# Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:00 AM EST

| | | |
|---|---|---|
| PDB ID | : | 7R81 |
| EMDB ID | : | EMD-24307 |
| Title | : | Structure of the translating Neurospora crassa ribosome arrested by cycloheximide |
| Authors | : | Shen, L.; Su, Z.; Yang, K.; Wu, C.; Becker, T.; Bell-Pedersen, D.; Zhang, J.; Sachs, M.S. |
| Deposited on | : | 2021-06-25 |
| Resolution | : | 2.70 Å(reported) |

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.

---

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

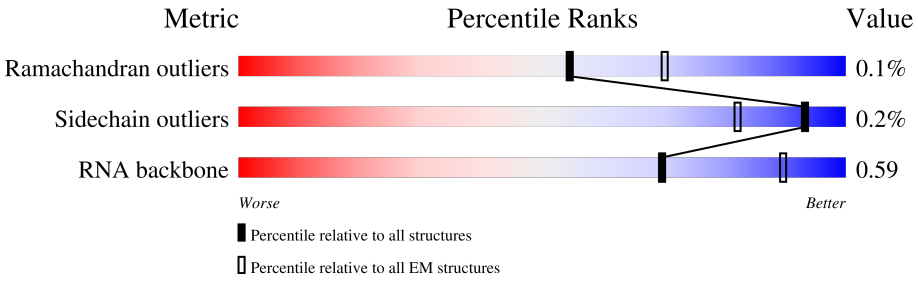
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 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 2.70 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A1 | 3338 | 6% 80% 13% 6% |
| 2 | A2 | 1796 | 25% 85% 14% |
| 3 | B1 | 120 | 92% 8% |
| 4 | B2 | 290 | 48% 72% 28% |
| 5 | C1 | 158 | 9% 87% 13% |
| 6 | C2 | 256 | 53% 82% 17% |
| 7 | D1 | 254 | 96% |
| 8 | D2 | 265 | 30% 79% 21% |

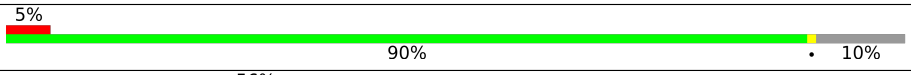
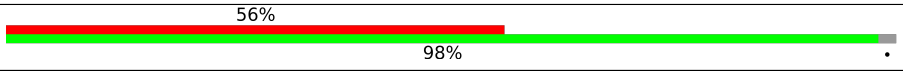
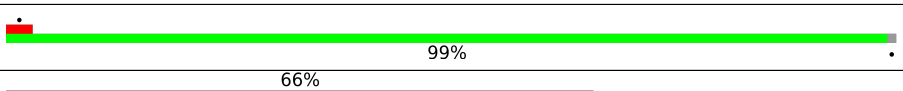
