LEU:HA | 4:E:455:GLY:HA3 | 1.83 | 0.60 |
| 14:P:183:GLU:HA | 14:P:186:ASN:HB2 | 1.82 | 0.60 |
| 20:W:1113:A:H1' | 20:W:1114:U:P | 2.41 | 0.60 |
| 6:G:13:ARG:NH2 | 24:y:34:C:O2 | 2.34 | 0.60 |
| 10:L:66:VAL:HG22 | 10:L:96:ALA:HB1 | 1.83 | 0.60 |
| 32:f:41:VAL:HG13 | 32:f:42:LYS:HG3 | 1.83 | 0.60 |
| 1:A:397:GLU:OE1 | 1:A:402:LYS:NZ | 2.34 | 0.60 |
| 35:i:94:LEU:O | 35:i:96:ARG:NH1 | 2.34 | 0.60 |
| 45:v:33:ARG:NH1 | 45:v:36:GLU:OE2 | 2.34 | 0.60 |
| 10:L:154:ILE:HB | 10:L:185:VAL:HG22 | 1.83 | 0.60 |
| 32:f:34:SER:HA | 44:s:55:VAL:HG23 | 1.84 | 0.60 |
| 14:P:56:LYS:NZ | 20:W:952:G:OP1 | 2.35 | 0.59 |
| 23:Z:65:GLU:O | 23:Z:66:LYS:HB2 | 2.01 | 0.59 |
| 14:P:214:LYS:NZ | 20:W:943:U:OP1 | 2.34 | 0.59 |
| 10:L:60:ILE:HB | 10:L:92:VAL:HG12 | 1.83 | 0.59 |
| 17:S:213:LEU:HG | 17:S:217:MET:HE2 | 1.83 | 0.59 |
| 33:g:44:PRO:HG2 | 33:g:81:ILE:HD11 | 1.84 | 0.59 |
| 2:B:291:PRO:HG2 | 2:B:318:VAL:HG11 | 1.84 | 0.59 |
| 34:h:64:ARG:NH2 | 35:i:93:THR:OG1 | 2.36 | 0.59 |
| 17:S:98:ARG:NH2 | 17:S:103:ASP:OD1 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:520:GLN:NE2 | 8:I:572:PRO:O | 2.36 | 0.59 |
| 37:k:256:ILE:HB | 37:k:270:LEU:HB2 | 1.84 | 0.59 |
| 20:W:614:C:H2' | 20:W:626:G:C8 | 2.38 | 0.59 |
| 34:h:40:ARG:NH1 | 34:h:47:GLU:OE1 | 2.36 | 0.59 |
| 4:E:97:PRO:HG2 | 4:E:100:GLU:HB3 | 1.85 | 0.58 |
| 10:L:170:VAL:HG13 | 10:L:187:PHE:HB2 | 1.85 | 0.58 |
| 4:E:105:CYS:SG | 4:E:106:GLY:N | 2.77 | 0.58 |
| 35:i:94:LEU:HD23 | 35:i:95:ARG:HB2 | 1.84 | 0.58 |
| 53:5:244:LEU:O | 53:5:436:HIS:N | 2.36 | 0.58 |
| 1:A:492:SER:HG | 1:A:495:SER:HG | 1.50 | 0.58 |
| 18:T:83:GLN:NE2 | 18:T:87:GLU:OE1 | 2.37 | 0.58 |
| 20:W:60:G:H22 | 20:W:316:G:H21 | 1.50 | 0.58 |
| 1:A:175:HIS:HB2 | 1:A:228:MET:HE2 | 1.86 | 0.58 |
| 5:F:233:ASN:H | 5:F:248:GLY:HA3 | 1.69 | 0.57 |
| 17:S:140:ARG:NH1 | 20:W:170:A:OP2 | 2.37 | 0.57 |
| 19:V:104:ARG:NH2 | 20:W:1007:C:O2' | 2.37 | 0.57 |
| 8:I:548:ARG:HH12 | 8:I:550:ARG:HB3 | 1.69 | 0.57 |
| 49:6:351:TYR:O | 49:6:355:ASN:ND2 | 2.37 | 0.57 |
| 3:D:182:ARG:NH2 | 24:y:55:U:O2' | 2.36 | 0.57 |
| 15:Q:128:ARG:NH2 | 15:Q:151:ASP:O | 2.38 | 0.57 |
| 18:T:86:LYS:NZ | 18:T:122:SER:O | 2.34 | 0.57 |
| 20:W:72:C:OP2 | 20:W:73:C:N4 | 2.37 | 0.57 |
| 8:I:380:ASP:HB3 | 8:I:426:TRP:HH2 | 1.70 | 0.57 |
| 17:S:57:ASP:HA | 17:S:106:LEU:HA | 1.85 | 0.57 |
| 23:Z:18:ARG:O | 23:Z:24:ARG:NH1 | 2.37 | 0.57 |
| 20:W:1462:U:H5' | 20:W:1462:U:C6 | 2.39 | 0.57 |
| 30:d:57:ALA:HB2 | 30:d:183:GLY:HA2 | 1.86 | 0.57 |
| 20:W:1281:G:OP2 | 43:q:101:ARG:NH2 | 2.37 | 0.57 |
| 22:Y:139:LEU:HD23 | 22:Y:150:PRO:HB3 | 1.87 | 0.57 |
| 51:8:150:LEU:HA | 51:8:166:ALA:HA | 1.87 | 0.57 |
| 13:O:65:LYS:HE2 | 15:Q:118:GLU:HG3 | 1.86 | 0.56 |
| 4:E:177:ILE:HG23 | 4:E:182:LEU:HB3 | 1.86 | 0.56 |
| 9:J:565:ARG:HB3 | 48:x:69:TYR:HE1 | 1.69 | 0.56 |
| 12:N:32:ILE:HD12 | 12:N:34:MET:HB2 | 1.87 | 0.56 |
| 20:W:1396:A:O2' | 20:W:1398:G:N7 | 2.38 | 0.56 |
| 32:f:102:LEU:HD21 | 39:m:100:VAL:HG21 | 1.85 | 0.56 |
| 2:B:280:VAL:HG23 | 2:B:281:ILE:HG23 | 1.87 | 0.56 |
| 47:z:115:G:H3' | 47:z:115:G:N3 | 2.20 | 0.56 |
| 1:A:559:LYS:HA | 1:A:562:ARG:HG2 | 1.86 | 0.56 |
| 17:S:49:VAL:HB | 17:S:115:LYS:HB3 | 1.88 | 0.56 |
| 20:W:1563:G:OP1 | 38:l:121:ARG:NH1 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:e:98:GLU:OE2 | 31:e:101:LYS:NZ | 2.38 | 0.56 |
| 3:D:183:ARG:HH12 | 24:y:57:G:H1 | 1.52 | 0.56 |
| 15:Q:12:GLU:O | 15:Q:13:GLU:C | 2.47 | 0.56 |
| 25:7:287:PHE:O | 25:7:288:HIS:ND1 | 2.39 | 0.56 |
| 48:x:200:GLU:H | 48:x:355:SER:HB3 | 1.71 | 0.56 |
| 33:g:53:GLU:OE1 | 33:g:85:ARG:NH2 | 2.36 | 0.56 |
| 48:x:227:VAL:O | 48:x:374:ARG:NH2 | 2.36 | 0.56 |
| 7:H:31:ILE:HA | 7:H:49:GLY:HA3 | 1.86 | 0.55 |
| 20:W:616:A:OP1 | 27:a:68:LYS:NZ | 2.39 | 0.55 |
| 17:S:94:ARG:NH2 | 20:W:1737:G:OP1 | 2.39 | 0.55 |
| 20:W:1522:A:OP2 | 40:n:144:ARG:NE | 2.39 | 0.55 |
| 26:9:16:LYS:HG2 | 26:9:20:MET:HE2 | 1.87 | 0.55 |
| 34:h:136:VAL:HG22 | 34:h:186:VAL:HG12 | 1.88 | 0.55 |
| 2:B:247:GLN:HG2 | 2:B:250:CYS:H | 1.71 | 0.55 |
| 9:J:567:CYS:SG | 9:J:605:VAL:HG22 | 2.46 | 0.55 |
| 1:A:298:ARG:HH22 | 1:A:361:LEU:HD13 | 1.71 | 0.55 |
| 1:A:384:VAL:HG12 | 1:A:386:GLU:H | 1.71 | 0.55 |
| 4:E:255:ARG:NH1 | 4:E:436:GLU:OE2 | 2.39 | 0.55 |
| 17:S:170:ARG:NH2 | 20:W:72:C:C4 | 2.75 | 0.55 |
| 38:l:104:LEU:HD13 | 38:l:121:ARG:HD2 | 1.89 | 0.55 |
| 4:E:165:CYS:HB2 | 4:E:166:PRO:HA | 1.89 | 0.55 |
| 6:G:44:ASN:ND2 | 20:W:1710:C:O2 | 2.40 | 0.55 |
| 8:I:461:SER:O | 8:I:463:LYS:NZ | 2.39 | 0.55 |
| 1:A:483:ARG:HH22 | 9:J:845:HIS:HB3 | 1.71 | 0.55 |
| 4:E:47:ILE:HD12 | 4:E:173:HIS:HB3 | 1.89 | 0.55 |
| 14:P:39:PHE:HB3 | 14:P:74:LEU:O | 2.06 | 0.55 |
| 20:W:1115:U:H2' | 20:W:1118:C:C4 | 2.42 | 0.55 |
| 20:W:1454:A:H5" | 45:v:3:ARG:HD2 | 1.89 | 0.55 |
| 20:W:1780:G:O6 | 20:W:1782:G:N2 | 2.35 | 0.55 |
| 1:A:301:HIS:HB2 | 1:A:304:ARG:HH21 | 1.72 | 0.55 |
| 9:J:595:GLN:HB3 | 48:x:41:LYS:HD2 | 1.88 | 0.54 |
| 11:M:11:SER:OG | 11:M:14:GLU:OE1 | 2.24 | 0.54 |
| 37:k:237:ASN:ND2 | 37:k:286:CYS:O | 2.40 | 0.54 |
| 3:D:71:VAL:HG21 | 3:D:85:LEU:HD13 | 1.89 | 0.54 |
| 9:J:565:ARG:HB3 | 48:x:69:TYR:CE1 | 2.42 | 0.54 |
| 7:H:32:HIS:HB2 | 7:H:48:GLN:HB3 | 1.90 | 0.54 |
| 39:m:48:VAL:HG21 | 40:n:23:ARG:HB3 | 1.87 | 0.54 |
| 7:H:76:HIS:ND1 | 24:y:24:G:O2' | 2.39 | 0.54 |
| 4:E:240:VAL:HG13 | 4:E:241:LYS:HG2 | 1.90 | 0.54 |
| 7:H:56:LYS:HA | 7:H:59:LEU:HD12 | 1.88 | 0.54 |
| 11:M:56:CYS:O | 11:M:60:SER:HA | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:c:6:VAL:HG12 | 29:c:34:ILE:HD11 | 1.89 | 0.54 |
| 34:h:32:ASP:OD2 | 34:h:65:ARG:NH1 | 2.39 | 0.54 |
| 37:k:201:SER:HB2 | 37:k:206:LEU:HB2 | 1.88 | 0.54 |
| 40:n:118:ARG:HE | 40:n:123:LEU:HD21 | 1.73 | 0.54 |
| 3:D:112:LEU:HD12 | 3:D:130:LEU:HB3 | 1.87 | 0.54 |
| 20:W:882:U:O4 | 20:W:904:A:N6 | 2.41 | 0.54 |
| 20:W:1192:U:OP2 | 27:a:119:ARG:NH2 | 2.40 | 0.54 |
| 37:k:120:ILE:HB | 37:k:132:TRP:HB2 | 1.90 | 0.54 |
| 3:D:25:ARG:NH2 | 3:D:35:SER:OG | 2.41 | 0.54 |
| 4:E:256:LEU:HD23 | 4:E:358:LEU:HD22 | 1.90 | 0.54 |
| 20:W:1462:U:H3' | 20:W:1463:U:H5" | 1.89 | 0.54 |
| 1:A:201:LEU:O | 1:A:233:ARG:NH2 | 2.41 | 0.54 |
| 4:E:400:LYS:HE3 | 4:E:419:ALA:HA | 1.89 | 0.54 |
| 14:P:26:SER:O | 14:P:51:ARG:NH2 | 2.41 | 0.54 |
| 22:Y:122:LYS:NZ | 22:Y:143:ASP:OD2 | 2.40 | 0.54 |
| 25:7:308:LEU:HD12 | 34:h:59:LEU:HD21 | 1.88 | 0.54 |
| 15:Q:13:GLU:HG2 | 15:Q:14:ASP:N | 2.23 | 0.54 |
| 4:E:355:GLY:HA3 | 4:E:411:LEU:HB3 | 1.90 | 0.53 |
| 27:a:123:VAL:HG12 | 27:a:124:LYS:HG3 | 1.89 | 0.53 |
| 1:A:619:ARG:HA | 12:N:45:ARG:HH12 | 1.72 | 0.53 |
| 20:W:1851:MA6:OP1 | 26:9:9:ARG:NH2 | 2.39 | 0.53 |
| 6:G:24:ARG:NH2 | 6:G:99:GLU:OE2 | 2.41 | 0.53 |
| 9:J:597:ASN:HB3 | 48:x:70:ALA:HB2 | 1.91 | 0.53 |
| 15:Q:80:ARG:NH2 | 15:Q:165:ASN:O | 2.41 | 0.53 |
| 20:W:373:G:H4' | 21:X:85:THR:HG21 | 1.91 | 0.53 |
| 20:W:1117:C:H2' | 20:W:1118:C:O4' | 2.08 | 0.53 |
| 3:D:244:ARG:HG2 | 3:D:248:LEU:HD23 | 1.91 | 0.53 |
| 1:A:55:LEU:HD13 | 1:A:93:TYR:HB2 | 1.90 | 0.53 |
| 10:L:123:THR:HG23 | 20:W:688:U:OP2 | 2.08 | 0.53 |
| 20:W:534:G:H1 | 20:W:549:C:H42 | 1.57 | 0.53 |
| 38:l:6:VAL:O | 38:l:11:GLN:NE2 | 2.42 | 0.53 |
| 48:x:364:LYS:HB3 | 48:x:370:ASP:HB3 | 1.90 | 0.53 |
| 22:Y:44:LEU:HD21 | 22:Y:72:ILE:HD11 | 1.90 | 0.53 |
| 9:J:492:GLU:HG2 | 9:J:493:LYS:HG3 | 1.90 | 0.53 |
| 20:W:201:C:H3' | 20:W:202:G:H21 | 1.73 | 0.53 |
| 50:4:110:ASN:HA | 51:8:110:VAL:HA | 1.91 | 0.53 |
| 10:L:66:VAL:N | 10:L:67:PRO:HD2 | 2.24 | 0.53 |
| 20:W:84:A:H5' | 31:e:122:LYS:HD2 | 1.91 | 0.53 |
| 20:W:99:A2M:O5' | 20:W:99:A2M:H8 | 2.09 | 0.53 |
| 20:W:1619:A:OP2 | 36:j:47:ARG:NH2 | 2.38 | 0.53 |
| 48:x:248:THR:HA | 48:x:373:VAL:HA | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:L:148:LEU:HA | 29:c:42:MET:HE2 | 1.92 | 0.52 |
| 20:W:836:G:H1' | 20:W:837:A:C8 | 2.43 | 0.52 |
| 20:W:1490:OMG:H5' | 20:W:1490:OMG:H8 | 1.74 | 0.52 |
| 46:w:34:LYS:NZ | 46:w:107:GLU:OE2 | 2.41 | 0.52 |
| 1:A:385:PRO:HA | 1:A:388:LYS:HG3 | 1.91 | 0.52 |
| 9:J:834:SER:HA | 9:J:841:THR:HA | 1.91 | 0.52 |
| 44:s:39:SER:HA | 48:x:296:ASN:HD21 | 1.74 | 0.52 |
| 1:A:9:GLU:HG3 | 1:A:46:ILE:HG21 | 1.90 | 0.52 |
| 1:A:304:ARG:NH1 | 1:A:305:GLU:OE1 | 2.43 | 0.52 |
| 16:R:45:VAL:HG11 | 16:R:53:ILE:HG13 | 1.92 | 0.52 |
| 21:X:13:GLN:HE21 | 21:X:63:THR:HG23 | 1.74 | 0.52 |
| 34:h:94:ARG:O | 34:h:101:GLN:NE2 | 2.39 | 0.52 |
| 15:Q:37:TYR:OH | 15:Q:57:LYS:NZ | 2.38 | 0.52 |
| 20:W:1113:A:O4' | 20:W:1119:A:N6 | 2.42 | 0.52 |
| 39:m:58:LEU:O | 39:m:63:PRO:HD3 | 2.10 | 0.52 |
| 9:J:573:ILE:O | 9:J:574:TYR:C | 2.53 | 0.52 |
| 3:D:192:ARG:NH2 | 24:y:4:G:OP1 | 2.43 | 0.52 |
| 37:k:24:THR:HG23 | 37:k:27:PHE:H | 1.74 | 0.52 |
| 9:J:55:LYS:NZ | 20:W:1180:C:OP2 | 2.39 | 0.52 |
| 18:T:150:ARG:NH1 | 20:W:1854:U:OP1 | 2.43 | 0.52 |
| 9:J:636:ILE:HD13 | 48:x:42:VAL:HG22 | 1.92 | 0.52 |
| 48:x:246:PHE:HA | 48:x:371:LEU:HA | 1.91 | 0.52 |
| 1:A:515:PRO:O | 1:A:520:ARG:NH1 | 2.42 | 0.52 |
| 8:I:303:ARG:NH1 | 8:I:322:ASP:OD1 | 2.37 | 0.52 |
| 50:4:119:THR:HA | 50:4:172:TRP:HA | 1.91 | 0.52 |
| 1:A:478:CYS:HB3 | 1:A:507:ILE:HB | 1.92 | 0.52 |
| 8:I:507:ARG:NH1 | 8:I:508:ASN:O | 2.43 | 0.52 |
| 17:S:132:ARG:NH2 | 20:W:152:U:O4' | 2.43 | 0.52 |
| 20:W:322:C:N4 | 20:W:323:C:O2 | 2.43 | 0.52 |
| 20:W:1391:OMC:H4' | 41:o:55:LEU:HD13 | 1.92 | 0.52 |
| 20:W:1391:OMC:HM22 | 20:W:1392:U:H5' | 1.92 | 0.52 |
| 1:A:384:VAL:HB | 1:A:387:VAL:HG22 | 1.91 | 0.51 |
| 2:B:230:ASP:HA | 2:B:234:ASP:HB2 | 1.92 | 0.51 |
| 12:N:61:ARG:NH1 | 15:Q:156:TYR:OH | 2.44 | 0.51 |
| 14:P:146:ARG:HE | 14:P:206:PRO:HG2 | 1.74 | 0.51 |
| 20:W:753:C:H41 | 20:W:790:C:H3' | 1.75 | 0.51 |
| 36:j:83:MET:HB3 | 36:j:116:LEU:HD13 | 1.91 | 0.51 |
| 37:k:219:TRP:HA | 37:k:226:HIS:HA | 1.92 | 0.51 |
| 42:p:103:LEU:O | 43:q:36:ARG:NH2 | 2.42 | 0.51 |
| 6:G:66:ARG:NH2 | 20:W:1825:A:OP2 | 2.43 | 0.51 |
| 8:I:510:PHE:O | 8:I:532:ARG:NE | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:510:PHE:HE2 | 23:Z:125:HIS:HE1 | 1.57 | 0.51 |
| 13:O:108:LYS:HD2 | 13:O:233:LEU:HD13 | 1.93 | 0.51 |
| 20:W:1775:U:O2' | 20:W:1776:G:N2 | 2.44 | 0.51 |
| 34:h:117:ARG:NH2 | 47:z:118:G:OP1 | 2.43 | 0.51 |
| 4:E:373:ILE:HG22 | 4:E:459:ILE:HG12 | 1.93 | 0.51 |
| 9:J:373:LYS:HG3 | 9:J:431:LEU:HD23 | 1.92 | 0.51 |
| 20:W:1116:C:H2' | 20:W:1117:C:H5 | 1.72 | 0.51 |
| 37:k:124:SER:OG | 37:k:126:ASP:OD1 | 2.28 | 0.51 |
| 48:x:289:LEU:HD23 | 48:x:431:LYS:HE2 | 1.92 | 0.51 |
| 9:J:641:ARG:NH2 | 9:J:644:GLU:OE1 | 2.44 | 0.51 |
| 17:S:219:GLU:HA | 17:S:222:GLU:HB2 | 1.92 | 0.51 |
| 34:h:45:ARG:NH1 | 34:h:82:GLY:O | 2.44 | 0.51 |
| 37:k:82:SER:OG | 37:k:83:TRP:N | 2.44 | 0.51 |
| 38:l:108:GLU:OE2 | 38:l:121:ARG:NE | 2.37 | 0.51 |
| 1:A:502:ARG:NH1 | 51:8:247:MET:O | 2.44 | 0.51 |
| 1:A:527:SER:HA | 1:A:530:LEU:HB2 | 1.93 | 0.51 |
| 21:X:78:THR:HG22 | 21:X:79:LYS:HG3 | 1.91 | 0.51 |
| 34:h:94:ARG:NH2 | 47:z:122:A:OP1 | 2.43 | 0.51 |
| 17:S:18:VAL:HG21 | 17:S:24:LEU:HD21 | 1.93 | 0.51 |
| 22:Y:124:CYS:HB3 | 22:Y:141:THR:HB | 1.93 | 0.51 |
| 2:B:341:PHE:HA | 2:B:344:PHE:HB3 | 1.92 | 0.51 |
| 20:W:324:C:OP2 | 20:W:329:G:N2 | 2.44 | 0.51 |
| 39:m:61:GLU:O | 39:m:62:VAL:C | 2.54 | 0.51 |
| 3:D:209:LYS:NZ | 4:E:272:ASP:OD1 | 2.44 | 0.50 |
| 7:H:48:GLN:HG2 | 7:H:49:GLY:H | 1.76 | 0.50 |
| 8:I:699:PHE:HZ | 8:I:702:LEU:HD22 | 1.76 | 0.50 |
| 20:W:320:G:H1 | 20:W:331:C:H42 | 1.59 | 0.50 |
| 20:W:886:A:H2' | 20:W:887:U:H4' | 1.93 | 0.50 |
| 42:p:132:MET:HE1 | 42:p:148:TYR:HD2 | 1.76 | 0.50 |
| 51:8:118:GLY:HA2 | 51:8:147:SER:HA | 1.92 | 0.50 |
| 1:A:481:GLN:NE2 | 1:A:496:ASP:O | 2.44 | 0.50 |
| 48:x:304:ASN:OD1 | 48:x:311:ASN:ND2 | 2.43 | 0.50 |
| 20:W:1307:U:O2' | 42:p:138:ARG:NH2 | 2.44 | 0.50 |
| 20:W:1610:G:OP1 | 40:n:121:ARG:NH2 | 2.44 | 0.50 |
| 2:B:399:SER:HA | 2:B:403:GLN:HB2 | 1.93 | 0.50 |
| 8:I:490:PRO:HB3 | 8:I:510:PHE:HE1 | 1.77 | 0.50 |
| 14:P:83:LYS:NZ | 18:T:130:GLU:OE2 | 2.41 | 0.50 |
| 20:W:493:A:H1' | 20:W:574:A:H5" | 1.93 | 0.50 |
| 20:W:837:A:H4' | 20:W:838:G:OP1 | 2.10 | 0.50 |
| 31:e:83:LYS:HE2 | 31:e:96:LEU:HD22 | 1.94 | 0.50 |
| 48:x:295:ALA:HB2 | 48:x:427:ASN:HA | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:6:220:PHE:O | 49:6:341:THR:OG1 | 2.29 | 0.50 |
| 49:6:333:VAL:HG12 | 49:6:334:VAL:HG23 | 1.92 | 0.50 |
| 7:H:39:ASN:HB2 | 24:y:37:T6A:H5" | 1.92 | 0.50 |
| 8:I:464:ILE:HB | 8:I:467:ILE:HD11 | 1.94 | 0.50 |
| 9:J:486:VAL:HG23 | 9:J:502:ILE:HD11 | 1.94 | 0.50 |
| 24:y:9:1MG:H8 | 24:y:11:C:H41 | 1.58 | 0.50 |
| 27:a:54:LYS:HG2 | 27:a:70:VAL:HG12 | 1.94 | 0.50 |
| 31:e:12:PHE:HZ | 31:e:21:LYS:HD2 | 1.76 | 0.50 |
| 37:k:247:TRP:HB3 | 37:k:258:ILE:HD11 | 1.93 | 0.50 |
| 9:J:504:LEU:HB2 | 9:J:564:ILE:HG23 | 1.94 | 0.50 |
| 20:W:202:G:H5' | 20:W:203:G:H5" | 1.92 | 0.50 |
| 1:A:172:ARG:HD2 | 1:A:228:MET:HE1 | 1.93 | 0.50 |
| 2:B:349:GLN:HB2 | 9:J:833:ALA:HB1 | 1.94 | 0.50 |
| 14:P:138:PHE:O | 14:P:213:ARG:N | 2.42 | 0.50 |
| 20:W:895:G:N2 | 20:W:898:U:OP2 | 2.45 | 0.50 |
| 20:W:535:G:N2 | 20:W:536:A:N7 | 2.52 | 0.49 |
| 35:i:13:GLU:O | 35:i:17:LYS:N | 2.41 | 0.49 |
| 36:j:18:ARG:NH1 | 36:j:36:LEU:O | 2.45 | 0.49 |
| 45:v:36:GLU:HB3 | 45:v:47:ARG:HD2 | 1.93 | 0.49 |
| 48:x:318:TYR:O | 48:x:322:ASN:ND2 | 2.45 | 0.49 |
| 53:5:270:GLY:HA2 | 53:5:276:GLY:H | 1.76 | 0.49 |
| 1:A:466:GLN:HA | 1:A:469:ARG:HG2 | 1.94 | 0.49 |
| 6:G:67:LYS:O | 47:z:109:G:N2 | 2.39 | 0.49 |
| 14:P:199:LYS:HG2 | 20:W:1114:U:H5" | 1.94 | 0.49 |
| 4:E:318:ILE:HG22 | 4:E:341:THR:HG22 | 1.93 | 0.49 |
| 20:W:624:C:H5" | 20:W:624:C:H6 | 1.77 | 0.49 |
| 36:j:16:THR:HG22 | 40:n:91:LYS:HE3 | 1.94 | 0.49 |
| 37:k:10:THR:HB | 37:k:306:LEU:HD12 | 1.94 | 0.49 |
| 2:B:249:MET:HE3 | 2:B:281:ILE:HG21 | 1.94 | 0.49 |
| 9:J:771:GLU:HB3 | 9:J:774:LYS:HD3 | 1.94 | 0.49 |
| 1:A:479:ASP:HB2 | 1:A:506:PRO:HB3 | 1.95 | 0.49 |
| 2:B:225:HIS:HB3 | 2:B:229:ARG:HH12 | 1.76 | 0.49 |
| 3:D:132:GLN:HA | 3:D:136:TRP:HB2 | 1.95 | 0.49 |
| 11:M:67:THR:OG1 | 11:M:70:LYS:O | 2.30 | 0.49 |
| 20:W:1568:C:OP1 | 38:l:96:SER:OG | 2.31 | 0.49 |
| 30:d:113:TYR:OH | 30:d:156:ALA:O | 2.31 | 0.49 |
| 36:j:18:ARG:HH11 | 40:n:88:LYS:HD2 | 1.76 | 0.49 |
| 10:L:83:LEU:HA | 10:L:86:LYS:HG2 | 1.95 | 0.49 |
| 19:V:55:ARG:HH11 | 20:W:1017:U:H5' | 1.77 | 0.49 |
| 21:X:75:GLY:HA3 | 21:X:88:ILE:HD12 | 1.95 | 0.49 |
| 2:B:345:CYS:HB2 | 2:B:393:MET:HE3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:E:254:PRO:HA | 4:E:286:GLY:HA3 | 1.95 | 0.49 |
| 9:J:490:LEU:HB3 | 9:J:499:VAL:HG22 | 1.95 | 0.49 |
| 11:M:22:LYS:HE3 | 20:W:1129:G:H5" | 1.94 | 0.49 |
| 13:O:123:ARG:NH2 | 20:W:1358:U:OP2 | 2.44 | 0.49 |
| 20:W:899:U:O2' | 20:W:900:C:O4' | 2.31 | 0.49 |
| 20:W:1422:G:H1' | 20:W:1424:G:O4' | 2.12 | 0.49 |
| 24:y:55:U:O2' | 24:y:57:G:N7 | 2.36 | 0.49 |
| 12:N:74:LYS:HB2 | 12:N:74:LYS:HE3 | 1.46 | 0.49 |
| 2:B:269:LYS:HE2 | 2:B:271:ARG:HB2 | 1.95 | 0.49 |
| 2:B:294:GLU:HA | 2:B:297:GLU:HB2 | 1.94 | 0.49 |
| 4:E:236:CYS:HA | 4:E:239:ILE:HD12 | 1.94 | 0.49 |
| 9:J:622:ARG:NH2 | 9:J:771:GLU:OE1 | 2.46 | 0.49 |
| 13:O:196:ILE:HB | 13:O:223:TYR:HB2 | 1.94 | 0.49 |
| 1:A:708:PRO:O | 1:A:712:SER:N | 2.45 | 0.48 |
| 23:Z:69:ARG:O | 23:Z:70:ARG:C | 2.55 | 0.48 |
| 48:x:286:PHE:HD2 | 48:x:288:LEU:HD22 | 1.77 | 0.48 |
| 20:W:160:U:O2' | 20:W:162:C:OP2 | 2.30 | 0.48 |
| 1:A:280:SER:OG | 1:A:321:ARG:NH2 | 2.46 | 0.48 |
| 11:M:58:GLY:O | 11:M:59:CYS:C | 2.56 | 0.48 |
| 46:w:21:ARG:HD3 | 46:w:88:LEU:HD22 | 1.95 | 0.48 |
| 4:E:348:CYS:N | 24:y:75:C:O2 | 2.46 | 0.48 |
| 1:A:445:GLN:O | 1:A:448:GLN:NE2 | 2.45 | 0.48 |
| 4:E:157:LEU:HD12 | 4:E:187:ILE:HG12 | 1.94 | 0.48 |
| 8:I:526:LEU:HB3 | 8:I:547:PHE:HB2 | 1.94 | 0.48 |
| 9:J:543:ASP:HB3 | 9:J:546:VAL:HG12 | 1.94 | 0.48 |
| 20:W:1252:C:OP1 | 46:w:75:LYS:NZ | 2.40 | 0.48 |
| 29:c:30:CYS:SG | 29:c:31:SER:N | 2.86 | 0.48 |
| 1:A:390:LEU:HD21 | 1:A:410:VAL:HG21 | 1.94 | 0.48 |
| 3:D:196:GLU:HB3 | 3:D:270:ASN:HB3 | 1.96 | 0.48 |
| 9:J:786:GLU:OE1 | 9:J:789:ARG:NH1 | 2.47 | 0.48 |
| 20:W:72:C:O3' | 20:W:73:C:O4' | 2.32 | 0.48 |
| 2:B:211:ARG:HG2 | 2:B:239:GLN:HE22 | 1.79 | 0.48 |
| 2:B:322:ASP:HB3 | 2:B:325:LEU:HB2 | 1.96 | 0.48 |
| 3:D:156:ALA:HB1 | 3:D:163:LEU:HD23 | 1.96 | 0.48 |
| 6:G:33:GLN:HB2 | 6:G:80:GLY:HA2 | 1.96 | 0.48 |
| 17:S:147:LEU:HD12 | 17:S:151:ASP:HB2 | 1.96 | 0.48 |
| 23:Z:64:ASP:O | 23:Z:65:GLU:C | 2.57 | 0.48 |
| 45:v:94:GLU:HG2 | 45:v:95:ILE:HG12 | 1.96 | 0.48 |
| 9:J:324:ILE:HG23 | 9:J:328:VAL:HG11 | 1.96 | 0.48 |
| 9:J:556:TYR:HE1 | 9:J:569:ILE:HG22 | 1.78 | 0.48 |
| 30:d:142:SER:OG | 30:d:145:ILE:HG12 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:x:362:ARG:HB2 | 48:x:370:ASP:HB2 | 1.94 | 0.48 |
| 8:I:396:ASP:OD1 | 8:I:396:ASP:N | 2.47 | 0.48 |
| 13:O:146:GLU:OE1 | 34:h:120:TYR:OH | 2.24 | 0.48 |
| 20:W:955:A:N1 | 20:W:968:U:O2' | 2.40 | 0.48 |
| 35:i:17:LYS:HG2 | 35:i:18:GLU:HG3 | 1.96 | 0.48 |
| 40:n:24:ARG:NH1 | 40:n:28:PHE:O | 2.47 | 0.48 |
| 48:x:407:VAL:HG22 | 48:x:423:THR:HG21 | 1.95 | 0.48 |
| 15:Q:52:LYS:HG3 | 45:v:109:LEU:HD12 | 1.95 | 0.48 |
| 19:V:55:ARG:HD3 | 20:W:1017:U:H5' | 1.95 | 0.48 |
| 20:W:1139:C:H2' | 20:W:1140:G:O4' | 2.14 | 0.48 |
| 20:W:1803:U:H2' | 20:W:1804:OMU:H6 | 1.95 | 0.48 |
| 34:h:105:LEU:HB2 | 34:h:122:VAL:HG21 | 1.96 | 0.48 |
| 37:k:83:TRP:HA | 37:k:107:ASP:HB2 | 1.95 | 0.48 |
| 18:T:101:GLY:HA3 | 18:T:134:PRO:HG2 | 1.96 | 0.47 |
| 48:x:29:PRO:HG2 | 48:x:67:SER:HB3 | 1.96 | 0.47 |
| 48:x:38:ARG:HD3 | 48:x:55:TYR:HD2 | 1.77 | 0.47 |
| 8:I:184:ASP:OD1 | 8:I:184:ASP:N | 2.47 | 0.47 |
| 9:J:120:LEU:HD11 | 9:J:124:LYS:HA | 1.96 | 0.47 |
| 37:k:153:CYS:H | 37:k:168:CYS:HB3 | 1.78 | 0.47 |
| 1:A:552:LEU:O | 1:A:556:ALA:N | 2.42 | 0.47 |
| 3:D:25:ARG:HH12 | 3:D:43:GLU:HG3 | 1.78 | 0.47 |
| 17:S:131:ARG:NH2 | 20:W:168:C:O5' | 2.47 | 0.47 |
| 38:l:116:ASP:OD1 | 38:l:117:GLN:N | 2.48 | 0.47 |
| 24:y:7:G:O2' | 24:y:49:5MC:O5' | 2.32 | 0.47 |
| 37:k:20:GLN:NE2 | 37:k:68:ASP:OD1 | 2.39 | 0.47 |
| 2:B:405:ILE:HG12 | 9:J:855:LEU:HD21 | 1.96 | 0.47 |
| 20:W:874:G:H1 | 20:W:912:C:H42 | 1.62 | 0.47 |
| 34:h:107:TYR:HA | 34:h:110:LEU:HB2 | 1.96 | 0.47 |
| 43:q:34:GLY:H | 43:q:108:CYS:HB3 | 1.80 | 0.47 |
| 1:A:443:VAL:HG22 | 1:A:447:TYR:HB2 | 1.95 | 0.47 |
| 8:I:208:HIS:NE2 | 8:I:220:ASP:OD2 | 2.46 | 0.47 |
| 8:I:294:ARG:HB2 | 8:I:297:LEU:HD12 | 1.97 | 0.47 |
| 9:J:549:GLU:HA | 9:J:572:HIS:CE1 | 2.49 | 0.47 |
| 20:W:294:U:OP1 | 21:X:36:TYR:OH | 2.30 | 0.47 |
| 4:E:386:THR:OG1 | 4:E:389:ASP:OD1 | 2.30 | 0.47 |
| 9:J:518:ALA:HA | 9:J:522:GLN:HA | 1.97 | 0.47 |
| 9:J:573:ILE:O | 9:J:576:HIS:N | 2.48 | 0.47 |
| 13:O:169:TYR:OH | 13:O:175:GLY:O | 2.32 | 0.47 |
| 14:P:129:THR:OG1 | 14:P:179:ASN:O | 2.32 | 0.47 |
| 18:T:74:ALA:HB1 | 18:T:115:ALA:HB2 | 1.96 | 0.47 |
| 25:7:241:ILE:HG22 | 25:7:285:ILE:HB | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:6:345:GLN:HA | 49:6:348:GLN:HG2 | 1.97 | 0.47 |
| 1:A:208:ILE:HD13 | 1:A:218:ILE:HD11 | 1.97 | 0.47 |
| 6:G:61:ILE:HD13 | 6:G:71:ILE:HD13 | 1.95 | 0.47 |
| 25:7:243:VAL:HG22 | 25:7:312:VAL:HG12 | 1.97 | 0.47 |
| 31:e:8:ARG:HB2 | 31:e:26:ASP:HB2 | 1.96 | 0.47 |
| 8:I:502:GLN:NE2 | 8:I:503:GLU:O | 2.48 | 0.47 |
| 20:W:659:G:H2' | 20:W:659:G:N3 | 2.30 | 0.47 |
| 20:W:1115:U:O2' | 20:W:1117:C:OP2 | 2.30 | 0.47 |
| 1:A:561:SER:HA | 1:A:564:GLU:HG2 | 1.95 | 0.47 |
| 8:I:273:MET:HE2 | 8:I:274:THR:HG22 | 1.96 | 0.47 |
| 9:J:500:CYS:SG | 9:J:555:ILE:HG12 | 2.54 | 0.47 |
| 18:T:121:ARG:NH1 | 44:s:40:ARG:HH11 | 2.12 | 0.47 |
| 37:k:18:VAL:O | 37:k:287:THR:OG1 | 2.26 | 0.47 |
| 1:A:483:ARG:O | 1:A:492:SER:N | 2.48 | 0.46 |
| 4:E:444:SER:HB3 | 4:E:451:TRP:HB2 | 1.96 | 0.46 |
| 8:I:475:GLY:HA3 | 8:I:523:GLY:HA3 | 1.97 | 0.46 |
| 22:Y:54:TYR:O | 31:e:15:ASN:ND2 | 2.47 | 0.46 |
| 24:y:1:A:H2' | 24:y:2:G:O4' | 2.15 | 0.46 |
| 46:w:27:ARG:HD2 | 46:w:82:MET:HE2 | 1.97 | 0.46 |
| 1:A:28:LEU:HD12 | 1:A:57:LEU:HB3 | 1.95 | 0.46 |
| 1:A:135:GLU:OE2 | 1:A:140:ARG:NH2 | 2.48 | 0.46 |
| 1:A:193:GLU:HA | 1:A:196:LYS:HD2 | 1.97 | 0.46 |
| 2:B:208:LEU:HD21 | 2:B:245:ALA:HB1 | 1.97 | 0.46 |
| 20:W:72:C:H5" | 20:W:73:C:C4 | 2.49 | 0.46 |
| 22:Y:11:ARG:HA | 22:Y:28:ALA:HB2 | 1.97 | 0.46 |
| 30:d:143:LYS:O | 30:d:144:LYS:C | 2.58 | 0.46 |
| 36:j:89:MET:HE1 | 36:j:116:LEU:HD11 | 1.97 | 0.46 |
| 40:n:86:ARG:NH1 | 40:n:110:ASP:OD2 | 2.47 | 0.46 |
| 47:z:110:C:H2' | 47:z:111:C:C6 | 2.50 | 0.46 |
| 50:4:159:LEU:O | 50:4:163:VAL:N | 2.47 | 0.46 |
| 1:A:48:GLU:HG2 | 1:A:49:PRO:HD3 | 1.97 | 0.46 |
| 3:D:196:GLU:HG3 | 3:D:233:PRO:HG2 | 1.97 | 0.46 |
| 9:J:643:LYS:HZ1 | 9:J:652:LEU:HA | 1.79 | 0.46 |
| 20:W:203:G:O2' | 20:W:204:G:O4' | 2.34 | 0.46 |
| 45:v:77:GLU:OE2 | 45:v:80:ARG:NH2 | 2.46 | 0.46 |
| 45:v:109:LEU:HD23 | 45:v:111:PHE:HD1 | 1.80 | 0.46 |
| 14:P:38:MET:HE3 | 14:P:185:VAL:HG21 | 1.98 | 0.46 |
| 20:W:53:C:O2' | 20:W:507:G:N7 | 2.40 | 0.46 |
| 1:A:205:LEU:HD21 | 1:A:233:ARG:HH12 | 1.81 | 0.46 |
| 9:J:568:ALA:HA | 9:J:571:CYS:SG | 2.56 | 0.46 |
| 9:J:592:SER:HB2 | 9:J:594:LEU:HD23 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:W:1058:A:OP1 | 24:y:38:A:O2' | 2.30 | 0.46 |
| 1:A:207:GLN:O | 1:A:211:HIS:N | 2.44 | 0.46 |
| 20:W:476:A:N3 | 20:W:488:U:O2' | 2.43 | 0.46 |
| 20:W:1228:A:H2' | 20:W:1229:G:C8 | 2.51 | 0.46 |
| 30:d:103:LEU:HD13 | 30:d:170:LYS:HD2 | 1.96 | 0.46 |
| 50:4:93:ARG:HA | 50:4:237:VAL:HA | 1.98 | 0.46 |
| 20:W:71:G:H3' | 20:W:72:C:C6 | 2.50 | 0.46 |
| 36:j:108:LYS:HB2 | 36:j:111:MET:HG3 | 1.98 | 0.46 |
| 11:M:59:CYS:HB3 | 11:M:61:THR:HG23 | 1.98 | 0.46 |
| 15:Q:5:LEU:O | 15:Q:9:GLN:HG2 | 2.16 | 0.46 |
| 20:W:74:G:H4' | 20:W:75:G:H5' | 1.97 | 0.46 |
| 20:W:1828:C:H2' | 20:W:1829:G:O4' | 2.16 | 0.46 |
| 30:d:157:LYS:HA | 30:d:157:LYS:HD3 | 1.76 | 0.46 |
| 37:k:39:THR:HG22 | 37:k:60:ARG:HG2 | 1.98 | 0.46 |
| 40:n:71:MET:HG2 | 40:n:99:LEU:HD11 | 1.97 | 0.46 |
| 1:A:409:LYS:HA | 1:A:412:ASN:HB2 | 1.97 | 0.46 |
| 7:H:48:GLN:HG3 | 7:H:82:VAL:HG12 | 1.97 | 0.46 |
| 8:I:440:ARG:HD3 | 8:I:447:SER:HB3 | 1.96 | 0.46 |
| 8:I:485:GLU:OE2 | 8:I:511:ASN:N | 2.49 | 0.46 |
| 9:J:426:GLU:N | 9:J:426:GLU:OE1 | 2.49 | 0.46 |
| 20:W:159:A2M:HM'2 | 20:W:159:A2M:H1' | 1.71 | 0.46 |
| 20:W:681:PSU:H4' | 27:a:9:THR:HG22 | 1.96 | 0.46 |
| 20:W:857:U:H2' | 20:W:858:A:C8 | 2.51 | 0.46 |
| 20:W:1060:A:O2' | 20:W:1062:A:N7 | 2.47 | 0.46 |
| 51:8:89:GLU:H | 51:8:92:ALA:HB2 | 1.81 | 0.46 |
| 5:F:109:MET:HA | 5:F:124:PHE:HA | 1.97 | 0.45 |
| 20:W:1301:A:O2' | 41:o:2:GLY:N | 2.44 | 0.45 |
| 36:j:31:GLU:HA | 36:j:34:MET:HG2 | 1.98 | 0.45 |
| 1:A:523:LEU:O | 1:A:527:SER:OG | 2.26 | 0.45 |
| 3:D:1:MET:HG2 | 3:D:113:ARG:HH22 | 1.81 | 0.45 |
| 4:E:367:ILE:HG12 | 4:E:434:CYS:HB2 | 1.98 | 0.45 |
| 7:H:34:ARG:HH22 | 24:y:26:M2G:H4' | 1.81 | 0.45 |
| 1:A:400:PRO:HG3 | 1:A:442:GLN:HG3 | 1.97 | 0.45 |
| 20:W:166:A2M:O2' | 20:W:167:G:H5' | 2.16 | 0.45 |
| 37:k:147:HIS:CD2 | 37:k:151:VAL:HG12 | 2.51 | 0.45 |
| 9:J:383:TYR:CE2 | 9:J:450:ARG:HG2 | 2.52 | 0.45 |
| 18:T:98:ARG:HB3 | 18:T:132:VAL:HG23 | 1.98 | 0.45 |
| 36:j:81:ARG:NH2 | 36:j:117:GLY:O | 2.50 | 0.45 |
| 37:k:213:ASP:N | 37:k:213:ASP:OD1 | 2.48 | 0.45 |
| 1:A:331:ILE:HA | 1:A:367:ARG:HD3 | 1.99 | 0.45 |
| 7:H:48:GLN:HE22 | 7:H:79:TYR:HB2 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:M:77:CYS:O | 48:x:83:VAL:HG23 | 2.17 | 0.45 |
| 17:S:161:PRO:HA | 17:S:171:THR:HG22 | 1.97 | 0.45 |
| 2:B:38:LEU:H | 2:B:252:HIS:CE1 | 2.35 | 0.45 |
| 4:E:183:LYS:HG3 | 4:E:184:HIS:CD2 | 2.51 | 0.45 |
| 19:V:127:ARG:NH2 | 20:W:678:U:OP1 | 2.50 | 0.45 |
| 20:W:543:C:H3' | 20:W:544:G:H8 | 1.81 | 0.45 |
| 20:W:1113:A:C1' | 20:W:1114:U:P | 3.05 | 0.45 |
| 32:f:33:ILE:HD13 | 48:x:479:GLN:HB3 | 1.97 | 0.45 |
| 41:o:2:GLY:O | 41:o:3:HIS:C | 2.58 | 0.45 |
| 3:D:193:ALA:HB3 | 3:D:237:MET:HB2 | 1.99 | 0.45 |
| 9:J:603:PRO:HA | 48:x:45:TRP:HE1 | 1.82 | 0.45 |
| 48:x:423:THR:O | 48:x:427:ASN:ND2 | 2.35 | 0.45 |
| 49:6:154:TRP:O | 49:6:158:THR:N | 2.47 | 0.45 |
| 2:B:233:ILE:HD11 | 2:B:273:VAL:HB | 1.99 | 0.45 |
| 11:M:54:VAL:HG12 | 11:M:64:CYS:SG | 2.57 | 0.45 |
| 19:V:94:LYS:HB2 | 19:V:94:LYS:HE2 | 1.81 | 0.45 |
| 19:V:107:LYS:NZ | 20:W:1076:G:OP2 | 2.47 | 0.45 |
| 20:W:1120:U:OP2 | 20:W:1120:U:H4' | 2.16 | 0.45 |
| 20:W:1314:U:H2' | 35:i:2:LEU:HD12 | 1.99 | 0.45 |
| 38:l:42:HIS:ND1 | 38:l:93:SER:OG | 2.50 | 0.45 |
| 39:m:58:LEU:HD12 | 39:m:62:VAL:HG21 | 1.99 | 0.45 |
| 10:L:160:LYS:HD2 | 10:L:191:GLU:HA | 1.99 | 0.45 |
| 20:W:71:G:N3 | 20:W:71:G:H2' | 2.31 | 0.45 |
| 35:i:12:TYR:HB3 | 35:i:79:LEU:HD11 | 1.99 | 0.45 |
| 37:k:164:ILE:HG21 | 37:k:185:LYS:HE2 | 1.99 | 0.45 |
| 17:S:67:VAL:HG12 | 17:S:69:THR:HG22 | 1.99 | 0.45 |
| 22:Y:106:LYS:NZ | 22:Y:251:GLU:OE2 | 2.50 | 0.45 |
| 30:d:34:ALA:HB2 | 30:d:56:ARG:HD2 | 1.99 | 0.45 |
| 40:n:92:ASP:OD1 | 40:n:94:LYS:NZ | 2.48 | 0.45 |
| 3:D:255:MET:HA | 3:D:258:ILE:HB | 1.98 | 0.44 |
| 20:W:344:U:H2' | 20:W:345:U:C6 | 2.52 | 0.44 |
| 24:y:9:1MG:O2' | 24:y:10:2MG:N7 | 2.49 | 0.44 |
| 34:h:222:PRO:HG2 | 37:k:226:HIS:CE1 | 2.52 | 0.44 |
| 48:x:389:SER:OG | 48:x:390:PHE:N | 2.49 | 0.44 |
| 2:B:406:GLU:O | 2:B:410:SER:N | 2.48 | 0.44 |
| 7:H:43:THR:OG1 | 7:H:44:LEU:N | 2.51 | 0.44 |
| 9:J:421:GLY:HA2 | 9:J:440:VAL:HA | 2.00 | 0.44 |
| 9:J:593:HIS:O | 9:J:597:ASN:ND2 | 2.48 | 0.44 |
| 20:W:1587:G:C5 | 38:l:78:ILE:HD11 | 2.52 | 0.44 |
| 2:B:251:PRO:HA | 2:B:254:LEU:HB2 | 1.99 | 0.44 |
| 20:W:1369:A:OP1 | 45:v:2:GLY:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:h:132:LYS:HB2 | 34:h:189:MET:HG2 | 1.98 | 0.44 |
| 37:k:191:HIS:CE1 | 37:k:217:MET:HG3 | 2.53 | 0.44 |
| 51:8:66:VAL:HA | 51:8:119:TRP:HA | 2.00 | 0.44 |
| 1:A:515:PRO:HB3 | 1:A:519:ILE:HB | 1.99 | 0.44 |
| 4:E:179:ILE:HG23 | 4:E:440:LYS:HD2 | 2.00 | 0.44 |
| 10:L:137:SER:HB3 | 10:L:166:VAL:HG21 | 1.98 | 0.44 |
| 36:j:85:ILE:HD13 | 36:j:111:MET:HB3 | 1.98 | 0.44 |
| 48:x:409:TRP:HE3 | 48:x:466:LEU:HD12 | 1.83 | 0.44 |
| 1:A:83:ILE:HG13 | 1:A:169:ARG:HD3 | 1.99 | 0.44 |
| 5:F:173:TYR:HA | 5:F:180:VAL:HA | 2.00 | 0.44 |
| 9:J:691:MET:HE1 | 9:J:741:SER:HB2 | 2.00 | 0.44 |
| 9:J:732:SER:OG | 9:J:735:GLU:OE1 | 2.30 | 0.44 |
| 20:W:839:C:H4' | 20:W:840:C:H5' | 1.99 | 0.44 |
| 20:W:1113:A:C2 | 20:W:1118:C:C4 | 3.05 | 0.44 |
| 8:I:392:SER:OG | 8:I:403:ALA:O | 2.28 | 0.44 |
| 20:W:1456:G:OP1 | 45:v:59:LYS:NZ | 2.48 | 0.44 |
| 20:W:1678:A2M:HM'3 | 20:W:1678:A2M:H1' | 1.81 | 0.44 |
| 22:Y:107:GLY:HA2 | 22:Y:189:LEU:HG | 1.99 | 0.44 |
| 38:l:35:ASP:HB2 | 40:n:46:ARG:HG2 | 1.99 | 0.44 |
| 1:A:447:TYR:HD2 | 1:A:450:ILE:HG12 | 1.82 | 0.44 |
| 17:S:159:ARG:HG2 | 17:S:173:ALA:HB2 | 1.98 | 0.44 |
| 20:W:71:G:H3' | 20:W:72:C:H6 | 1.82 | 0.44 |
| 20:W:1211:G:H8 | 20:W:1211:G:C5' | 2.31 | 0.44 |
| 20:W:1418:C:N4 | 20:W:1421:A:N3 | 2.65 | 0.44 |
| 20:W:1698:C:N4 | 47:z:112:A:C4 | 2.86 | 0.44 |
| 23:Z:172:ARG:HA | 23:Z:175:ARG:HH21 | 1.82 | 0.44 |
| 35:i:12:TYR:HB3 | 35:i:83:LEU:HD11 | 2.00 | 0.44 |
| 20:W:1274:G:H4' | 35:i:47:LYS:HE2 | 1.98 | 0.44 |
| 20:W:1354:G:N2 | 20:W:1357:A:OP2 | 2.46 | 0.44 |
| 20:W:1681:U:H2' | 20:W:1682:C:C6 | 2.53 | 0.44 |
| 20:W:1843:G:OP1 | 26:9:7:LYS:NZ | 2.48 | 0.44 |
| 22:Y:122:LYS:HG3 | 22:Y:164:LEU:HD21 | 2.00 | 0.44 |
| 4:E:89:TYR:HB3 | 4:E:124:PHE:HB3 | 2.00 | 0.44 |
| 8:I:528:VAL:HG12 | 8:I:545:GLU:HB2 | 2.00 | 0.44 |
| 13:O:114:LYS:HD2 | 20:W:1358:U:H5' | 2.00 | 0.44 |
| 20:W:1597:C:OP2 | 39:m:85:ARG:NH2 | 2.42 | 0.44 |
| 37:k:205:SER:HA | 37:k:221:LEU:HB2 | 2.00 | 0.44 |
| 43:q:22:LEU:HD21 | 43:q:89:VAL:HA | 1.99 | 0.44 |
| 48:x:365:LEU:HB2 | 48:x:369:ILE:HD11 | 2.00 | 0.44 |
| 4:E:408:ILE:HG21 | 4:E:459:ILE:HD11 | 1.99 | 0.43 |
| 20:W:166:A2M:H1' | 20:W:166:A2M:HM'3 | 1.72 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:W:887:U:H2' | 20:W:888:U:H2' | 1.99 | 0.43 |
| 37:k:240:CYS:HB3 | 37:k:249:CYS:HB2 | 1.19 | 0.43 |
| 40:n:34:LYS:HE2 | 40:n:103:LEU:HD23 | 2.00 | 0.43 |
| 40:n:88:LYS:HA | 40:n:95:TYR:HE1 | 1.83 | 0.43 |
| 9:J:366:LEU:HD21 | 9:J:430:ASN:HD22 | 1.83 | 0.43 |
| 9:J:802:ILE:O | 9:J:841:THR:OG1 | 2.31 | 0.43 |
| 15:Q:77:ILE:HG21 | 15:Q:133:PRO:HG2 | 1.99 | 0.43 |
| 37:k:197:THR:HG21 | 37:k:238:ALA:HA | 2.00 | 0.43 |
| 50:4:122:GLY:HA3 | 50:4:131:VAL:HA | 1.99 | 0.43 |
| 1:A:13:LYS:HZ1 | 14:P:76:ASN:HB3 | 1.81 | 0.43 |
| 2:B:331:ASP:OD1 | 2:B:331:ASP:N | 2.51 | 0.43 |
| 9:J:410:ASP:OD1 | 9:J:485:ARG:NH2 | 2.46 | 0.43 |
| 20:W:484:A2M:O5' | 20:W:484:A2M:H8 | 2.18 | 0.43 |
| 20:W:1808:U:H2' | 20:W:1809:A:C8 | 2.54 | 0.43 |
| 30:d:146:GLN:O | 30:d:150:ASP:N | 2.50 | 0.43 |
| 37:k:87:LEU:HD21 | 37:k:122:SER:HB3 | 2.00 | 0.43 |
| 1:A:14:ARG:CZ | 1:A:14:ARG:HB2 | 2.49 | 0.43 |
| 5:F:263:GLY:HA2 | 5:F:285:PHE:HA | 2.00 | 0.43 |
| 9:J:570:LEU:HD12 | 9:J:570:LEU:HA | 1.75 | 0.43 |
| 20:W:751:G:N2 | 20:W:789:G:O3' | 2.51 | 0.43 |
| 25:7:256:GLN:HG2 | 25:7:265:ILE:HG21 | 2.00 | 0.43 |
| 1:A:502:ARG:HH21 | 9:J:850:THR:HG21 | 1.83 | 0.43 |
| 8:I:573:ASN:ND2 | 8:I:619:GLN:O | 2.49 | 0.43 |
| 20:W:537:C:N4 | 20:W:548:C:O2 | 2.52 | 0.43 |
| 20:W:1119:A:H4' | 20:W:1120:U:O5' | 2.17 | 0.43 |
| 20:W:1619:A:H4' | 36:j:44:ARG:HH12 | 1.83 | 0.43 |
| 21:X:111:VAL:HG11 | 21:X:128:VAL:HG11 | 1.99 | 0.43 |
| 37:k:153:CYS:HB2 | 37:k:197:THR:HA | 2.01 | 0.43 |
| 1:A:266:PRO:HA | 1:A:267:PRO:HD3 | 1.87 | 0.43 |
| 2:B:369:ARG:NH1 | 53:5:474:LYS:O | 2.51 | 0.43 |
| 3:D:121:TYR:CE2 | 3:D:126:GLN:HB3 | 2.54 | 0.43 |
| 14:P:75:GLN:HE21 | 14:P:189:ILE:HG21 | 1.84 | 0.43 |
| 17:S:10:THR:HB | 17:S:128:THR:HA | 2.00 | 0.43 |
| 20:W:641:A:OP1 | 23:Z:40:LYS:NZ | 2.44 | 0.43 |
| 30:d:56:ARG:NH1 | 30:d:180:GLY:O | 2.52 | 0.43 |
| 41:o:52:PHE:HB3 | 46:w:80:PHE:HB3 | 1.99 | 0.43 |
| 1:A:323:LEU:HD12 | 1:A:383:VAL:HG11 | 2.00 | 0.43 |
| 2:B:349:GLN:N | 9:J:834:SER:O | 2.51 | 0.43 |
| 4:E:184:HIS:CE1 | 4:E:244:PRO:HD2 | 2.54 | 0.43 |
| 9:J:632:ALA:HA | 48:x:40:GLY:HA3 | 2.01 | 0.43 |
| 10:L:57:ARG:HH22 | 10:L:91:HIS:CG | 2.36 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:L:69:LEU:HD21 | 10:L:132:ASP:OD1 | 2.19 | 0.43 |
| 12:N:17:CYS:HB2 | 12:N:56:CYS:HB3 | 2.00 | 0.43 |
| 20:W:1328:OMG:HM23 | 20:W:1328:OMG:H1' | 1.72 | 0.43 |
| 20:W:1639:G7M:H2' | 20:W:1640:A:C8 | 2.54 | 0.43 |
| 9:J:760:LYS:HG2 | 9:J:764:LYS:HE2 | 2.01 | 0.43 |
| 9:J:793:PHE:HE1 | 9:J:825:MET:HG2 | 1.82 | 0.43 |
| 15:Q:14:ASP:O | 15:Q:15:VAL:C | 2.60 | 0.43 |
| 15:Q:126:ASP:HB3 | 15:Q:129:ALA:HB3 | 2.00 | 0.43 |
| 20:W:1113:A:N3 | 20:W:1118:C:N4 | 2.66 | 0.43 |
| 20:W:1210:G:H3' | 20:W:1211:G:H5" | 2.01 | 0.43 |
| 23:Z:107:GLU:HA | 23:Z:112:THR:HG21 | 2.00 | 0.43 |
| 34:h:135:GLU:HG3 | 34:h:153:VAL:HG12 | 2.00 | 0.43 |
| 43:q:51:VAL:HG12 | 43:q:109:VAL:HB | 2.00 | 0.43 |
| 51:8:69:GLY:HA3 | 51:8:78:ILE:HA | 2.00 | 0.43 |
| 8:I:388:LEU:HB2 | 8:I:409:ILE:HG12 | 2.00 | 0.43 |
| 10:L:116:ARG:NH2 | 20:W:687:C:O2' | 2.52 | 0.43 |
| 15:Q:11:LYS:HB3 | 15:Q:11:LYS:HE2 | 1.78 | 0.43 |
| 20:W:1524:G:O2' | 24:y:30:G:OP1 | 2.34 | 0.43 |
| 34:h:75:LYS:NZ | 35:i:34:GLU:OE1 | 2.48 | 0.43 |
| 1:A:191:LYS:NZ | 1:A:243:MET:O | 2.51 | 0.43 |
| 1:A:247:GLN:NE2 | 9:J:735:GLU:OE2 | 2.52 | 0.43 |
| 3:D:16:VAL:HG12 | 3:D:17:GLU:HG2 | 2.00 | 0.43 |
| 13:O:102:LEU:HD22 | 13:O:130:ILE:HG12 | 2.01 | 0.43 |
| 14:P:165:ARG:HG2 | 14:P:169:MET:HE3 | 2.01 | 0.43 |
| 15:Q:184:ARG:HD3 | 15:Q:191:ARG:HG3 | 2.01 | 0.43 |
| 17:S:137:ARG:HH21 | 17:S:140:ARG:HH21 | 1.66 | 0.43 |
| 20:W:1101:U:H2' | 20:W:1102:G:C8 | 2.54 | 0.43 |
| 46:w:17:ILE:HG22 | 46:w:94:PRO:HD3 | 2.01 | 0.43 |
| 48:x:37:ASP:OD1 | 48:x:37:ASP:N | 2.50 | 0.43 |
| 48:x:439:ALA:O | 48:x:444:SER:OG | 2.28 | 0.43 |
| 1:A:414:VAL:O | 1:A:425:GLN:NE2 | 2.52 | 0.42 |
| 4:E:256:LEU:N | 4:E:358:LEU:O | 2.50 | 0.42 |
| 8:I:490:PRO:HB2 | 8:I:508:ASN:HB3 | 2.01 | 0.42 |
| 8:I:660:ASP:OD2 | 8:I:662:THR:OG1 | 2.37 | 0.42 |
| 8:I:685:THR:OG1 | 8:I:689:ARG:N | 2.48 | 0.42 |
| 20:W:1463:U:H5" | 20:W:1463:U:C6 | 2.53 | 0.42 |
| 34:h:123:LEU:HD22 | 34:h:152:PHE:HB3 | 2.01 | 0.42 |
| 37:k:15:ASN:N | 37:k:37:ASP:OD2 | 2.42 | 0.42 |
| 41:o:10:HIS:HA | 41:o:11:PRO:HD3 | 1.93 | 0.42 |
| 9:J:590:LEU:O | 9:J:593:HIS:NE2 | 2.52 | 0.42 |
| 23:Z:151:LEU:HD23 | 23:Z:151:LEU:HA | 1.89 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:d:158:ILE:HG13 | 30:d:159:SER:H | 1.84 | 0.42 |
| 37:k:89:LEU:HB2 | 37:k:101:PHE:HE1 | 1.84 | 0.42 |
| 8:I:274:THR:OG1 | 8:I:275:ILE:N | 2.52 | 0.42 |
| 9:J:444:ILE:HA | 9:J:447:LEU:HB2 | 2.02 | 0.42 |
| 15:Q:76:VAL:HG12 | 15:Q:123:VAL:HB | 2.01 | 0.42 |
| 20:W:920:A:O2' | 20:W:922:A:OP1 | 2.35 | 0.42 |
| 20:W:929:G:H2' | 20:W:930:C:O4' | 2.19 | 0.42 |
| 20:W:1037:G:H4' | 20:W:1845:A:H4' | 2.01 | 0.42 |
| 20:W:1210:G:C3' | 20:W:1211:G:H5" | 2.50 | 0.42 |
| 27:a:68:LYS:HG2 | 27:a:91:LEU:HD22 | 2.02 | 0.42 |
| 40:n:79:ILE:HA | 40:n:80:PRO:HD3 | 1.93 | 0.42 |
| 3:D:126:GLN:HB3 | 3:D:126:GLN:HE21 | 1.71 | 0.42 |
| 20:W:1463:U:OP1 | 20:W:1463:U:H4' | 2.20 | 0.42 |
| 53:5:281:HIS:O | 53:5:285:GLY:N | 2.46 | 0.42 |
| 1:A:723:ASP:O | 1:A:727:GLN:N | 2.49 | 0.42 |
| 2:B:417:MET:O | 2:B:421:ASN:ND2 | 2.53 | 0.42 |
| 4:E:327:ASP:OD1 | 4:E:327:ASP:N | 2.49 | 0.42 |
| 7:H:34:ARG:NH1 | 7:H:78:GLU:HB2 | 2.34 | 0.42 |
| 8:I:625:LEU:HB2 | 8:I:636:ALA:HB3 | 2.02 | 0.42 |
| 9:J:549:GLU:HA | 9:J:572:HIS:HE1 | 1.85 | 0.42 |
| 19:V:16:LEU:HD12 | 20:W:919:A:H5" | 2.01 | 0.42 |
| 37:k:302:TYR:HE2 | 37:k:308:ARG:HB2 | 1.84 | 0.42 |
| 39:m:56:ASP:O | 39:m:60:LYS:HG2 | 2.19 | 0.42 |
| 49:6:319:LYS:HD3 | 49:6:335:SER:HB2 | 2.01 | 0.42 |
| 50:4:250:ASP:O | 50:4:254:LYS:N | 2.45 | 0.42 |
| 1:A:313:ASP:OD1 | 1:A:316:GLN:NE2 | 2.53 | 0.42 |
| 6:G:62:ARG:NH2 | 20:W:615:C:OP2 | 2.52 | 0.42 |
| 10:L:119:SER:OG | 10:L:120:ARG:NH1 | 2.51 | 0.42 |
| 12:N:25:GLY:O | 13:O:85:SER:OG | 2.34 | 0.42 |
| 20:W:639:C:H2' | 20:W:640:A:C8 | 2.55 | 0.42 |
| 20:W:1579:A:O2' | 20:W:1581:C:OP2 | 2.34 | 0.42 |
| 50:4:118:GLY:N | 50:4:173:TYR:O | 2.52 | 0.42 |
| 10:L:25:GLN:HA | 10:L:28:LEU:HB3 | 2.01 | 0.42 |
| 14:P:72:ALA:HA | 14:P:76:ASN:O | 2.20 | 0.42 |
| 17:S:42:GLY:O | 17:S:46:LYS:NZ | 2.52 | 0.42 |
| 20:W:494:C:N4 | 20:W:509:OMG:HN22 | 2.18 | 0.42 |
| 11:M:53:VAL:HG13 | 11:M:62:VAL:HG13 | 2.01 | 0.42 |
| 20:W:71:G:C6 | 20:W:72:C:H1' | 2.55 | 0.42 |
| 21:X:104:LYS:O | 27:a:11:ARG:NH2 | 2.33 | 0.42 |
| 34:h:213:PRO:HD3 | 45:v:19:LYS:HD3 | 2.01 | 0.42 |
| 48:x:370:ASP:OD1 | 48:x:370:ASP:N | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:319:LEU:HD12 | 2:B:325:LEU:HB3 | 2.02 | 0.42 |
| 3:D:76:VAL:HG12 | 3:D:83:ILE:HG23 | 2.01 | 0.42 |
| 11:M:56:CYS:HB3 | 11:M:60:SER:H | 1.85 | 0.42 |
| 14:P:75:GLN:NE2 | 14:P:189:ILE:HD13 | 2.35 | 0.42 |
| 14:P:120:MET:HE1 | 20:W:987:A:C6 | 2.55 | 0.42 |
| 15:Q:11:LYS:O | 15:Q:12:GLU:C | 2.63 | 0.42 |
| 20:W:384:U:O4 | 30:d:5:ARG:NH1 | 2.41 | 0.42 |
| 23:Z:107:GLU:O | 23:Z:113:GLN:NE2 | 2.44 | 0.42 |
| 14:P:108:ASP:OD1 | 14:P:109:LYS:N | 2.53 | 0.42 |
| 15:Q:12:GLU:N | 45:v:111:PHE:CE2 | 2.88 | 0.42 |
| 20:W:70:G:C2' | 20:W:79:A:H61 | 2.33 | 0.42 |
| 20:W:484:A2M:HM'3 | 20:W:484:A2M:H1' | 1.80 | 0.42 |
| 24:y:53:G:H2' | 24:y:54:A:H8 | 1.84 | 0.42 |
| 37:k:20:GLN:HG2 | 37:k:69:VAL:H | 1.85 | 0.42 |
| 37:k:152:SER:OG | 37:k:196:ASN:O | 2.32 | 0.42 |
| 37:k:201:SER:HB3 | 37:k:205:SER:H | 1.84 | 0.42 |
| 1:A:290:LEU:HD21 | 1:A:335:ARG:HE | 1.85 | 0.41 |
| 3:D:111:ILE:HG22 | 3:D:183:ARG:HG3 | 2.02 | 0.41 |
| 8:I:311:GLU:N | 8:I:698:ARG:O | 2.50 | 0.41 |
| 10:L:100:ILE:HD13 | 10:L:122:LEU:HD12 | 2.02 | 0.41 |
| 14:P:122:GLU:HG2 | 14:P:140:VAL:HG23 | 2.01 | 0.41 |
| 14:P:123:ALA:HB2 | 14:P:165:ARG:HG3 | 2.01 | 0.41 |
| 20:W:1758:G:N7 | 20:W:1771:G:N2 | 2.68 | 0.41 |
| 43:q:52:LEU:HD21 | 43:q:65:VAL:HG11 | 2.02 | 0.41 |
| 7:H:56:LYS:NZ | 7:H:81:GLU:O | 2.53 | 0.41 |
| 8:I:369:GLN:NE2 | 8:I:409:ILE:O | 2.52 | 0.41 |
| 15:Q:81:ASN:HA | 15:Q:84:GLN:HB2 | 2.02 | 0.41 |
| 27:a:91:LEU:HD21 | 28:b:80:LEU:HD23 | 2.01 | 0.41 |
| 1:A:13:LYS:HZ3 | 14:P:76:ASN:HB3 | 1.83 | 0.41 |
| 1:A:132:VAL:O | 9:J:678:ASN:ND2 | 2.52 | 0.41 |
| 8:I:225:GLU:HB2 | 8:I:230:LYS:HE2 | 2.02 | 0.41 |
| 20:W:1115:U:C2' | 20:W:1118:C:N3 | 2.83 | 0.41 |
| 20:W:1223:A:OP1 | 32:f:79:HIS:HA | 2.20 | 0.41 |
| 20:W:1482:C:OP1 | 41:o:54:LYS:NZ | 2.49 | 0.41 |
| 20:W:1490:OMG:HM23 | 20:W:1490:OMG:H1' | 1.56 | 0.41 |
| 20:W:1636:G:H1' | 32:f:164:ARG:NH1 | 2.34 | 0.41 |
| 25:7:302:GLY:HA2 | 25:7:309:ILE:HB | 2.00 | 0.41 |
| 27:a:95:GLU:OE1 | 27:a:140:ARG:NH2 | 2.54 | 0.41 |
| 32:f:19:LEU:HD21 | 32:f:69:VAL:HG21 | 2.02 | 0.41 |
| 37:k:99:ARG:HE | 37:k:99:ARG:HB2 | 1.76 | 0.41 |
| 8:I:666:VAL:HB | 8:I:684:TRP:HB2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:R:58:VAL:HG21 | 18:T:28:PHE:HZ | 1.85 | 0.41 |
| 17:S:142:ARG:HG3 | 17:S:147:LEU:HB2 | 2.02 | 0.41 |
| 18:T:25:GLU:H | 18:T:25:GLU:HG3 | 1.52 | 0.41 |
| 20:W:104:A:OP1 | 30:d:12:ARG:NH1 | 2.54 | 0.41 |
| 20:W:851:C:H5" | 20:W:852:G:H5' | 2.01 | 0.41 |
| 20:W:1113:A:C2 | 20:W:1118:C:C5 | 3.09 | 0.41 |
| 20:W:1415:C:H2' | 20:W:1416:C:C6 | 2.55 | 0.41 |
| 20:W:1550:G:H3' | 20:W:1579:A:H61 | 1.86 | 0.41 |
| 20:W:1736:G:H2' | 20:W:1737:G:C8 | 2.56 | 0.41 |
| 24:y:64:RIA:H2A | 24:y:64:RIA:H2' | 1.62 | 0.41 |
| 32:f:40:ALA:HB1 | 32:f:45:TYR:CG | 2.56 | 0.41 |
| 37:k:32:LEU:HD12 | 37:k:71:ILE:HG12 | 2.03 | 0.41 |
| 37:k:59:LEU:HD23 | 37:k:90:TRP:CD2 | 2.55 | 0.41 |
| 37:k:161:SER:O | 37:k:162:ASN:C | 2.63 | 0.41 |
| 37:k:191:HIS:CG | 37:k:195:LEU:HD21 | 2.55 | 0.41 |
| 48:x:21:VAL:HG13 | 48:x:26:ARG:HH12 | 1.85 | 0.41 |
| 7:H:79:TYR:O | 24:y:12:G:O2' | 2.32 | 0.41 |
| 9:J:687:LEU:HD13 | 9:J:737:VAL:HG11 | 2.03 | 0.41 |
| 17:S:57:ASP:HB3 | 17:S:98:ARG:HG2 | 2.02 | 0.41 |
| 23:Z:110:LEU:HB2 | 23:Z:147:PHE:HB3 | 2.01 | 0.41 |
| 37:k:153:CYS:HB3 | 37:k:198:VAL:HG12 | 2.01 | 0.41 |
| 1:A:43:TRP:O | 1:A:47:HIS:ND1 | 2.53 | 0.41 |
| 14:P:74:LEU:C | 14:P:75:GLN:HG2 | 2.45 | 0.41 |
| 27:a:101:LEU:HB3 | 27:a:124:LYS:HB2 | 2.01 | 0.41 |
| 34:h:29:LEU:HB2 | 34:h:34:TYR:HB2 | 2.02 | 0.41 |
| 45:v:105:MET:HB3 | 45:v:105:MET:HE3 | 1.83 | 0.41 |
| 49:6:207:CYS:O | 49:6:211:ALA:N | 2.46 | 0.41 |
| 4:E:151:VAL:HG11 | 4:E:282:SER:HB3 | 2.03 | 0.41 |
| 20:W:116:OMU:H6 | 20:W:116:OMU:O5' | 2.20 | 0.41 |
| 21:X:147:LYS:HD2 | 21:X:147:LYS:HA | 1.88 | 0.41 |
| 35:i:3:MET:HE3 | 35:i:3:MET:HB2 | 1.88 | 0.41 |
| 52:3:36:GLN:HA | 52:3:41:ALA:HB3 | 2.02 | 0.41 |
| 9:J:749:TRP:HA | 9:J:752:CYS:HB2 | 2.03 | 0.41 |
| 15:Q:77:ILE:HG13 | 15:Q:99:ILE:HB | 2.03 | 0.41 |
| 20:W:99:A2M:H2' | 20:W:100:PSU:O4' | 2.21 | 0.41 |
| 30:d:6:ASP:OD1 | 30:d:9:HIS:ND1 | 2.53 | 0.41 |
| 40:n:40:TYR:HA | 40:n:83:PHE:HE2 | 1.86 | 0.41 |
| 43:q:52:LEU:HB3 | 43:q:53:ALA:H | 1.78 | 0.41 |
| 45:v:24:LEU:HB2 | 45:v:58:MET:HE2 | 2.03 | 0.41 |
| 48:x:57:ASN:OD1 | 48:x:58:LYS:N | 2.54 | 0.41 |
| 51:8:326:TYR:O | 51:8:330:ILE:N | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:308:LYS:HD2 | 1:A:308:LYS:HA | 1.81 | 0.41 |
| 9:J:754:SER:O | 9:J:758:ASN:ND2 | 2.54 | 0.41 |
| 9:J:835:LEU:HG | 9:J:838:PRO:HD2 | 2.02 | 0.41 |
| 20:W:608:C:H2' | 20:W:609:PSU:C6 | 2.56 | 0.41 |
| 20:W:668:A2M:H8 | 20:W:668:A2M:H2' | 1.93 | 0.41 |
| 20:W:1536:G:H2' | 20:W:1537:A:C8 | 2.55 | 0.41 |
| 36:j:17:TYR:HB3 | 36:j:25:LEU:HD11 | 2.03 | 0.41 |
| 37:k:289:LEU:HD22 | 37:k:298:LEU:HD12 | 2.03 | 0.41 |
| 45:v:114:LEU:HD12 | 45:v:114:LEU:HA | 1.90 | 0.41 |
| 49:6:329:GLN:HE22 | 49:6:331:LYS:HE2 | 1.85 | 0.41 |
| 51:8:274:LYS:O | 51:8:279:GLN:N | 2.48 | 0.41 |
| 2:B:251:PRO:O | 2:B:255:ARG:N | 2.48 | 0.41 |
| 3:D:9:TYR:HE2 | 3:D:38:GLU:HG3 | 1.86 | 0.41 |
| 9:J:383:TYR:CD2 | 9:J:450:ARG:HG2 | 2.55 | 0.41 |
| 9:J:566:THR:O | 9:J:569:ILE:HG12 | 2.21 | 0.41 |
| 17:S:20:ASP:OD1 | 17:S:20:ASP:N | 2.48 | 0.41 |
| 20:W:428:OMU:H2' | 20:W:428:OMU:H6 | 1.86 | 0.41 |
| 20:W:1031:A2M:HM'3 | 20:W:1031:A2M:H1' | 1.91 | 0.41 |
| 20:W:1447:OMG:H1' | 20:W:1447:OMG:HM23 | 1.73 | 0.41 |
| 42:p:132:MET:HE1 | 42:p:148:TYR:CD2 | 2.56 | 0.41 |
| 48:x:330:MET:N | 48:x:330:MET:SD | 2.94 | 0.41 |
| 17:S:7:PHE:HB2 | 17:S:124:LEU:HD12 | 2.03 | 0.40 |
| 20:W:140:U:O2' | 20:W:143:U:OP1 | 2.39 | 0.40 |
| 20:W:736:C:H2' | 20:W:737:G:C8 | 2.55 | 0.40 |
| 20:W:1144:A:H2' | 20:W:1145:A:C8 | 2.57 | 0.40 |
| 21:X:110:SER:HB2 | 21:X:137:THR:HG22 | 2.02 | 0.40 |
| 27:a:68:LYS:HB3 | 27:a:91:LEU:HD13 | 2.02 | 0.40 |
| 30:d:67:TRP:HA | 30:d:189:VAL:HG22 | 2.03 | 0.40 |
| 34:h:132:LYS:HE2 | 34:h:191:PRO:HA | 2.02 | 0.40 |
| 35:i:24:LYS:NZ | 35:i:65:ARG:HH21 | 2.20 | 0.40 |
| 37:k:166:VAL:HG23 | 37:k:176:VAL:HG22 | 2.03 | 0.40 |
| 38:l:56:ARG:HG3 | 38:l:103:VAL:HG21 | 2.03 | 0.40 |
| 48:x:379:GLY:N | 48:x:391:ILE:O | 2.49 | 0.40 |
| 5:F:303:GLY:HA2 | 5:F:309:VAL:HA | 2.03 | 0.40 |
| 9:J:505:LEU:HD12 | 9:J:505:LEU:HA | 1.94 | 0.40 |
| 11:M:20:LYS:HG3 | 11:M:21:LYS:HG2 | 2.03 | 0.40 |
| 13:O:185:THR:OG1 | 20:W:1155:U:OP1 | 2.28 | 0.40 |
| 15:Q:10:MET:HE1 | 45:v:109:LEU:HD11 | 2.03 | 0.40 |
| 20:W:576:A2M:HM'3 | 20:W:576:A2M:H1' | 1.83 | 0.40 |
| 20:W:867:OMG:HM23 | 20:W:867:OMG:H1' | 1.91 | 0.40 |
| 29:c:42:MET:HE3 | 29:c:49:GLU:HA | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:c:55:ASP:C | 29:c:57:ARG:H | 2.30 | 0.40 |
| 30:d:62:VAL:HA | 30:d:77:ARG:HA | 2.03 | 0.40 |
| 36:j:41:GLN:HG3 | 36:j:84:ILE:HD12 | 2.03 | 0.40 |
| 37:k:10:THR:HG22 | 37:k:308:ARG:HG2 | 2.04 | 0.40 |
| 37:k:125:ARG:HG2 | 37:k:150:TRP:CG | 2.56 | 0.40 |
| 43:q:55:ASN:HD21 | 43:q:82:ASN:H | 1.69 | 0.40 |
| 51:8:211:ILE:O | 51:8:215:MET:N | 2.51 | 0.40 |
| 4:E:277:GLY:H | 4:E:343:ILE:HG21 | 1.86 | 0.40 |
| 8:I:607:ASP:N | 8:I:607:ASP:OD1 | 2.54 | 0.40 |
| 9:J:551:LEU:O | 9:J:555:ILE:HD12 | 2.21 | 0.40 |
| 10:L:66:VAL:C | 10:L:68:GLN:H | 2.29 | 0.40 |
| 14:P:204:ILE:O | 20:W:1121:G:O2' | 2.36 | 0.40 |
| 16:R:49:ALA:HB2 | 18:T:117:ARG:HD2 | 2.03 | 0.40 |
| 20:W:530:U:H2' | 20:W:531:A:H8 | 1.87 | 0.40 |
| 20:W:541:U:OP1 | 20:W:544:G:N1 | 2.53 | 0.40 |
| 34:h:64:ARG:HH11 | 35:i:94:LEU:HD12 | 1.86 | 0.40 |
| 35:i:65:ARG:NH1 | 41:o:25:SER:OG | 2.54 | 0.40 |
| 40:n:86:ARG:HH11 | 40:n:86:ARG:HD3 | 1.74 | 0.40 |
| 4:E:371:LEU:HB3 | 4:E:373:ILE:HG23 | 2.03 | 0.40 |
| 6:G:17:ASN:OD1 | 6:G:18:GLU:N | 2.54 | 0.40 |
| 9:J:594:LEU:HA | 9:J:597:ASN:HB2 | 2.04 | 0.40 |
| 13:O:191:VAL:HG11 | 13:O:236:PHE:HA | 2.03 | 0.40 |
| 15:Q:57:LYS:HE2 | 15:Q:159:ILE:HG23 | 2.03 | 0.40 |
| 20:W:557:U:H2' | 20:W:558:G:C8 | 2.56 | 0.40 |
| 20:W:1356:G:H2' | 20:W:1357:A:C8 | 2.57 | 0.40 |
| 33:g:132:PHE:O | 33:g:140:ARG:NH1 | 2.53 | 0.40 |
| 43:q:31:LEU:HA | 43:q:111:VAL:HA | 2.02 | 0.40 |
| 46:w:56:MET:HE3 | 46:w:88:LEU:HD12 | 2.04 | 0.40 |
| 1:A:201:LEU:HD23 | 1:A:201:LEU:HA | 1.93 | 0.40 |
| 9:J:330:ILE:HD13 | 9:J:431:LEU:HD21 | 2.04 | 0.40 |
| 20:W:535:G:H1' | 20:W:536:A:H2' | 2.04 | 0.40 |
| 20:W:1210:G:H5" | 20:W:1210:G:H8 | 1.87 | 0.40 |
| 20:W:1442:OMU:H5" | 20:W:1442:OMU:H6 | 2.03 | 0.40 |
| 22:Y:104:ASP:HB3 | 22:Y:110:ALA:HB2 | 2.04 | 0.40 |
| 36:j:28:MET:HE3 | 36:j:28:MET:HB2 | 1.86 | 0.40 |
| 50:4:117:ILE:HA | 50:4:174:ALA:HA | 2.02 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 731/1382 (53%) | 687 (94%) | 44 (6%) | 0 | 100 | 100 |
| 2 | B | 380/445 (85%) | 344 (90%) | 36 (10%) | 0 | 100 | 100 |
| 3 | D | 276/315 (88%) | 260 (94%) | 15 (5%) | 1 (0%) | 30 | 65 |
| 4 | E | 462/472 (98%) | 435 (94%) | 26 (6%) | 1 (0%) | 43 | 75 |
| 5 | F | 323/325 (99%) | 305 (94%) | 18 (6%) | 0 | 100 | 100 |
| 6 | G | 95/147 (65%) | 89 (94%) | 6 (6%) | 0 | 100 | 100 |
| 7 | H | 83/116 (72%) | 65 (78%) | 18 (22%) | 0 | 100 | 100 |
| 8 | I | 573/814 (70%) | 538 (94%) | 35 (6%) | 0 | 100 | 100 |
| 9 | J | 639/913 (70%) | 601 (94%) | 38 (6%) | 0 | 100 | 100 |
| 10 | L | 172/194 (89%) | 161 (94%) | 11 (6%) | 0 | 100 | 100 |
| 11 | M | 79/84 (94%) | 74 (94%) | 5 (6%) | 0 | 100 | 100 |
| 12 | N | 81/83 (98%) | 80 (99%) | 1 (1%) | 0 | 100 | 100 |
| 13 | O | 218/293 (74%) | 214 (98%) | 4 (2%) | 0 | 100 | 100 |
| 14 | P | 209/264 (79%) | 201 (96%) | 6 (3%) | 2 (1%) | 12 | 45 |
| 15 | Q | 211/295 (72%) | 203 (96%) | 8 (4%) | 0 | 100 | 100 |
| 16 | R | 97/115 (84%) | 96 (99%) | 1 (1%) | 0 | 100 | 100 |
| 17 | S | 228/249 (92%) | 213 (93%) | 15 (7%) | 0 | 100 | 100 |
| 18 | T | 131/151 (87%) | 120 (92%) | 11 (8%) | 0 | 100 | 100 |
| 19 | V | 148/151 (98%) | 146 (99%) | 2 (1%) | 0 | 100 | 100 |
| 21 | X | 138/158 (87%) | 135 (98%) | 3 (2%) | 0 | 100 | 100 |
| 22 | Y | 255/263 (97%) | 251 (98%) | 4 (2%) | 0 | 100 | 100 |
| 23 | Z | 175/194 (90%) | 173 (99%) | 2 (1%) | 0 | 100 | 100 |
| 25 | 7 | 75/320 (23%) | 68 (91%) | 7 (9%) | 0 | 100 | 100 |
| 26 | 9 | 22/25 (88%) | 22 (100%) | 0 | 0 | 100 | 100 |
| 27 | a | 138/143 (96%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 28 | b | 55/59 (93%) | 50 (91%) | 5 (9%) | 0 | 100 | 100 |
| 29 | c | 127/130 (98%) | 123 (97%) | 4 (3%) | 0 | 100 | 100 |
| 30 | d | 194/208 (93%) | 184 (95%) | 10 (5%) | 0 | 100 | 100 |
| 31 | e | 123/133 (92%) | 122 (99%) | 1 (1%) | 0 | 100 | 100 |
| 32 | f | 180/204 (88%) | 173 (96%) | 7 (4%) | 0 | 100 | 100 |
| 33 | g | 139/146 (95%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 34 | h | 223/243 (92%) | 220 (99%) | 3 (1%) | 0 | 100 | 100 |
| 35 | i | 97/165 (59%) | 92 (95%) | 5 (5%) | 0 | 100 | 100 |
| 36 | j | 112/145 (77%) | 111 (99%) | 1 (1%) | 0 | 100 | 100 |
| 37 | k | 311/317 (98%) | 282 (91%) | 29 (9%) | 0 | 100 | 100 |
| 38 | l | 140/145 (97%) | 131 (94%) | 9 (6%) | 0 | 100 | 100 |
| 39 | m | 68/125 (54%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 40 | n | 140/152 (92%) | 137 (98%) | 3 (2%) | 0 | 100 | 100 |
| 41 | o | 53/56 (95%) | 53 (100%) | 0 | 0 | 100 | 100 |
| 42 | p | 49/80 (61%) | 46 (94%) | 3 (6%) | 0 | 100 | 100 |
| 43 | q | 120/132 (91%) | 105 (88%) | 15 (12%) | 0 | 100 | 100 |
| 44 | s | 61/69 (88%) | 57 (93%) | 4 (7%) | 0 | 100 | 100 |
| 45 | v | 129/135 (96%) | 126 (98%) | 3 (2%) | 0 | 100 | 100 |
| 46 | w | 101/119 (85%) | 95 (94%) | 6 (6%) | 0 | 100 | 100 |
| 48 | x | 434/548 (79%) | 384 (88%) | 48 (11%) | 2 (0%) | 24 | 60 |
| 49 | 6 | 348/374 (93%) | 315 (90%) | 33 (10%) | 0 | 100 | 100 |
| 50 | 4 | 251/357 (70%) | 233 (93%) | 18 (7%) | 0 | 100 | 100 |
| 51 | 8 | 313/352 (89%) | 281 (90%) | 32 (10%) | 0 | 100 | 100 |
| 52 | 3 | 209/218 (96%) | 200 (96%) | 9 (4%) | 0 | 100 | 100 |
| 53 | 5 | 307/564 (54%) | 290 (94%) | 17 (6%) | 0 | 100 | 100 |
| All | All | 10223/13087 (78%) | 9627 (94%) | 590 (6%) | 6 (0%) | 49 | 81 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | x | 13 | PRO |
| 4 | E | 324 | GLU |
| 48 | x | 80 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | P | 77 | ASP |
| 14 | P | 79 | VAL |
| 3 | D | 233 | PRO |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 525/1259 (42%) | 525 (100%) | 0 | 100 100 |
| 2 | B | 206/406 (51%) | 206 (100%) | 0 | 100 100 |
| 3 | D | 249/280 (89%) | 249 (100%) | 0 | 100 100 |
| 4 | E | 394/397 (99%) | 394 (100%) | 0 | 100 100 |
| 6 | G | 83/124 (67%) | 83 (100%) | 0 | 100 100 |
| 7 | H | 74/97 (76%) | 74 (100%) | 0 | 100 100 |
| 8 | I | 470/702 (67%) | 470 (100%) | 0 | 100 100 |
| 9 | J | 489/811 (60%) | 488 (100%) | 1 (0%) | 87 87 |
| 10 | L | 160/174 (92%) | 159 (99%) | 1 (1%) | 78 81 |
| 11 | M | 73/76 (96%) | 72 (99%) | 1 (1%) | 59 71 |
| 12 | N | 67/67 (100%) | 66 (98%) | 1 (2%) | 57 70 |
| 13 | O | 186/225 (83%) | 186 (100%) | 0 | 100 100 |
| 14 | P | 192/231 (83%) | 191 (100%) | 1 (0%) | 81 82 |
| 15 | Q | 179/243 (74%) | 179 (100%) | 0 | 100 100 |
| 16 | R | 86/98 (88%) | 86 (100%) | 0 | 100 100 |
| 17 | S | 200/218 (92%) | 200 (100%) | 0 | 100 100 |
| 18 | T | 104/119 (87%) | 104 (100%) | 0 | 100 100 |
| 19 | V | 130/131 (99%) | 130 (100%) | 0 | 100 100 |
| 21 | X | 129/142 (91%) | 129 (100%) | 0 | 100 100 |
| 22 | Y | 220/225 (98%) | 219 (100%) | 1 (0%) | 81 82 |
| 23 | Z | 158/168 (94%) | 158 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 25 | 7 | 64/277 (23%) | 64 (100%) | 0 | 100 100 |
| 26 | 9 | 23/24 (96%) | 23 (100%) | 0 | 100 100 |
| 27 | a | 112/115 (97%) | 112 (100%) | 0 | 100 100 |
| 28 | b | 46/48 (96%) | 44 (96%) | 2 (4%) | 26 48 |
| 29 | c | 112/113 (99%) | 112 (100%) | 0 | 100 100 |
| 30 | d | 172/180 (96%) | 172 (100%) | 0 | 100 100 |
| 31 | e | 107/115 (93%) | 107 (100%) | 0 | 100 100 |
| 32 | f | 156/170 (92%) | 156 (100%) | 0 | 100 100 |
| 33 | g | 117/121 (97%) | 117 (100%) | 0 | 100 100 |
| 34 | h | 189/202 (94%) | 189 (100%) | 0 | 100 100 |
| 35 | i | 90/136 (66%) | 90 (100%) | 0 | 100 100 |
| 36 | j | 104/130 (80%) | 104 (100%) | 0 | 100 100 |
| 37 | k | 272/275 (99%) | 269 (99%) | 3 (1%) | 65 74 |
| 38 | l | 112/115 (97%) | 112 (100%) | 0 | 100 100 |
| 39 | m | 62/103 (60%) | 61 (98%) | 1 (2%) | 55 70 |
| 40 | n | 123/132 (93%) | 123 (100%) | 0 | 100 100 |
| 41 | o | 48/49 (98%) | 47 (98%) | 1 (2%) | 47 65 |
| 42 | p | 47/72 (65%) | 47 (100%) | 0 | 100 100 |
| 43 | q | 104/108 (96%) | 104 (100%) | 0 | 100 100 |
| 44 | s | 56/62 (90%) | 56 (100%) | 0 | 100 100 |
| 45 | v | 119/122 (98%) | 117 (98%) | 2 (2%) | 53 68 |
| 46 | w | 94/107 (88%) | 94 (100%) | 0 | 100 100 |
| 48 | x | 205/494 (42%) | 204 (100%) | 1 (0%) | 81 82 |
| 49 | 6 | 49/335 (15%) | 49 (100%) | 0 | 100 100 |
| All | All | 6957/9798 (71%) | 6941 (100%) | 16 (0%) | 85 87 |

All (16) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | J | 570 | LEU |
| 10 | L | 64 | VAL |
| 11 | M | 56 | CYS |
| 12 | N | 74 | LYS |
| 14 | P | 76 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | Y | 139 | LEU |
| 28 | b | 122 | THR |
| 28 | b | 125 | LYS |
| 37 | k | 160 | SER |
| 37 | k | 161 | SER |
| 37 | k | 162 | ASN |
| 39 | m | 58 | LEU |
| 41 | o | 6 | LEU |
| 45 | v | 105 | MET |
| 45 | v | 114 | LEU |
| 48 | x | 73 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 82 | ASN |
| 1 | A | 109 | GLN |
| 1 | A | 110 | GLN |
| 1 | A | 122 | GLN |
| 1 | A | 167 | ASN |
| 1 | A | 277 | ASN |
| 1 | A | 512 | GLN |
| 1 | A | 544 | GLN |
| 2 | B | 225 | HIS |
| 2 | B | 373 | ASN |
| 2 | B | 402 | GLN |
| 3 | D | 41 | ASN |
| 3 | D | 60 | ASN |
| 3 | D | 126 | GLN |
| 4 | E | 123 | ASN |
| 4 | E | 265 | ASN |
| 7 | H | 48 | GLN |
| 7 | H | 86 | GLN |
| 8 | I | 249 | ASN |
| 8 | I | 581 | HIS |
| 8 | I | 609 | GLN |
| 9 | J | 433 | ASN |
| 9 | J | 465 | HIS |
| 9 | J | 467 | GLN |
| 9 | J | 472 | HIS |
| 9 | J | 606 | GLN |
| 9 | J | 623 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | J | 758 | ASN |
| 9 | J | 784 | GLN |
| 9 | J | 840 | GLN |
| 9 | J | 858 | GLN |
| 10 | L | 157 | HIS |
| 13 | O | 115 | GLN |
| 14 | P | 53 | GLN |
| 14 | P | 76 | ASN |
| 15 | Q | 169 | HIS |
| 16 | R | 8 | ASN |
| 19 | V | 58 | HIS |
| 19 | V | 62 | GLN |
| 19 | V | 69 | ASN |
| 21 | X | 11 | GLN |
| 21 | X | 121 | GLN |
| 22 | Y | 36 | HIS |
| 22 | Y | 216 | ASN |
| 23 | Z | 140 | GLN |
| 27 | a | 61 | GLN |
| 29 | c | 70 | ASN |
| 30 | d | 111 | GLN |
| 30 | d | 116 | HIS |
| 32 | f | 36 | GLN |
| 32 | f | 137 | GLN |
| 32 | f | 165 | ASN |
| 32 | f | 203 | ASN |
| 34 | h | 57 | ASN |
| 35 | i | 42 | ASN |
| 37 | k | 119 | GLN |
| 37 | k | 188 | HIS |
| 37 | k | 272 | GLN |
| 37 | k | 311 | GLN |
| 38 | l | 10 | ASN |
| 38 | l | 12 | GLN |
| 39 | m | 46 | ASN |
| 39 | m | 64 | ASN |
| 40 | n | 17 | ASN |
| 40 | n | 85 | ASN |
| 40 | n | 97 | GLN |
| 41 | o | 26 | ASN |
| 45 | v | 74 | GLN |
| 45 | v | 83 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | x | 31 | GLN |
| 48 | x | 296 | ASN |
| 48 | x | 416 | GLN |
| 48 | x | 428 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 20 | W | 1709/1869 (91%) | 375 (21%) | 24 (1%) |
| 24 | y | 74/75 (98%) | 17 (22%) | 0 |
| 47 | z | 26/774 (3%) | 15 (57%) | 0 |
| All | All | 1809/2718 (66%) | 407 (22%) | 24 (1%) |

All (407) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 4 | C |
| 20 | W | 17 | C |
| 20 | W | 33 | G |
| 20 | W | 41 | G |
| 20 | W | 44 | U |
| 20 | W | 45 | A |
| 20 | W | 46 | A |
| 20 | W | 56 | G |
| 20 | W | 64 | A |
| 20 | W | 65 | C |
| 20 | W | 67 | C |
| 20 | W | 68 | A |
| 20 | W | 71 | G |
| 20 | W | 72 | C |
| 20 | W | 73 | C |
| 20 | W | 74 | G |
| 20 | W | 77 | A |
| 20 | W | 103 | A |
| 20 | W | 113 | G |
| 20 | W | 114 | G |
| 20 | W | 115 | U |
| 20 | W | 126 | G |
| 20 | W | 127 | C |
| 20 | W | 129 | C |
| 20 | W | 130 | G |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 143 | U |
| 20 | W | 155 | G |
| 20 | W | 159 | A2M |
| 20 | W | 160 | U |
| 20 | W | 175 | A |
| 20 | W | 190 | G |
| 20 | W | 192 | C |
| 20 | W | 198 | U |
| 20 | W | 199 | C |
| 20 | W | 200 | G |
| 20 | W | 201 | C |
| 20 | W | 203 | G |
| 20 | W | 204 | G |
| 20 | W | 205 | G |
| 20 | W | 209 | A |
| 20 | W | 298 | G |
| 20 | W | 302 | A |
| 20 | W | 306 | C |
| 20 | W | 307 | G |
| 20 | W | 308 | G |
| 20 | W | 309 | G |
| 20 | W | 312 | G |
| 20 | W | 313 | A |
| 20 | W | 314 | U |
| 20 | W | 319 | C |
| 20 | W | 320 | G |
| 20 | W | 323 | C |
| 20 | W | 324 | C |
| 20 | W | 325 | C |
| 20 | W | 326 | C |
| 20 | W | 327 | G |
| 20 | W | 329 | G |
| 20 | W | 339 | A |
| 20 | W | 340 | C |
| 20 | W | 347 | G |
| 20 | W | 360 | A |
| 20 | W | 362 | C |
| 20 | W | 364 | A |
| 20 | W | 367 | U |
| 20 | W | 368 | U |
| 20 | W | 369 | C |
| 20 | W | 370 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 377 | G |
| 20 | W | 385 | G |
| 20 | W | 386 | C |
| 20 | W | 409 | C |
| 20 | W | 421 | G |
| 20 | W | 434 | G |
| 20 | W | 448 | A |
| 20 | W | 449 | A |
| 20 | W | 450 | C |
| 20 | W | 452 | G |
| 20 | W | 459 | C |
| 20 | W | 465 | A |
| 20 | W | 470 | G |
| 20 | W | 472 | C |
| 20 | W | 473 | A |
| 20 | W | 474 | G |
| 20 | W | 482 | G |
| 20 | W | 487 | U |
| 20 | W | 492 | C |
| 20 | W | 493 | A |
| 20 | W | 516 | A |
| 20 | W | 525 | A |
| 20 | W | 530 | U |
| 20 | W | 531 | A |
| 20 | W | 533 | A |
| 20 | W | 535 | G |
| 20 | W | 536 | A |
| 20 | W | 537 | C |
| 20 | W | 538 | U |
| 20 | W | 542 | U |
| 20 | W | 544 | G |
| 20 | W | 545 | A |
| 20 | W | 546 | G |
| 20 | W | 547 | G |
| 20 | W | 548 | C |
| 20 | W | 549 | C |
| 20 | W | 552 | G |
| 20 | W | 553 | U |
| 20 | W | 554 | A |
| 20 | W | 555 | A |
| 20 | W | 557 | U |
| 20 | W | 558 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 559 | G |
| 20 | W | 560 | A |
| 20 | W | 563 | G |
| 20 | W | 568 | C |
| 20 | W | 574 | A |
| 20 | W | 576 | A2M |
| 20 | W | 589 | G |
| 20 | W | 590 | A2M |
| 20 | W | 591 | U |
| 20 | W | 606 | G |
| 20 | W | 607 | U |
| 20 | W | 608 | C |
| 20 | W | 609 | PSU |
| 20 | W | 614 | C |
| 20 | W | 617 | G |
| 20 | W | 627 | U |
| 20 | W | 628 | A |
| 20 | W | 629 | A |
| 20 | W | 631 | U |
| 20 | W | 643 | A |
| 20 | W | 655 | A |
| 20 | W | 668 | A2M |
| 20 | W | 669 | A |
| 20 | W | 671 | A |
| 20 | W | 672 | A |
| 20 | W | 673 | G |
| 20 | W | 687 | C |
| 20 | W | 689 | U |
| 20 | W | 691 | G |
| 20 | W | 696 | G |
| 20 | W | 697 | G |
| 20 | W | 735 | C |
| 20 | W | 737 | G |
| 20 | W | 749 | U |
| 20 | W | 750 | C |
| 20 | W | 751 | G |
| 20 | W | 752 | G |
| 20 | W | 753 | C |
| 20 | W | 791 | C |
| 20 | W | 792 | C |
| 20 | W | 797 | C |
| 20 | W | 798 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 799 | U |
| 20 | W | 801 | PSU |
| 20 | W | 809 | A |
| 20 | W | 821 | G |
| 20 | W | 822 | PSU |
| 20 | W | 827 | A |
| 20 | W | 830 | A |
| 20 | W | 836 | G |
| 20 | W | 837 | A |
| 20 | W | 838 | G |
| 20 | W | 839 | C |
| 20 | W | 840 | C |
| 20 | W | 841 | G |
| 20 | W | 847 | A |
| 20 | W | 859 | G |
| 20 | W | 862 | A |
| 20 | W | 868 | G |
| 20 | W | 869 | A |
| 20 | W | 870 | A |
| 20 | W | 871 | U |
| 20 | W | 872 | A |
| 20 | W | 873 | G |
| 20 | W | 881 | G |
| 20 | W | 886 | A |
| 20 | W | 887 | U |
| 20 | W | 891 | G |
| 20 | W | 895 | G |
| 20 | W | 896 | U |
| 20 | W | 897 | U |
| 20 | W | 898 | U |
| 20 | W | 899 | U |
| 20 | W | 900 | C |
| 20 | W | 901 | G |
| 20 | W | 903 | A |
| 20 | W | 908 | A |
| 20 | W | 909 | G |
| 20 | W | 913 | A |
| 20 | W | 920 | A |
| 20 | W | 922 | A |
| 20 | W | 930 | C |
| 20 | W | 933 | G |
| 20 | W | 943 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 954 | U |
| 20 | W | 955 | A |
| 20 | W | 965 | U |
| 20 | W | 971 | G |
| 20 | W | 990 | A |
| 20 | W | 992 | A |
| 20 | W | 1002 | U |
| 20 | W | 1017 | U |
| 20 | W | 1023 | A |
| 20 | W | 1049 | A |
| 20 | W | 1053 | C |
| 20 | W | 1061 | U |
| 20 | W | 1062 | A |
| 20 | W | 1083 | A |
| 20 | W | 1085 | C |
| 20 | W | 1089 | G |
| 20 | W | 1109 | C |
| 20 | W | 1114 | U |
| 20 | W | 1115 | U |
| 20 | W | 1116 | C |
| 20 | W | 1117 | C |
| 20 | W | 1119 | A |
| 20 | W | 1120 | U |
| 20 | W | 1121 | G |
| 20 | W | 1138 | C |
| 20 | W | 1153 | C |
| 20 | W | 1154 | U |
| 20 | W | 1195 | A |
| 20 | W | 1207 | G |
| 20 | W | 1208 | A |
| 20 | W | 1211 | G |
| 20 | W | 1215 | C |
| 20 | W | 1224 | G |
| 20 | W | 1242 | U |
| 20 | W | 1243 | U |
| 20 | W | 1248 | C4J |
| 20 | W | 1249 | C |
| 20 | W | 1251 | A |
| 20 | W | 1253 | A |
| 20 | W | 1256 | G |
| 20 | W | 1257 | G |
| 20 | W | 1259 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 1269 | G |
| 20 | W | 1274 | G |
| 20 | W | 1275 | G |
| 20 | W | 1284 | A |
| 20 | W | 1285 | G |
| 20 | W | 1286 | G |
| 20 | W | 1288 | OMU |
| 20 | W | 1301 | A |
| 20 | W | 1302 | G |
| 20 | W | 1303 | C |
| 20 | W | 1309 | C |
| 20 | W | 1313 | A |
| 20 | W | 1315 | U |
| 20 | W | 1319 | U |
| 20 | W | 1327 | G |
| 20 | W | 1330 | G |
| 20 | W | 1348 | G |
| 20 | W | 1371 | U |
| 20 | W | 1372 | U |
| 20 | W | 1378 | A |
| 20 | W | 1397 | U |
| 20 | W | 1402 | A |
| 20 | W | 1405 | A |
| 20 | W | 1406 | G |
| 20 | W | 1419 | C |
| 20 | W | 1420 | G |
| 20 | W | 1421 | A |
| 20 | W | 1422 | G |
| 20 | W | 1423 | C |
| 20 | W | 1428 | G |
| 20 | W | 1429 | G |
| 20 | W | 1430 | C |
| 20 | W | 1433 | C |
| 20 | W | 1434 | C |
| 20 | W | 1435 | C |
| 20 | W | 1436 | C |
| 20 | W | 1437 | C |
| 20 | W | 1438 | A |
| 20 | W | 1439 | A |
| 20 | W | 1442 | OMU |
| 20 | W | 1454 | A |
| 20 | W | 1462 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 1463 | U |
| 20 | W | 1464 | C |
| 20 | W | 1465 | A |
| 20 | W | 1477 | U |
| 20 | W | 1487 | A |
| 20 | W | 1489 | A |
| 20 | W | 1490 | OMG |
| 20 | W | 1491 | G |
| 20 | W | 1494 | U |
| 20 | W | 1495 | G |
| 20 | W | 1497 | G |
| 20 | W | 1498 | A |
| 20 | W | 1508 | A |
| 20 | W | 1509 | U |
| 20 | W | 1521 | C |
| 20 | W | 1522 | A |
| 20 | W | 1523 | C |
| 20 | W | 1533 | A |
| 20 | W | 1537 | A |
| 20 | W | 1545 | A |
| 20 | W | 1548 | G |
| 20 | W | 1552 | G |
| 20 | W | 1553 | C |
| 20 | W | 1556 | A |
| 20 | W | 1557 | C |
| 20 | W | 1567 | G |
| 20 | W | 1570 | G |
| 20 | W | 1578 | U |
| 20 | W | 1579 | A |
| 20 | W | 1580 | A |
| 20 | W | 1585 | U |
| 20 | W | 1588 | A |
| 20 | W | 1600 | G |
| 20 | W | 1601 | A |
| 20 | W | 1606 | G |
| 20 | W | 1607 | A |
| 20 | W | 1612 | G |
| 20 | W | 1614 | A |
| 20 | W | 1621 | U |
| 20 | W | 1623 | A |
| 20 | W | 1624 | U |
| 20 | W | 1629 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 1637 | A |
| 20 | W | 1639 | G7M |
| 20 | W | 1647 | A |
| 20 | W | 1648 | G |
| 20 | W | 1654 | G |
| 20 | W | 1661 | A |
| 20 | W | 1665 | G |
| 20 | W | 1669 | G |
| 20 | W | 1671 | G |
| 20 | W | 1679 | A |
| 20 | W | 1680 | G |
| 20 | W | 1698 | C |
| 20 | W | 1699 | A |
| 20 | W | 1719 | A |
| 20 | W | 1721 | U |
| 20 | W | 1722 | G |
| 20 | W | 1723 | G |
| 20 | W | 1738 | C |
| 20 | W | 1742 | C |
| 20 | W | 1744 | G |
| 20 | W | 1748 | G |
| 20 | W | 1752 | C |
| 20 | W | 1753 | C |
| 20 | W | 1754 | G |
| 20 | W | 1755 | C |
| 20 | W | 1756 | C |
| 20 | W | 1757 | G |
| 20 | W | 1758 | G |
| 20 | W | 1759 | G |
| 20 | W | 1760 | G |
| 20 | W | 1772 | C |
| 20 | W | 1773 | C |
| 20 | W | 1774 | C |
| 20 | W | 1775 | U |
| 20 | W | 1779 | G |
| 20 | W | 1780 | G |
| 20 | W | 1781 | A |
| 20 | W | 1782 | G |
| 20 | W | 1783 | C |
| 20 | W | 1800 | A |
| 20 | W | 1805 | G |
| 20 | W | 1813 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 1823 | A |
| 20 | W | 1824 | A |
| 20 | W | 1829 | G |
| 20 | W | 1834 | A |
| 20 | W | 1835 | A |
| 20 | W | 1837 | G |
| 20 | W | 1838 | U |
| 20 | W | 1849 | G |
| 20 | W | 1851 | MA6 |
| 20 | W | 1861 | G |
| 20 | W | 1862 | G |
| 20 | W | 1863 | A |
| 20 | W | 1864 | U |
| 20 | W | 1865 | C |
| 24 | y | 11 | C |
| 24 | y | 12 | G |
| 24 | y | 14 | A |
| 24 | y | 16 | H2U |
| 24 | y | 26 | M2G |
| 24 | y | 32 | C |
| 24 | y | 47 | H2U |
| 24 | y | 48 | 5MC |
| 24 | y | 49 | 5MC |
| 24 | y | 58 | 1MA |
| 24 | y | 64 | RIA |
| 24 | y | 65 | G |
| 24 | y | 69 | C |
| 24 | y | 71 | C |
| 24 | y | 73 | A |
| 24 | y | 75 | C |
| 24 | y | 76 | A |
| 47 | z | 97 | C |
| 47 | z | 99 | A |
| 47 | z | 101 | A |
| 47 | z | 108 | G |
| 47 | z | 109 | G |
| 47 | z | 111 | C |
| 47 | z | 112 | A |
| 47 | z | 113 | A |
| 47 | z | 115 | G |
| 47 | z | 116 | U |
| 47 | z | 117 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | z | 118 | G |
| 47 | z | 119 | U |
| 47 | z | 120 | C |
| 47 | z | 121 | A |

All (24) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | W | 72 | C |
| 20 | W | 368 | U |
| 20 | W | 433 | A |
| 20 | W | 536 | A |
| 20 | W | 607 | U |
| 20 | W | 688 | U |
| 20 | W | 837 | A |
| 20 | W | 1113 | A |
| 20 | W | 1114 | U |
| 20 | W | 1115 | U |
| 20 | W | 1119 | A |
| 20 | W | 1215 | C |
| 20 | W | 1318 | G |
| 20 | W | 1419 | C |
| 20 | W | 1420 | G |
| 20 | W | 1421 | A |
| 20 | W | 1428 | G |
| 20 | W | 1429 | G |
| 20 | W | 1463 | U |
| 20 | W | 1490 | OMG |
| 20 | W | 1520 | G |
| 20 | W | 1679 | A |
| 20 | W | 1698 | C |
| 20 | W | 1782 | G |

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

106 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 | $\#\|Z\| > 2$ |
| 20 | PSU | W | 1643 | 55,20 | 18,21,22 | 1.08 | 1 (5%) | 22,30,33 | 0.69 | 0 |
| 20 | PSU | W | 1596 | 20 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 0.76 | 0 |
| 24 | 5MC | y | 48 | 24 | 18,22,23 | 0.35 | 0 | 26,32,35 | 0.54 | 0 |
| 20 | A2M | W | 668 | 55,20 | 22,25,26 | 0.22 | 0 | 31,36,39 | 1.22 | 1 (3%) |
| 20 | PSU | W | 651 | 20 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 0.75 | 0 |
| 24 | T6A | y | 37 | 24 | 31,34,35 | 0.52 | 0 | 44,49,52 | 1.36 | 2 (4%) |
| 20 | PSU | W | 572 | 20 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 0.71 | 0 |
| 20 | PSU | W | 1081 | 20 | 18,21,22 | 1.06 | 2 (11%) | 22,30,33 | 0.80 | 0 |
| 20 | PSU | W | 1445 | 20 | 18,21,22 | 0.88 | 1 (5%) | 22,30,33 | 0.69 | 0 |
| 20 | OMG | W | 436 | 20 | 23,26,27 | 0.44 | 0 | 33,38,41 | 0.49 | 0 |
| 20 | OMU | W | 172 | 20 | 19,22,23 | 0.31 | 0 | 26,31,34 | 1.11 | 1 (3%) |
| 24 | M2G | y | 26 | 24 | 24,27,28 | 0.45 | 0 | 35,40,43 | 0.47 | 0 |
| 20 | JMH | W | 1219 | 55,20 | 18,22,23 | 0.70 | 1 (5%) | 21,32,35 | 0.68 | 0 |
| 20 | 5MU | W | 814 | 20 | 19,22,23 | 0.46 | 0 | 28,32,35 | 0.51 | 0 |
| 20 | OMU | W | 121 | 20 | 19,22,23 | 0.46 | 0 | 26,31,34 | 0.57 | 0 |
| 20 | PSU | W | 966 | 20 | 18,21,22 | 1.01 | 1 (5%) | 22,30,33 | 0.75 | 0 |
| 20 | PSU | W | 1045 | 20 | 18,21,22 | 0.96 | 1 (5%) | 22,30,33 | 0.84 | 0 |
| 20 | OMU | W | 1442 | 20 | 19,22,23 | 0.49 | 0 | 26,31,34 | 0.56 | 0 |
| 20 | A2M | W | 590 | 20 | 22,25,26 | 0.20 | 0 | 31,36,39 | 0.50 | 0 |
| 20 | PSU | W | 34 | 20 | 18,21,22 | 0.99 | 1 (5%) | 22,30,33 | 0.72 | 0 |
| 20 | PSU | W | 612 | 20 | 18,21,22 | 1.03 | 2 (11%) | 22,30,33 | 0.74 | 0 |
| 24 | H2U | y | 47 | 24 | 18,21,22 | 0.57 | 0 | 21,30,33 | 0.54 | 0 |
| 20 | PSU | W | 105 | 20 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 0.74 | 0 |
| 20 | OMU | W | 1288 | 20 | 19,22,23 | 0.50 | 0 | 26,31,34 | 0.69 | 0 |
| 24 | RIA | y | 64 | 24 | 35,38,39 | 0.30 | 0 | 53,57,60 | 0.73 | 1 (1%) |
| 20 | A2M | W | 576 | 20 | 22,25,26 | 0.22 | 0 | 31,36,39 | 1.51 | 4 (12%) |
| 20 | PSU | W | 296 | 20 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 0.80 | 0 |
| 20 | A2M | W | 484 | 20 | 22,25,26 | 0.22 | 0 | 31,36,39 | 1.36 | 3 (9%) |
| 20 | A2M | W | 99 | 55,20 | 22,25,26 | 0.25 | 0 | 31,36,39 | 0.44 | 0 |
| 20 | PSU | W | 109 | 20 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 0.71 | 0 |
| 20 | PSU | W | 1625 | 20 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 0.73 | 0 |
| 20 | PSU | W | 863 | 20 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 0.70 | 0 |
| 20 | PSU | W | 1186 | 20 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 0.79 | 0 |
| 20 | OMG | W | 867 | 20 | 23,26,27 | 0.39 | 0 | 33,38,41 | 0.38 | 0 |
| 20 | PSU | W | 119 | 20 | 18,21,22 | 0.99 | 1 (5%) | 22,30,33 | 0.68 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 24 | H2U | y | 16 | 24 | 18,21,22 | 0.52 | 0 | 21,30,33 | 0.73 | 0 |
| 20 | C4J | W | 1248 | 20 | 24,29,30 | 0.87 | 1 (4%) | 29,42,45 | 0.81 | 0 |
| 20 | OMG | W | 1490 | 55,20 | 23,26,27 | 0.35 | 0 | 33,38,41 | 0.40 | 0 |
| 20 | PSU | W | 649 | 20 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 0.84 | 0 |
| 20 | A2M | W | 1678 | 20 | 22,25,26 | 0.24 | 0 | 31,36,39 | 0.48 | 0 |
| 20 | OMC | W | 1703 | 20 | 19,22,23 | 0.48 | 0 | 26,31,34 | 0.60 | 0 |
| 20 | A2M | W | 1383 | 20 | 22,25,26 | 0.25 | 0 | 31,36,39 | 0.59 | 0 |
| 20 | PSU | W | 918 | 20 | 18,21,22 | 1.07 | 2 (11%) | 22,30,33 | 0.79 | 1 (4%) |
| 20 | PSU | W | 815 | 20 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 0.75 | 0 |
| 20 | OMC | W | 174 | 55,20 | 19,22,23 | 0.47 | 0 | 26,31,34 | 0.57 | 0 |
| 20 | 4AC | W | 1842 | 20 | 21,24,25 | 0.49 | 0 | 29,34,37 | 0.66 | 0 |
| 20 | 4AC | W | 1337 | 20 | 21,24,25 | 0.54 | 0 | 29,34,37 | 0.83 | 1 (3%) |
| 20 | PSU | W | 801 | 20 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 0.64 | 0 |
| 20 | OMC | W | 462 | 20 | 19,22,23 | 0.46 | 0 | 26,31,34 | 0.63 | 0 |
| 20 | PSU | W | 1004 | 20 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 0.72 | 0 |
| 20 | PSU | W | 1046 | 20 | 18,21,22 | 1.05 | 2 (11%) | 22,30,33 | 0.62 | 0 |
| 20 | PSU | W | 1238 | 20 | 18,21,22 | 0.89 | 1 (5%) | 22,30,33 | 0.75 | 1 (4%) |
| 20 | MA6 | W | 1851 | 20 | 23,26,27 | 0.36 | 0 | 34,38,41 | 0.79 | 1 (2%) |
| 20 | A2M | W | 159 | 20 | 22,25,26 | 0.24 | 0 | 31,36,39 | 1.21 | 3 (9%) |
| 20 | PSU | W | 1056 | 20 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 0.73 | 0 |
| 24 | 1MA | y | 58 | 24 | 21,25,26 | 0.40 | 0 | 31,37,40 | 0.68 | 0 |
| 20 | OMG | W | 601 | 20 | 23,26,27 | 0.40 | 0 | 33,38,41 | 0.39 | 0 |
| 20 | PSU | W | 406 | 20 | 18,21,22 | 0.87 | 1 (5%) | 22,30,33 | 0.67 | 0 |
| 20 | OMC | W | 517 | 20 | 19,22,23 | 0.50 | 0 | 26,31,34 | 0.59 | 0 |
| 20 | OMG | W | 644 | 20 | 23,26,27 | 0.44 | 0 | 33,38,41 | 0.46 | 0 |
| 20 | A2M | W | 512 | 20 | 22,25,26 | 0.22 | 0 | 31,36,39 | 1.64 | 5 (16%) |
| 20 | PSU | W | 1003 | 20 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 0.70 | 0 |
| 20 | OMU | W | 428 | 20 | 19,22,23 | 0.36 | 0 | 26,31,34 | 0.50 | 0 |
| 20 | PSU | W | 1692 | 20 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 0.70 | 0 |
| 20 | PSU | W | 686 | 20 | 18,21,22 | 0.88 | 1 (5%) | 22,30,33 | 0.74 | 0 |
| 20 | PSU | W | 681 | 20 | 18,21,22 | 1.07 | 1 (5%) | 22,30,33 | 0.77 | 0 |
| 20 | OMG | W | 1328 | 20 | 23,26,27 | 0.28 | 0 | 33,38,41 | 0.33 | 0 |
| 20 | OMU | W | 116 | 20 | 19,22,23 | 0.42 | 0 | 26,31,34 | 0.60 | 0 |
| 20 | PSU | W | 1360 | 56,55,20 | 18,21,22 | 1.08 | 2 (11%) | 22,30,33 | 0.76 | 0 |
| 20 | PSU | W | 822 | 20 | 18,21,22 | 0.85 | 1 (5%) | 22,30,33 | 0.77 | 1 (4%) |
| 20 | OMU | W | 354 | 20 | 19,22,23 | 0.49 | 0 | 26,31,34 | 0.79 | 1 (3%) |
| 24 | 7MG | y | 46 | 24 | 22,26,27 | 1.12 | 1 (4%) | 29,39,42 | 0.72 | 0 |
| 20 | A2M | W | 27 | 55,20 | 22,25,26 | 0.26 | 0 | 31,36,39 | 0.42 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 20 | OMG | W | 683 | 20 | 23,26,27 | 0.49 | 0 | 33,38,41 | 0.49 | 0 |
| 20 | PSU | W | 1174 | 20 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 0.77 | 0 |
| 20 | PSU | W | 63 | 20 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 0.87 | 0 |
| 24 | 2MG | y | 10 | 24 | 23,26,27 | 0.40 | 0 | 32,38,41 | 0.50 | 0 |
| 20 | PSU | W | 36 | 20 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 0.73 | 0 |
| 20 | A2M | W | 166 | 20 | 22,25,26 | 0.20 | 0 | 31,36,39 | 0.45 | 0 |
| 20 | OMG | W | 1447 | 20 | 23,26,27 | 0.30 | 0 | 33,38,41 | 0.39 | 0 |
| 20 | PSU | W | 218 | 20 | 18,21,22 | 1.00 | 1 (5%) | 22,30,33 | 0.72 | 0 |
| 20 | A2M | W | 468 | 20 | 22,25,26 | 0.23 | 0 | 31,36,39 | 0.60 | 0 |
| 20 | OMG | W | 509 | 55,20 | 23,26,27 | 0.42 | 0 | 33,38,41 | 0.51 | 0 |
| 24 | 5MC | y | 49 | 24 | 18,22,23 | 0.37 | 0 | 26,32,35 | 0.55 | 0 |
| 20 | PSU | W | 1244 | 20 | 18,21,22 | 0.84 | 1 (5%) | 22,30,33 | 0.64 | 0 |
| 20 | PSU | W | 1136 | 20 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 0.74 | 0 |
| 20 | PSU | W | 866 | 20 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 0.65 | 0 |
| 20 | PSU | W | 100 | 55,20 | 18,21,22 | 0.92 | 1 (5%) | 22,30,33 | 0.81 | 0 |
| 20 | 6MZ | W | 1832 | 55,20 | 22,25,26 | 0.40 | 0 | 30,36,39 | 0.67 | 0 |
| 24 | 1MG | y | 9 | 24 | 22,26,27 | 0.53 | 0 | 33,39,42 | 0.66 | 0 |
| 20 | PSU | W | 1177 | 20 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 0.73 | 0 |
| 20 | A2M | W | 1031 | 20 | 22,25,26 | 0.25 | 0 | 31,36,39 | 0.40 | 0 |
| 20 | G7M | W | 1639 | 20,24 | 23,26,27 | 0.66 | 0 | 35,39,42 | 0.55 | 0 |
| 20 | PSU | W | 300 | 20 | 18,21,22 | 1.01 | 1 (5%) | 22,30,33 | 0.77 | 0 |
| 20 | PSU | W | 667 | 20 | 18,21,22 | 1.11 | 2 (11%) | 22,30,33 | 0.70 | 0 |
| 20 | UY1 | W | 1326 | 55,20 | 19,22,23 | 0.84 | 1 (5%) | 22,31,34 | 0.70 | 0 |
| 20 | PSU | W | 1232 | 20 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 0.78 | 0 |
| 20 | OMC | W | 1272 | 20 | 19,22,23 | 0.50 | 0 | 26,31,34 | 0.61 | 0 |
| 20 | 5MC | W | 1374 | 20 | 18,22,23 | 0.46 | 0 | 26,32,35 | 0.52 | 0 |
| 20 | MA6 | W | 1850 | 20 | 23,26,27 | 0.35 | 0 | 34,38,41 | 0.65 | 1 (2%) |
| 20 | OMU | W | 1804 | 20 | 19,22,23 | 0.46 | 0 | 26,31,34 | 0.74 | 0 |
| 20 | PSU | W | 366 | 20 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 0.72 | 0 |
| 20 | PSU | W | 1347 | 20 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 0.73 | 0 |
| 20 | PSU | W | 609 | 20 | 18,21,22 | 0.87 | 1 (5%) | 22,30,33 | 0.71 | 0 |
| 20 | OMC | W | 1391 | 20 | 19,22,23 | 0.50 | 0 | 26,31,34 | 0.69 | 0 |
| 20 | PSU | W | 1367 | 20 | 18,21,22 | 1.01 | 1 (5%) | 22,30,33 | 0.78 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 20 | PSU | W | 1643 | 55,20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1596 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 5MC | y | 48 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | A2M | W | 668 | 55,20 | - | 4/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 651 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | T6A | y | 37 | 24 | - | 3/23/41/42 | 0/3/3/3 |
| 20 | PSU | W | 572 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1081 | 20 | - | 1/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1445 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMG | W | 436 | 20 | - | 0/9/27/28 | 0/3/3/3 |
| 20 | OMU | W | 172 | 20 | - | 1/9/27/28 | 0/2/2/2 |
| 24 | M2G | y | 26 | 24 | - | 2/11/29/30 | 0/3/3/3 |
| 20 | JMH | W | 1219 | 55,20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | 5MU | W | 814 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMU | W | 121 | 20 | - | 0/9/27/28 | 0/2/2/2 |
| 20 | PSU | W | 966 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1045 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMU | W | 1442 | 20 | - | 2/9/27/28 | 0/2/2/2 |
| 20 | A2M | W | 590 | 20 | - | 1/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 34 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 612 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | H2U | y | 47 | 24 | - | 5/7/38/39 | 0/2/2/2 |
| 20 | PSU | W | 105 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMU | W | 1288 | 20 | - | 2/9/27/28 | 0/2/2/2 |
| 24 | RIA | y | 64 | 24 | - | 2/17/51/52 | 0/4/4/4 |
| 20 | A2M | W | 576 | 20 | - | 2/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 296 | 20 | - | 2/7/25/26 | 0/2/2/2 |
| 20 | A2M | W | 484 | 20 | - | 1/9/27/28 | 0/3/3/3 |
| 20 | A2M | W | 99 | 55,20 | - | 0/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 109 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1625 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 863 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1186 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMG | W | 867 | 20 | - | 0/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 119 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | H2U | y | 16 | 24 | - | 5/7/38/39 | 0/2/2/2 |
| 20 | C4J | W | 1248 | 20 | - | 2/16/34/35 | 0/2/2/2 |
| 20 | OMG | W | 1490 | 55,20 | - | 3/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 649 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | A2M | W | 1678 | 20 | - | 0/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 20 | OMC | W | 1703 | 20 | - | 0/9/27/28 | 0/2/2/2 |
| 20 | A2M | W | 1383 | 20 | - | 0/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 918 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 815 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMC | W | 174 | 55,20 | - | 0/9/27/28 | 0/2/2/2 |
| 20 | 4AC | W | 1842 | 20 | - | 0/11/29/30 | 0/2/2/2 |
| 20 | 4AC | W | 1337 | 20 | - | 0/11/29/30 | 0/2/2/2 |
| 20 | PSU | W | 801 | 20 | - | 2/7/25/26 | 0/2/2/2 |
| 20 | OMC | W | 462 | 20 | - | 0/9/27/28 | 0/2/2/2 |
| 20 | PSU | W | 1004 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1046 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1238 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | MA6 | W | 1851 | 20 | - | 2/11/29/30 | 0/3/3/3 |
| 20 | A2M | W | 159 | 20 | - | 3/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 1056 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 1MA | y | 58 | 24 | - | 1/7/25/26 | 0/3/3/3 |
| 20 | OMG | W | 601 | 20 | - | 0/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 406 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMC | W | 517 | 20 | - | 0/9/27/28 | 0/2/2/2 |
| 20 | OMG | W | 644 | 20 | - | 1/9/27/28 | 0/3/3/3 |
| 20 | A2M | W | 512 | 20 | - | 3/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 1003 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMU | W | 428 | 20 | - | 6/9/27/28 | 0/2/2/2 |
| 20 | PSU | W | 1692 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 686 | 20 | - | 2/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 681 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMG | W | 1328 | 20 | - | 1/9/27/28 | 0/3/3/3 |
| 20 | OMU | W | 116 | 20 | - | 0/9/27/28 | 0/2/2/2 |
| 20 | PSU | W | 1360 | 56,55,20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 822 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMU | W | 354 | 20 | - | 0/9/27/28 | 0/2/2/2 |
| 24 | 7MG | y | 46 | 24 | - | 1/7/37/38 | 0/3/3/3 |
| 20 | A2M | W | 27 | 55,20 | - | 0/9/27/28 | 0/3/3/3 |
| 20 | OMG | W | 683 | 20 | - | 0/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 1174 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 63 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 2MG | y | 10 | 24 | - | 0/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 36 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | A2M | W | 166 | 20 | - | 1/9/27/28 | 0/3/3/3 |
| 20 | OMG | W | 1447 | 20 | - | 3/9/27/28 | 0/3/3/3 |
| 20 | PSU | W | 218 | 20 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 20 | A2M | W | 468 | 20 | - | 0/9/27/28 | 0/3/3/3 |
| 20 | OMG | W | 509 | 55,20 | - | 1/9/27/28 | 0/3/3/3 |
| 24 | 5MC | y | 49 | 24 | - | 2/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1244 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1136 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 866 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 100 | 55,20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | 6MZ | W | 1832 | 55,20 | - | 0/9/27/28 | 0/3/3/3 |
| 24 | 1MG | y | 9 | 24 | - | 2/7/25/26 | 0/3/3/3 |
| 20 | PSU | W | 1177 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | A2M | W | 1031 | 20 | - | 0/9/27/28 | 0/3/3/3 |
| 20 | G7M | W | 1639 | 20,24 | - | 2/7/25/26 | 0/3/3/3 |
| 20 | PSU | W | 300 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 667 | 20 | - | 1/7/25/26 | 0/2/2/2 |
| 20 | UY1 | W | 1326 | 55,20 | - | 1/9/27/28 | 0/2/2/2 |
| 20 | PSU | W | 1232 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | OMC | W | 1272 | 20 | - | 0/9/27/28 | 0/2/2/2 |
| 20 | 5MC | W | 1374 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | MA6 | W | 1850 | 20 | - | 0/11/29/30 | 0/3/3/3 |
| 20 | OMU | W | 1804 | 20 | - | 0/9/27/28 | 0/2/2/2 |
| 20 | PSU | W | 366 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 1347 | 20 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | PSU | W | 609 | 20 | - | 2/7/25/26 | 0/2/2/2 |
| 20 | OMC | W | 1391 | 20 | - | 1/9/27/28 | 0/2/2/2 |
| 20 | PSU | W | 1367 | 20 | - | 0/7/25/26 | 0/2/2/2 |

All (58) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | y | 46 | 7MG | C5-N7 | 4.69 | 1.41 | 1.35 |
| 20 | W | 1625 | PSU | C6-C5 | 3.41 | 1.39 | 1.35 |
| 20 | W | 866 | PSU | C6-C5 | 3.40 | 1.39 | 1.35 |
| 20 | W | 801 | PSU | C6-C5 | 3.36 | 1.39 | 1.35 |
| 20 | W | 1232 | PSU | C6-C5 | 3.34 | 1.39 | 1.35 |
| 20 | W | 651 | PSU | C6-C5 | 3.34 | 1.39 | 1.35 |
| 20 | W | 1596 | PSU | C6-C5 | 3.34 | 1.39 | 1.35 |
| 20 | W | 300 | PSU | C6-C5 | 3.33 | 1.39 | 1.35 |
| 20 | W | 105 | PSU | C6-C5 | 3.31 | 1.39 | 1.35 |
| 20 | W | 1177 | PSU | C6-C5 | 3.30 | 1.39 | 1.35 |
| 20 | W | 36 | PSU | C6-C5 | 3.30 | 1.39 | 1.35 |
| 20 | W | 366 | PSU | C6-C5 | 3.29 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | W | 1174 | PSU | C6-C5 | 3.28 | 1.39 | 1.35 |
| 20 | W | 815 | PSU | C6-C5 | 3.28 | 1.39 | 1.35 |
| 20 | W | 966 | PSU | C6-C5 | 3.27 | 1.39 | 1.35 |
| 20 | W | 1186 | PSU | C6-C5 | 3.27 | 1.39 | 1.35 |
| 20 | W | 1347 | PSU | C6-C5 | 3.27 | 1.39 | 1.35 |
| 20 | W | 1643 | PSU | C6-C5 | 3.26 | 1.39 | 1.35 |
| 20 | W | 296 | PSU | C6-C5 | 3.26 | 1.39 | 1.35 |
| 20 | W | 218 | PSU | C6-C5 | 3.26 | 1.39 | 1.35 |
| 20 | W | 863 | PSU | C6-C5 | 3.26 | 1.39 | 1.35 |
| 20 | W | 1004 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |
| 20 | W | 667 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |
| 20 | W | 1692 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |
| 20 | W | 119 | PSU | C6-C5 | 3.23 | 1.39 | 1.35 |
| 20 | W | 63 | PSU | C6-C5 | 3.23 | 1.39 | 1.35 |
| 20 | W | 1003 | PSU | C6-C5 | 3.23 | 1.39 | 1.35 |
| 20 | W | 1360 | PSU | C6-C5 | 3.23 | 1.39 | 1.35 |
| 20 | W | 1367 | PSU | C6-C5 | 3.23 | 1.39 | 1.35 |
| 20 | W | 681 | PSU | C6-C5 | 3.21 | 1.39 | 1.35 |
| 20 | W | 1238 | PSU | C6-C5 | 3.21 | 1.39 | 1.35 |
| 20 | W | 649 | PSU | C6-C5 | 3.21 | 1.39 | 1.35 |
| 20 | W | 109 | PSU | C6-C5 | 3.21 | 1.39 | 1.35 |
| 20 | W | 918 | PSU | C6-C5 | 3.20 | 1.39 | 1.35 |
| 20 | W | 572 | PSU | C6-C5 | 3.20 | 1.39 | 1.35 |
| 20 | W | 1056 | PSU | C6-C5 | 3.19 | 1.39 | 1.35 |
| 20 | W | 609 | PSU | C6-C5 | 3.18 | 1.39 | 1.35 |
| 20 | W | 1045 | PSU | C6-C5 | 3.17 | 1.39 | 1.35 |
| 20 | W | 34 | PSU | C6-C5 | 3.17 | 1.39 | 1.35 |
| 20 | W | 1445 | PSU | C6-C5 | 3.17 | 1.39 | 1.35 |
| 20 | W | 1046 | PSU | C6-C5 | 3.16 | 1.39 | 1.35 |
| 20 | W | 1136 | PSU | C6-C5 | 3.16 | 1.39 | 1.35 |
| 20 | W | 1081 | PSU | C6-C5 | 3.15 | 1.39 | 1.35 |
| 20 | W | 686 | PSU | C6-C5 | 3.14 | 1.39 | 1.35 |
| 20 | W | 612 | PSU | C6-C5 | 3.12 | 1.39 | 1.35 |
| 20 | W | 100 | PSU | C6-C5 | 3.12 | 1.39 | 1.35 |
| 20 | W | 822 | PSU | C6-C5 | 3.10 | 1.38 | 1.35 |
| 20 | W | 1244 | PSU | C6-C5 | 3.10 | 1.38 | 1.35 |
| 20 | W | 406 | PSU | C6-C5 | 3.08 | 1.38 | 1.35 |
| 20 | W | 1326 | UY1 | C6-C5 | 3.07 | 1.38 | 1.35 |
| 20 | W | 1248 | C4J | C6-C5 | 3.00 | 1.39 | 1.34 |
| 20 | W | 1081 | PSU | O4'-C1' | -2.47 | 1.40 | 1.43 |
| 20 | W | 1219 | JMH | C5-C4 | -2.36 | 1.37 | 1.42 |
| 20 | W | 918 | PSU | O4'-C1' | -2.34 | 1.40 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | W | 667 | PSU | O4'-C1' | -2.21 | 1.40 | 1.43 |
| 20 | W | 1360 | PSU | O4'-C1' | -2.08 | 1.40 | 1.43 |
| 20 | W | 612 | PSU | O4'-C1' | -2.05 | 1.41 | 1.43 |
| 20 | W | 1046 | PSU | O4'-C1' | -2.04 | 1.41 | 1.43 |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | y | 37 | T6A | C12-N11-C10 | 7.74 | 134.83 | 121.94 |
| 20 | W | 576 | A2M | C2'-C1'-N9 | -5.46 | 104.34 | 113.53 |
| 20 | W | 512 | A2M | O3'-C3'-C4' | 5.16 | 125.97 | 111.05 |
| 20 | W | 668 | A2M | O3'-C3'-C2' | 5.00 | 125.36 | 111.17 |
| 20 | W | 512 | A2M | C2'-C1'-N9 | -4.74 | 105.55 | 113.53 |
| 20 | W | 484 | A2M | O3'-C3'-C2' | 4.72 | 124.56 | 111.17 |
| 20 | W | 576 | A2M | O3'-C3'-C4' | 4.54 | 124.17 | 111.05 |
| 20 | W | 172 | OMU | O2'-C2'-C1' | 4.45 | 117.76 | 109.08 |
| 20 | W | 159 | A2M | O3'-C3'-C4' | 3.69 | 121.71 | 111.05 |
| 20 | W | 512 | A2M | O3'-C3'-C2' | 3.63 | 121.47 | 111.17 |
| 20 | W | 484 | A2M | C2'-C1'-N9 | -3.56 | 107.54 | 113.53 |
| 20 | W | 159 | A2M | C2'-C1'-N9 | -3.52 | 107.60 | 113.53 |
| 20 | W | 159 | A2M | O3'-C3'-C2' | 3.51 | 121.15 | 111.17 |
| 20 | W | 1851 | MA6 | C2-N1-C6 | 2.99 | 118.81 | 111.75 |
| 20 | W | 1850 | MA6 | C2-N1-C6 | 2.95 | 118.72 | 111.75 |
| 20 | W | 484 | A2M | O3'-C3'-C4' | 2.86 | 119.33 | 111.05 |
| 24 | y | 37 | T6A | C5-C6-N6 | 2.85 | 126.25 | 118.71 |
| 20 | W | 1337 | 4AC | C5-C4-N4 | 2.66 | 127.54 | 122.92 |
| 20 | W | 354 | OMU | C2'-C1'-N1 | -2.66 | 109.06 | 114.22 |
| 20 | W | 576 | A2M | O3'-C3'-C2' | 2.57 | 118.45 | 111.17 |
| 20 | W | 822 | PSU | C3'-C2'-C1' | 2.47 | 104.51 | 101.64 |
| 24 | y | 64 | RIA | C1'-C2'-C3' | -2.46 | 99.19 | 102.30 |
| 20 | W | 512 | A2M | C2'-C3'-C4' | 2.25 | 106.89 | 101.99 |
| 20 | W | 918 | PSU | O4'-C1'-C2' | 2.11 | 108.12 | 105.14 |
| 20 | W | 1238 | PSU | C2'-C3'-C4' | -2.09 | 98.59 | 102.64 |
| 20 | W | 576 | A2M | C2'-C3'-C4' | 2.01 | 106.36 | 101.99 |
| 20 | W | 512 | A2M | O4'-C1'-N9 | -2.00 | 104.11 | 108.06 |

There are no chirality outliers.

All (76) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | W | 159 | A2M | C1'-C2'-O2'-CM' |
| 20 | W | 166 | A2M | C1'-C2'-O2'-CM' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | W | 172 | OMU | C1'-C2'-O2'-CM2 |
| 20 | W | 296 | PSU | C3'-C4'-C5'-O5' |
| 20 | W | 484 | A2M | C1'-C2'-O2'-CM' |
| 20 | W | 512 | A2M | C3'-C4'-C5'-O5' |
| 20 | W | 576 | A2M | C1'-C2'-O2'-CM' |
| 20 | W | 609 | PSU | C3'-C4'-C5'-O5' |
| 20 | W | 609 | PSU | O4'-C4'-C5'-O5' |
| 20 | W | 668 | A2M | C1'-C2'-O2'-CM' |
| 20 | W | 801 | PSU | C3'-C4'-C5'-O5' |
| 20 | W | 1288 | OMU | C3'-C4'-C5'-O5' |
| 20 | W | 1288 | OMU | O4'-C4'-C5'-O5' |
| 20 | W | 1328 | OMG | C1'-C2'-O2'-CM2 |
| 20 | W | 1447 | OMG | C1'-C2'-O2'-CM2 |
| 20 | W | 1490 | OMG | C1'-C2'-O2'-CM2 |
| 20 | W | 1851 | MA6 | O4'-C4'-C5'-O5' |
| 24 | y | 26 | M2G | C3'-C4'-C5'-O5' |
| 24 | y | 46 | 7MG | C2'-C1'-N9-C8 |
| 24 | y | 47 | H2U | O4'-C1'-N1-C6 |
| 24 | y | 64 | RIA | O1'-C1'-O2A-C2A |
| 24 | y | 64 | RIA | C2'-C1'-O2A-C2A |
| 20 | W | 296 | PSU | O4'-C4'-C5'-O5' |
| 20 | W | 512 | A2M | O4'-C4'-C5'-O5' |
| 20 | W | 668 | A2M | O4'-C4'-C5'-O5' |
| 20 | W | 668 | A2M | C3'-C4'-C5'-O5' |
| 20 | W | 686 | PSU | C3'-C4'-C5'-O5' |
| 20 | W | 686 | PSU | O4'-C4'-C5'-O5' |
| 20 | W | 1442 | OMU | O4'-C4'-C5'-O5' |
| 20 | W | 1851 | MA6 | C3'-C4'-C5'-O5' |
| 24 | y | 47 | H2U | C4'-C5'-O5'-P |
| 20 | W | 801 | PSU | O4'-C4'-C5'-O5' |
| 20 | W | 1248 | C4J | C4'-C5'-O5'-P |
| 24 | y | 47 | H2U | O4'-C4'-C5'-O5' |
| 20 | W | 1447 | OMG | C3'-C4'-C5'-O5' |
| 24 | y | 47 | H2U | C3'-C4'-C5'-O5' |
| 20 | W | 428 | OMU | O4'-C4'-C5'-O5' |
| 24 | y | 16 | H2U | O4'-C4'-C5'-O5' |
| 24 | y | 26 | M2G | O4'-C4'-C5'-O5' |
| 20 | W | 428 | OMU | C2'-C1'-N1-C6 |
| 20 | W | 576 | A2M | C4'-C5'-O5'-P |
| 20 | W | 1447 | OMG | O4'-C4'-C5'-O5' |
| 20 | W | 1639 | G7M | O4'-C4'-C5'-O5' |
| 20 | W | 1490 | OMG | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | y | 49 | 5MC | O4'-C4'-C5'-O5' |
| 24 | y | 16 | H2U | C2'-C1'-N1-C6 |
| 20 | W | 668 | A2M | C2'-C1'-N9-C8 |
| 20 | W | 1391 | OMC | C3'-C2'-O2'-CM2 |
| 20 | W | 1442 | OMU | C3'-C4'-C5'-O5' |
| 20 | W | 1639 | G7M | C3'-C4'-C5'-O5' |
| 20 | W | 428 | OMU | O4'-C1'-N1-C6 |
| 20 | W | 159 | A2M | O4'-C4'-C5'-O5' |
| 20 | W | 644 | OMG | C4'-C5'-O5'-P |
| 24 | y | 47 | H2U | O4'-C1'-N1-C2 |
| 24 | y | 37 | T6A | N11-C12-C13-ODA |
| 24 | y | 37 | T6A | N11-C12-C13-ODB |
| 20 | W | 512 | A2M | C4'-C5'-O5'-P |
| 20 | W | 1490 | OMG | C4'-C5'-O5'-P |
| 20 | W | 159 | A2M | C3'-C4'-C5'-O5' |
| 24 | y | 16 | H2U | C3'-C4'-C5'-O5' |
| 24 | y | 9 | 1MG | C2'-C1'-N9-C4 |
| 20 | W | 428 | OMU | C3'-C4'-C5'-O5' |
| 20 | W | 667 | PSU | O4'-C1'-C5-C4 |
| 20 | W | 1326 | UY1 | O4'-C1'-C5-C4 |
| 20 | W | 590 | A2M | O4'-C1'-N9-C8 |
| 20 | W | 1248 | C4J | N33-C32-C34-O36 |
| 24 | y | 9 | 1MG | C2'-C1'-N9-C8 |
| 20 | W | 428 | OMU | O4'-C1'-N1-C2 |
| 20 | W | 428 | OMU | C2'-C1'-N1-C2 |
| 20 | W | 509 | OMG | O4'-C4'-C5'-O5' |
| 24 | y | 37 | T6A | C14-C12-N11-C10 |
| 20 | W | 1081 | PSU | C4'-C5'-O5'-P |
| 24 | y | 16 | H2U | O4'-C1'-N1-C2 |
| 24 | y | 49 | 5MC | C3'-C4'-C5'-O5' |
| 24 | y | 16 | H2U | C2'-C1'-N1-C2 |
| 24 | y | 58 | 1MA | C4'-C5'-O5'-P |

There are no ring outliers.

29 monomers are involved in 34 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 20 | W | 668 | A2M | 1 | 0 |
| 24 | y | 37 | T6A | 2 | 0 |
| 24 | y | 26 | M2G | 1 | 0 |
| 20 | W | 1442 | OMU | 1 | 0 |
| 24 | y | 64 | RIA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 20 | W | 576 | A2M | 1 | 0 |
| 20 | W | 484 | A2M | 2 | 0 |
| 20 | W | 99 | A2M | 2 | 0 |
| 20 | W | 867 | OMG | 1 | 0 |
| 20 | W | 1490 | OMG | 2 | 0 |
| 20 | W | 1678 | A2M | 1 | 0 |
| 20 | W | 1851 | MA6 | 1 | 0 |
| 20 | W | 159 | A2M | 1 | 0 |
| 20 | W | 428 | OMU | 1 | 0 |
| 20 | W | 681 | PSU | 1 | 0 |
| 20 | W | 1328 | OMG | 1 | 0 |
| 20 | W | 116 | OMU | 1 | 0 |
| 24 | y | 10 | 2MG | 1 | 0 |
| 20 | W | 166 | A2M | 2 | 0 |
| 20 | W | 1447 | OMG | 1 | 0 |
| 20 | W | 509 | OMG | 1 | 0 |
| 24 | y | 49 | 5MC | 1 | 0 |
| 20 | W | 100 | PSU | 1 | 0 |
| 24 | y | 9 | 1MG | 2 | 0 |
| 20 | W | 1031 | A2M | 1 | 0 |
| 20 | W | 1639 | G7M | 1 | 0 |
| 20 | W | 1804 | OMU | 1 | 0 |
| 20 | W | 609 | PSU | 1 | 0 |
| 20 | W | 1391 | OMC | 2 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 94 ligands modelled in this entry, 94 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

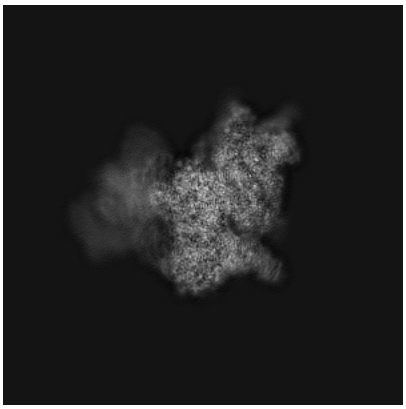
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54936. These allow visual inspection of the internal detail of the map and identification of artifacts.

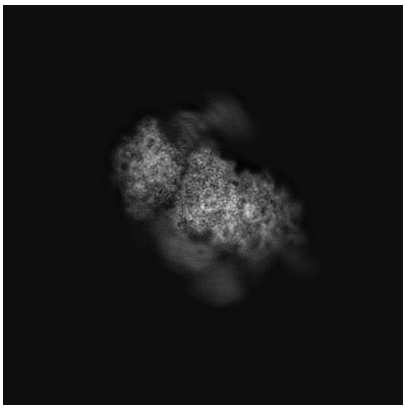
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

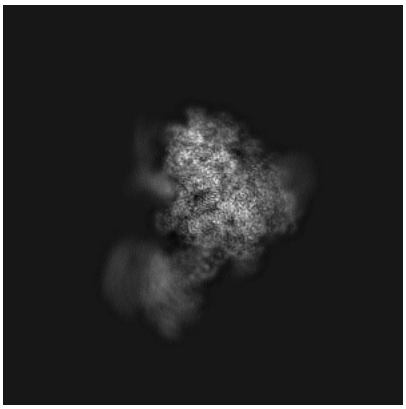
### 6.1.1 Primary map



X

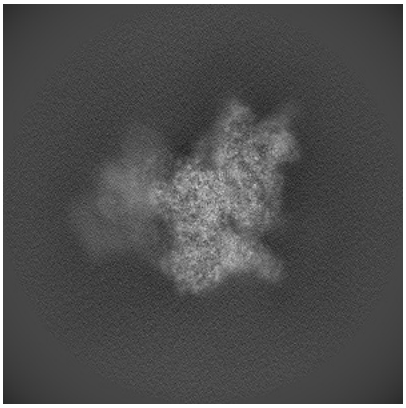


Y

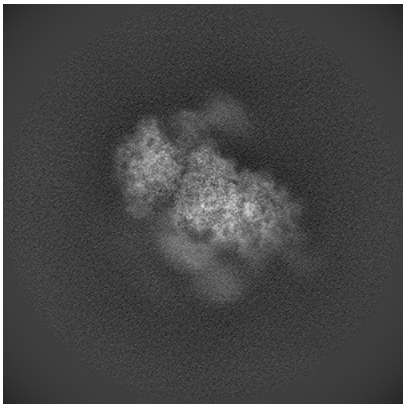


Z

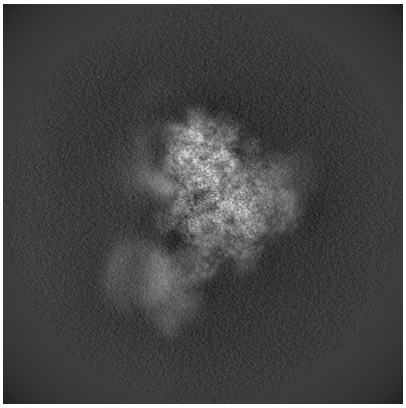
### 6.1.2 Raw map



X



Y



Z

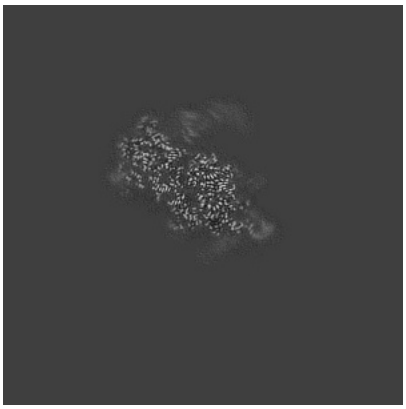
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

### 6.2.1 Primary map



X Index: 300

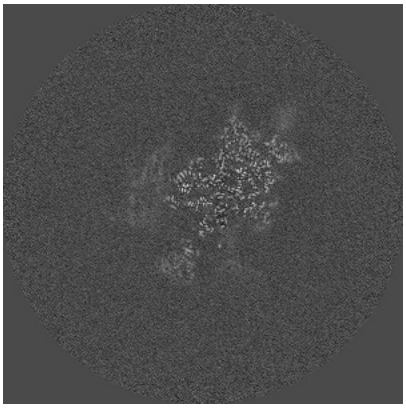


Y Index: 300

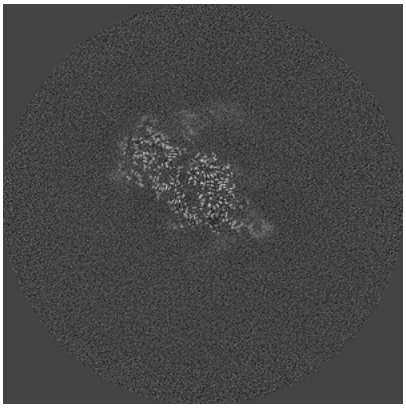


Z Index: 300

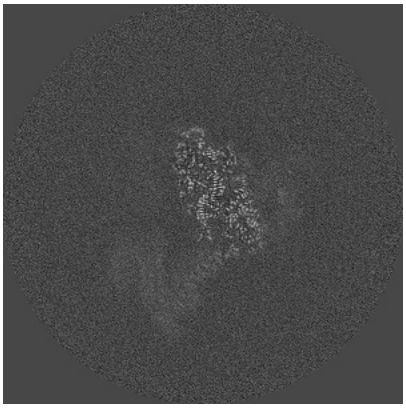
### 6.2.2 Raw map



X Index: 300



Y Index: 300

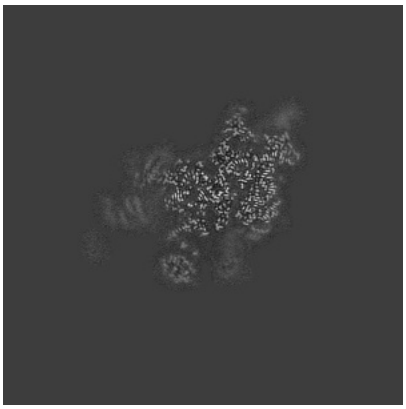


Z Index: 300

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

## 6.3 Largest variance slices (i)

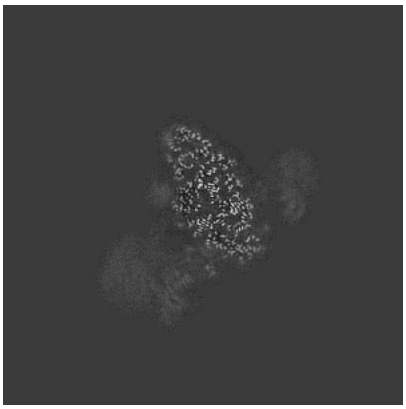
### 6.3.1 Primary map



X Index: 293

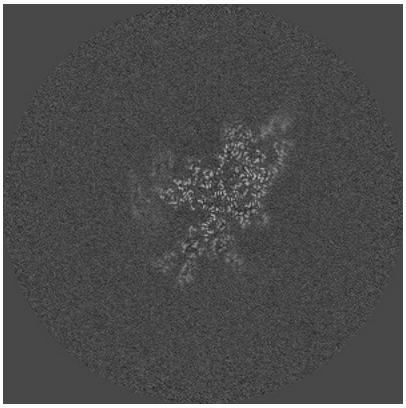


Y Index: 296

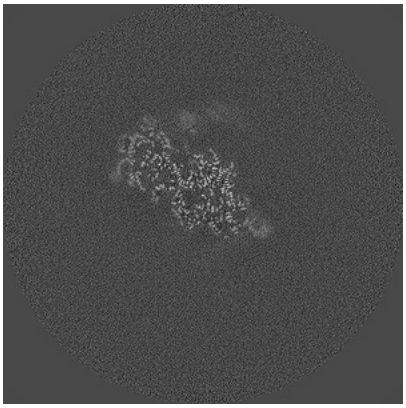


Z Index: 318

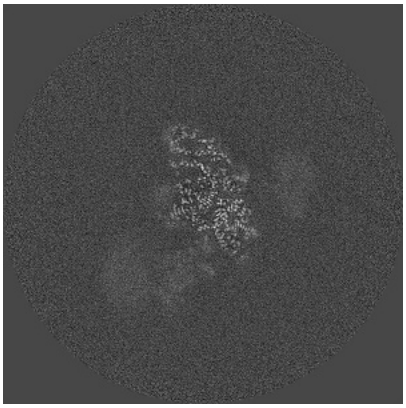
### 6.3.2 Raw map



X Index: 309



Y Index: 296

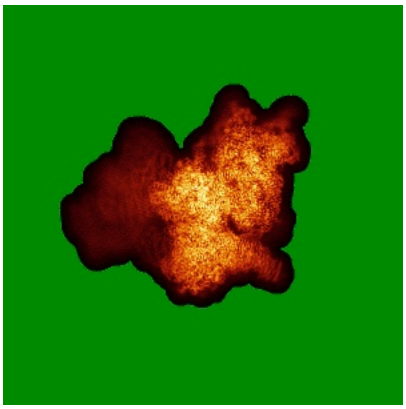


Z Index: 325

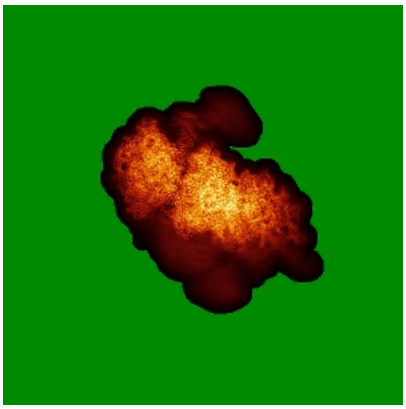
The images above show the largest variance slices of the map in three orthogonal directions.

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

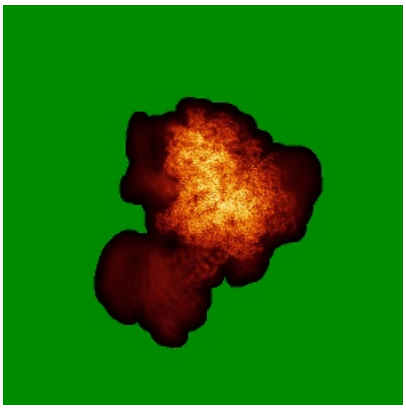
### 6.4.1 Primary map



X

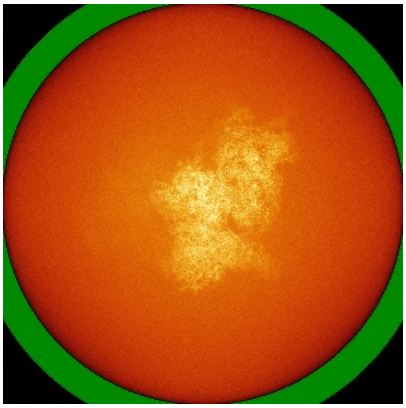


Y

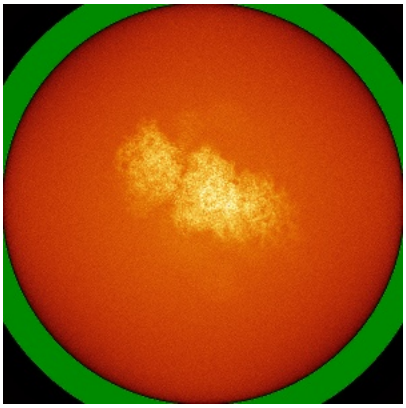


Z

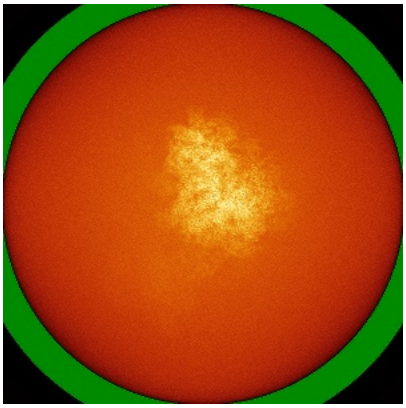
### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Orthogonal surface views (i)

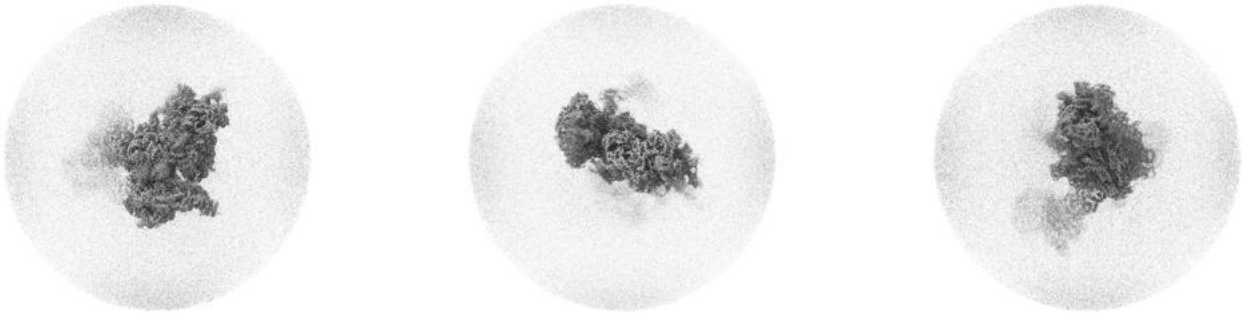
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

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

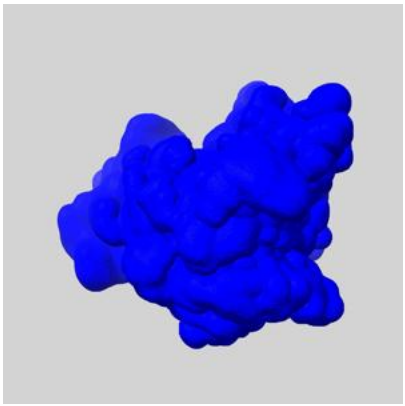
## 6.6 Mask visualisation

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

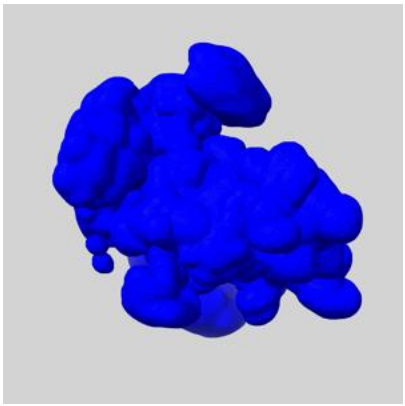
A mask typically either:

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

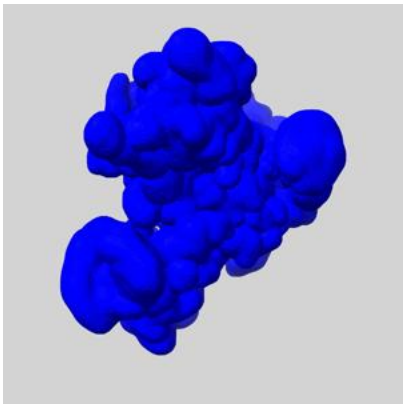
### 6.6.1 emd_54936_msk_1.map



X



Y

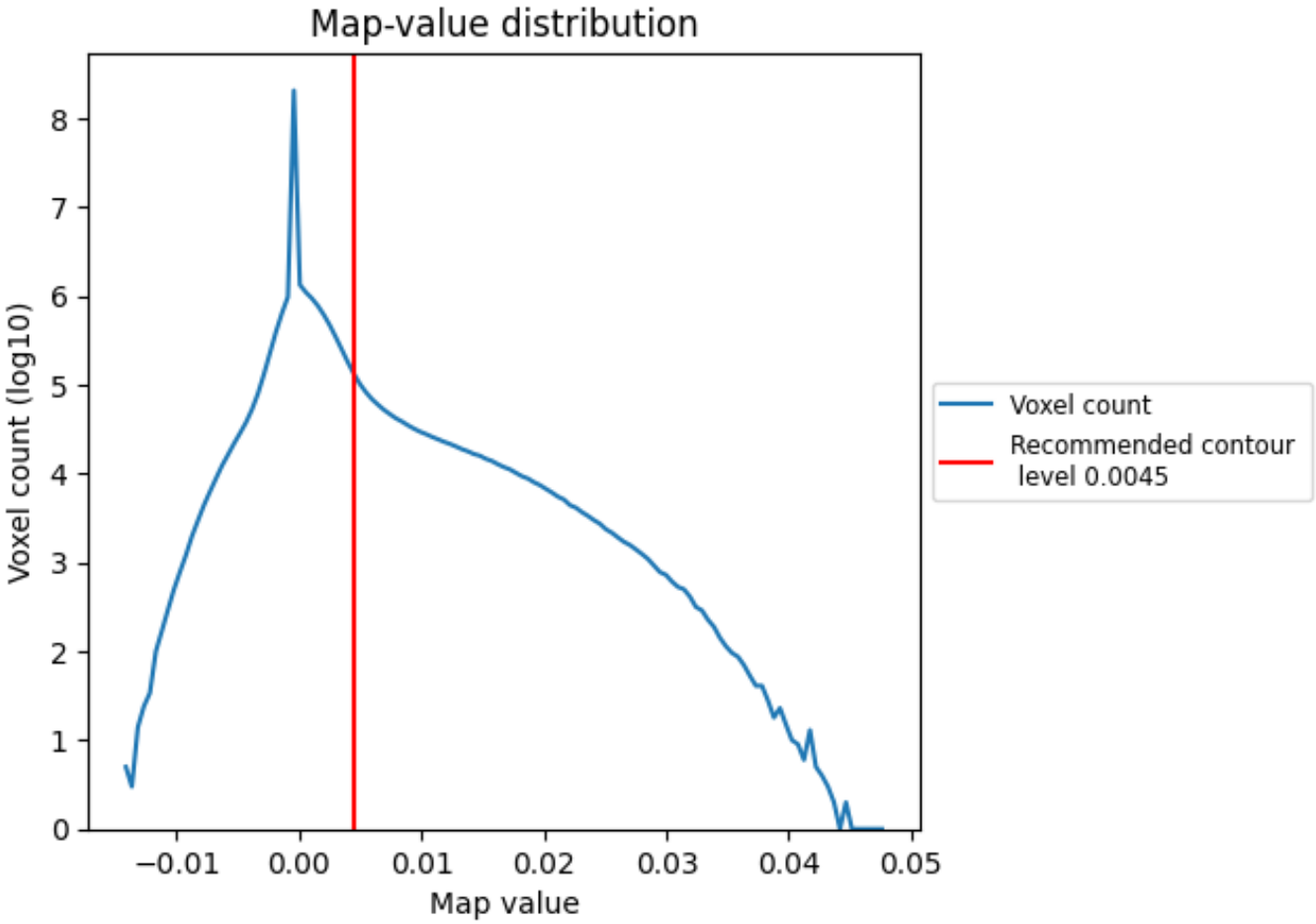


Z

# 7 Map analysis

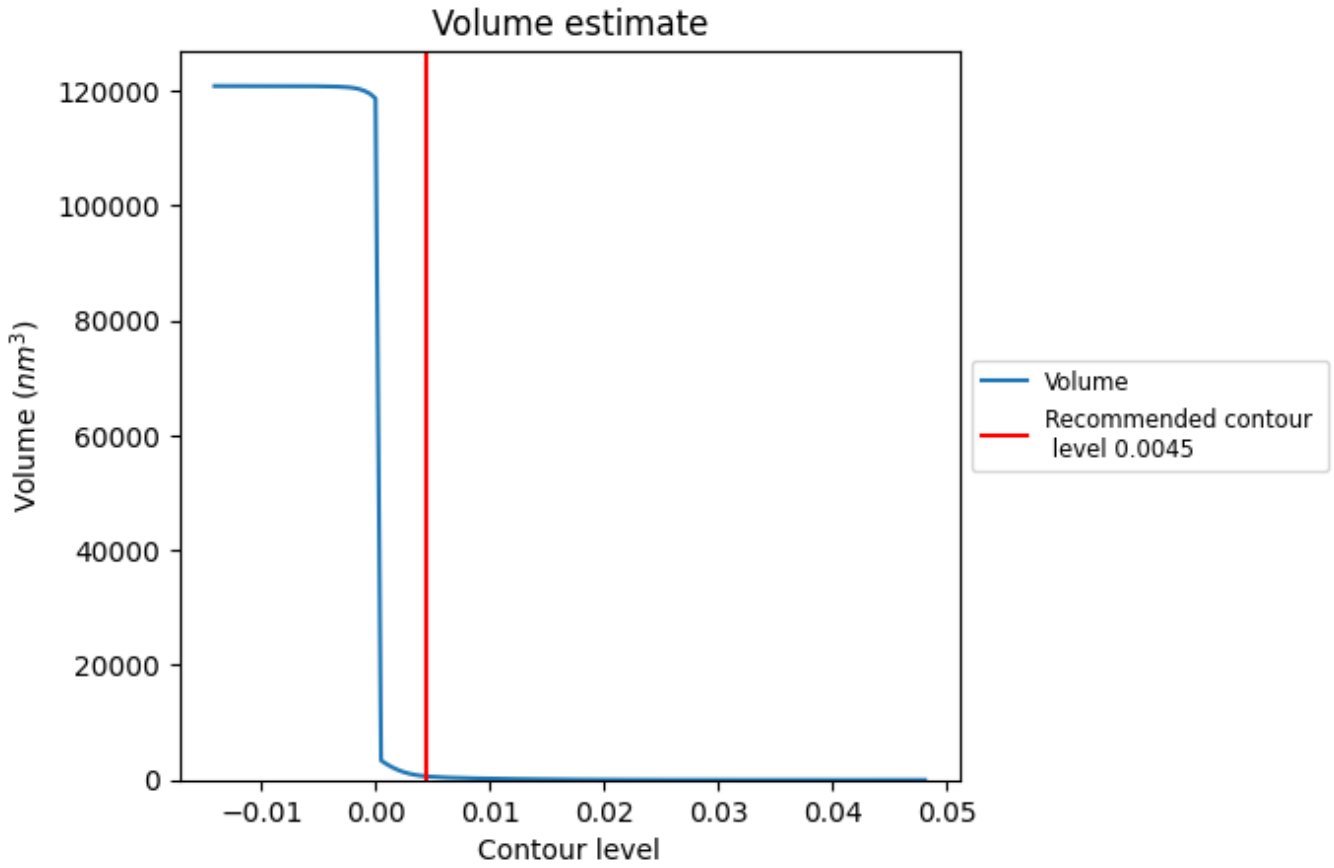
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

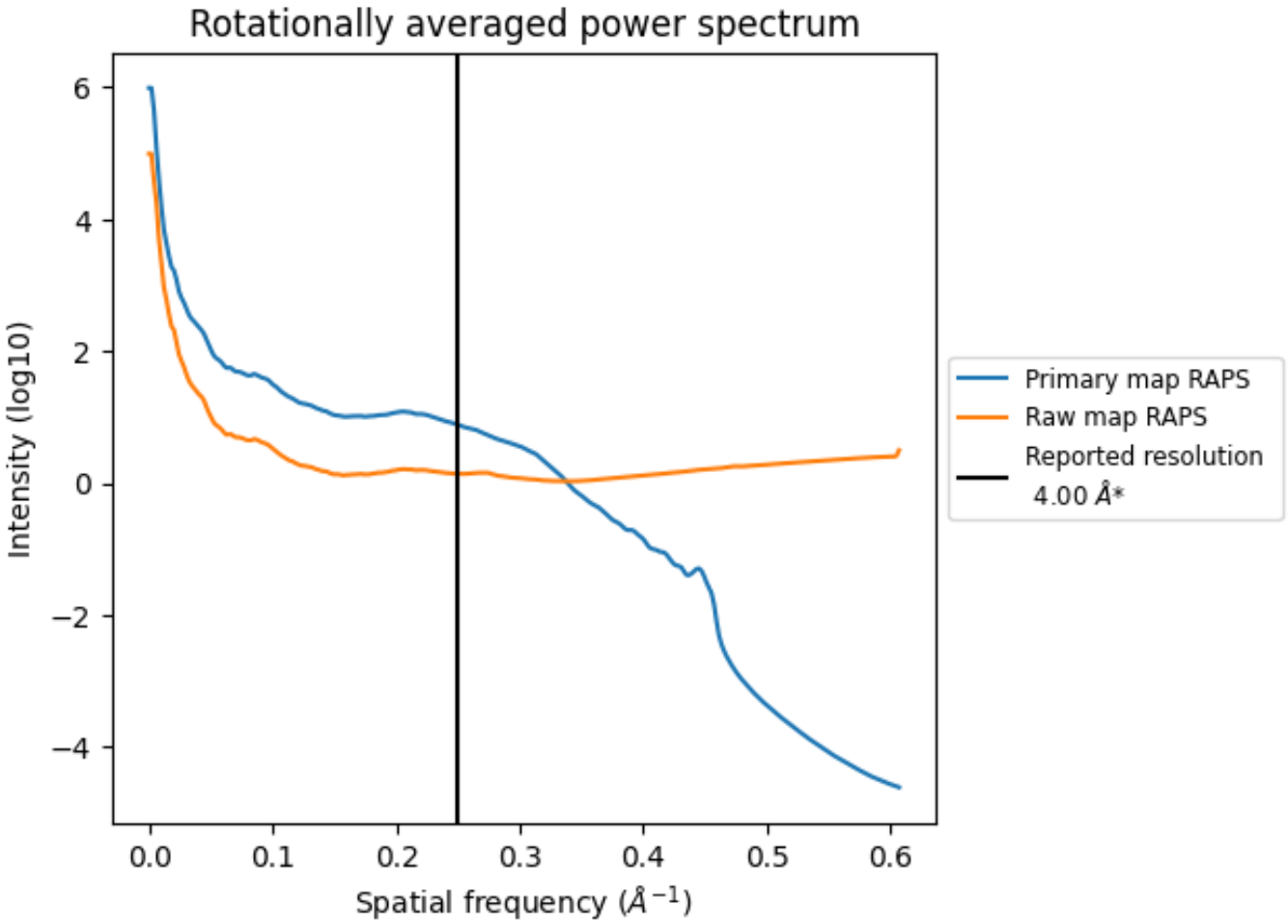
## 7.2 Volume estimate




The volume at the recommended contour level is 623 $nm^3$; this corresponds to an approximate mass of 563 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)

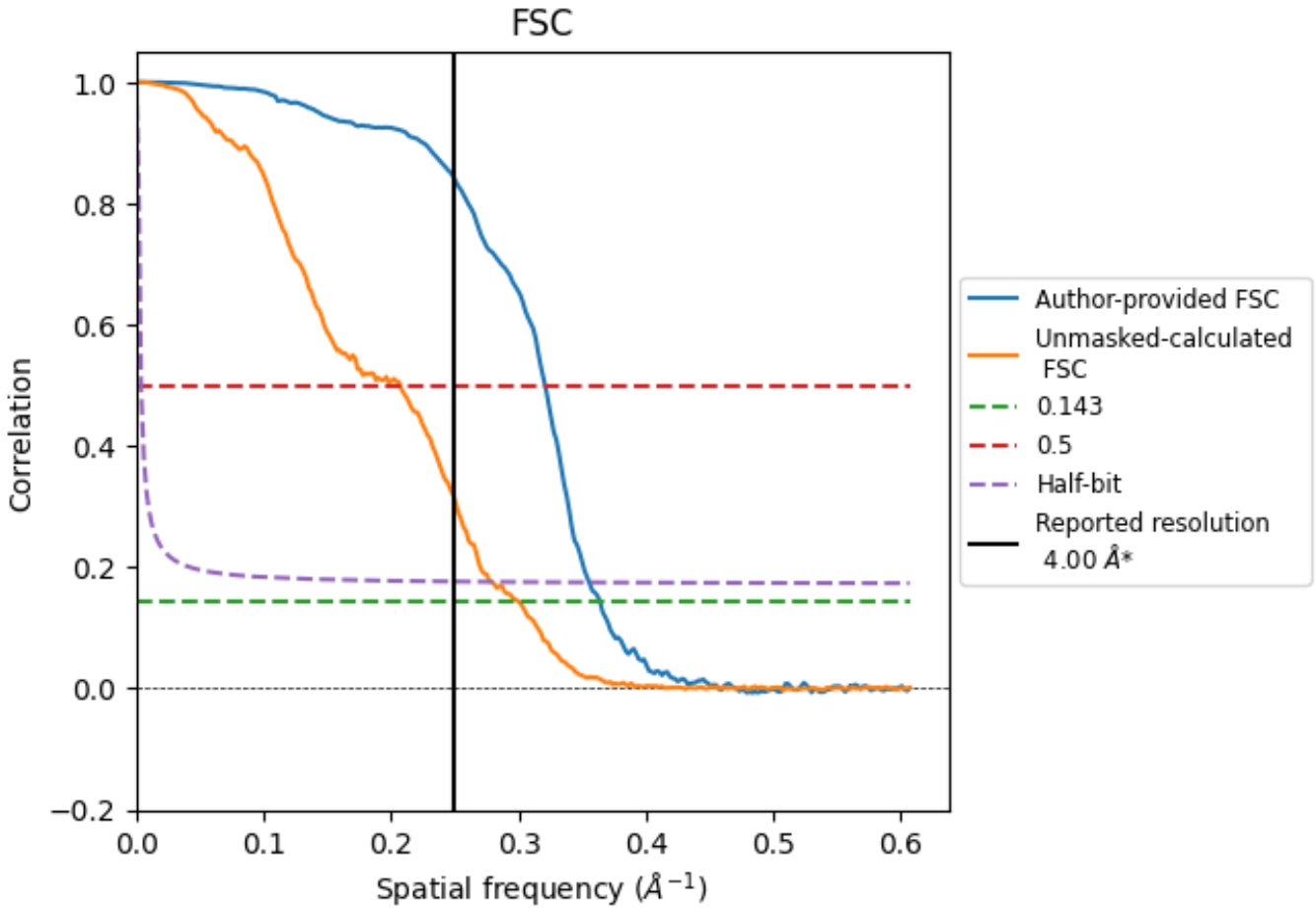



*Reported resolution corresponds to spatial frequency of 0.250 Å$^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.250 Å$^{-1}$

## 8.2 Resolution estimates (i)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.00 | - | - |
| Author-provided FSC curve | 2.75 | 3.12 | 2.81 |
| Unmasked-calculated* | 3.33 | 4.83 | 3.58 |

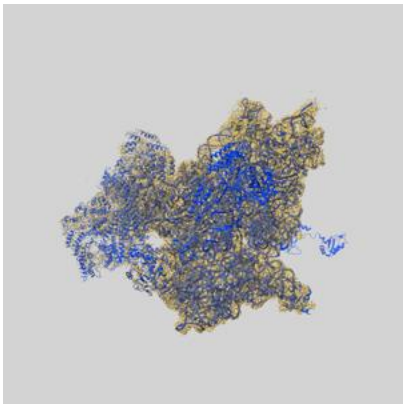
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.75 differs from the reported value 4.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.33 differs from the reported value 4.0 by more than 10 %

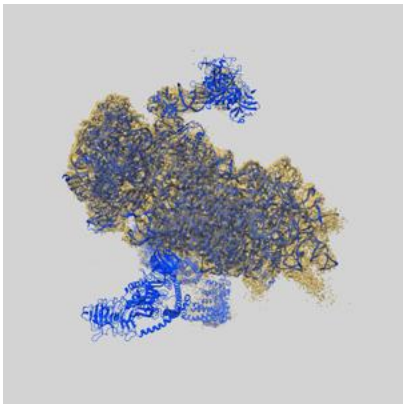
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54936 and PDB model 9SJ3. Per-residue inclusion information can be found in section 3 on page 14.

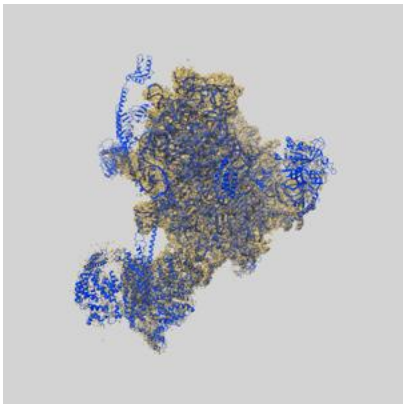
## 9.1 Map-model overlay



X



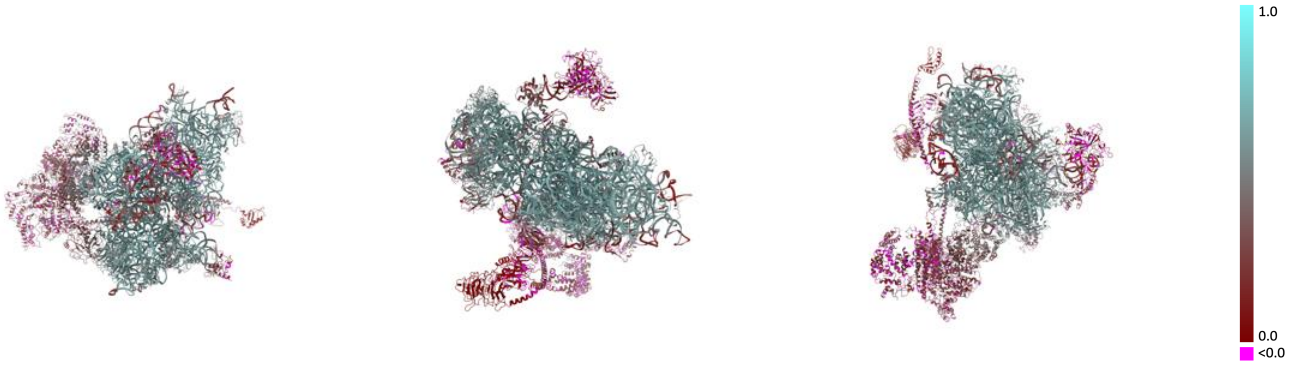
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0045 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.

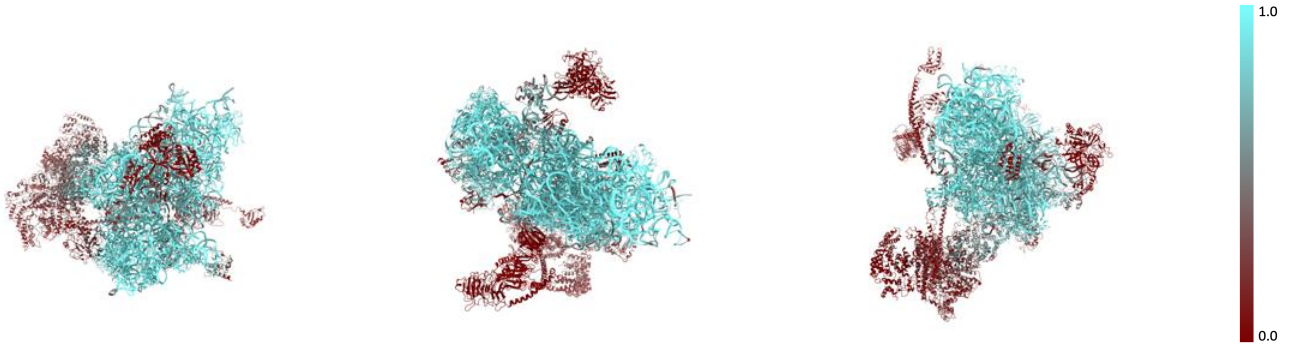
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according 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.

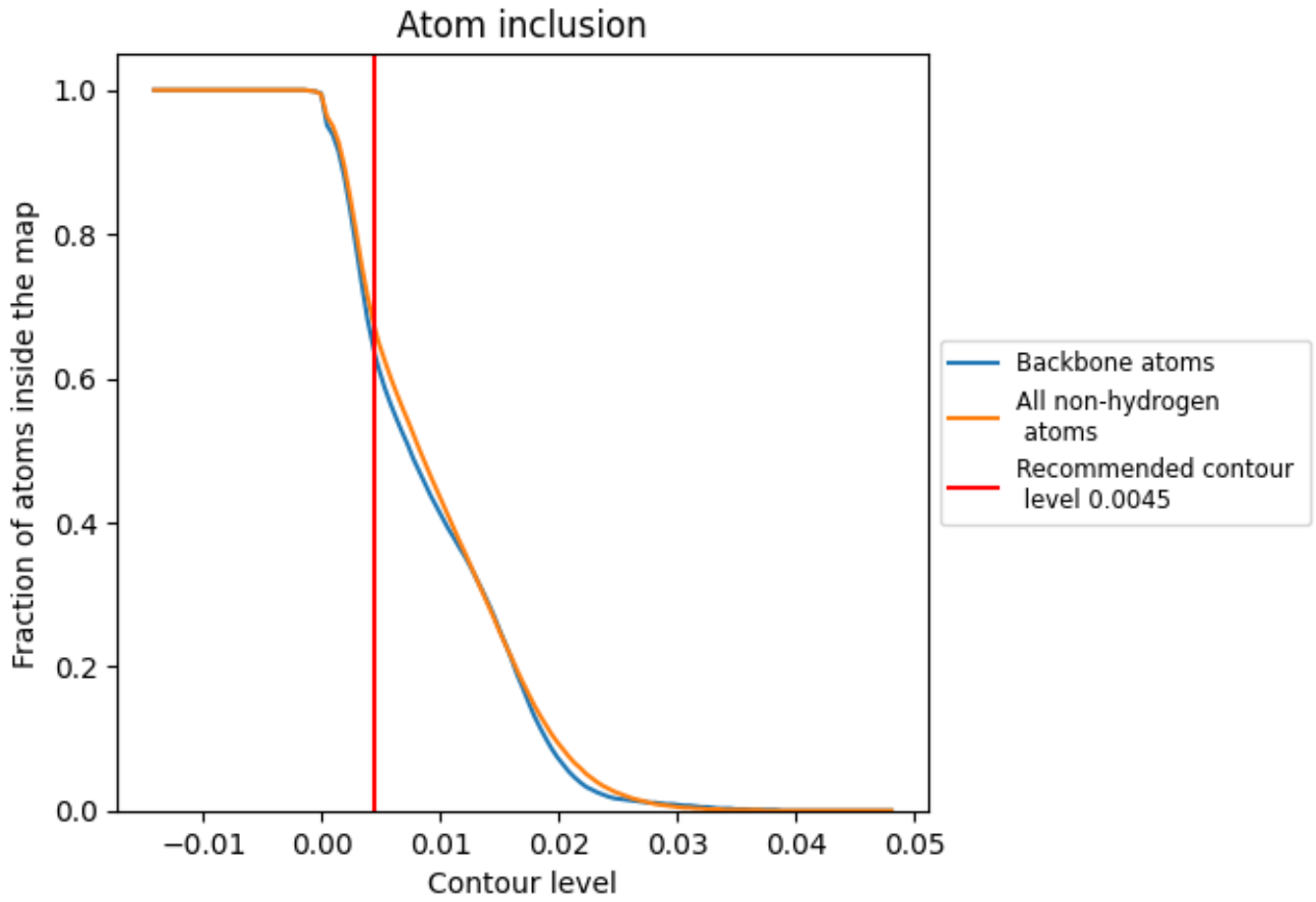
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

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 (0.0045).

## 9.4 Atom inclusion (i)




At the recommended contour level, 63% of all backbone atoms, 67% 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 (0.0045) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6690 | 0.4590 |
| 3 | 0.0290 | 0.1560 |
| 4 | 0.0730 | 0.1770 |
| 5 | 0.0410 | 0.1320 |
| 6 | 0.0740 | 0.1630 |
| 7 | 0.1400 | 0.2640 |
| 8 | 0.0450 | 0.1390 |
| 9 | 0.8610 | 0.5980 |
| A | 0.2570 | 0.2620 |
| B | 0.1000 | 0.1740 |
| D | 0.4000 | 0.3380 |
| E | 0.0140 | 0.1030 |
| F | 0.0000 | -0.0010 |
| G | 0.5030 | 0.4110 |
| H | 0.1130 | 0.2860 |
| I | 0.0040 | 0.1130 |
| J | 0.3320 | 0.3200 |
| L | 0.8020 | 0.5260 |
| M | 0.9080 | 0.6040 |
| N | 0.9340 | 0.6140 |
| O | 0.9430 | 0.6390 |
| P | 0.9330 | 0.6090 |
| Q | 0.9420 | 0.6200 |
| R | 0.9420 | 0.6240 |
| S | 0.9000 | 0.5410 |
| T | 0.9290 | 0.6140 |
| V | 0.9300 | 0.6100 |
| W | 0.9560 | 0.5880 |
| X | 0.9370 | 0.6290 |
| Y | 0.9600 | 0.6330 |
| Z | 0.9370 | 0.6280 |
| a | 0.9620 | 0.6380 |
| b | 0.8080 | 0.5750 |
| c | 0.9620 | 0.6480 |
| d | 0.9270 | 0.5910 |




*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| e | 0.9350 | 0.6100 |
| f | 0.9290 | 0.6080 |
| g | 0.9390 | 0.6170 |
| h | 0.8810 | 0.5820 |
| i | 0.8530 | 0.5450 |
| j | 0.8960 | 0.5660 |
| k | 0.8570 | 0.5320 |
| l | 0.9270 | 0.5920 |
| m | 0.8940 | 0.5680 |
| n | 0.8850 | 0.5560 |
| o | 0.9410 | 0.6310 |
| p | 0.5780 | 0.2630 |
| q | 0.4690 | 0.2730 |
| s | 0.8600 | 0.5770 |
| v | 0.8690 | 0.5730 |
| w | 0.8370 | 0.5430 |
| x | 0.2380 | 0.3250 |
| y | 0.6500 | 0.3620 |
| z | 0.4350 | 0.3690 |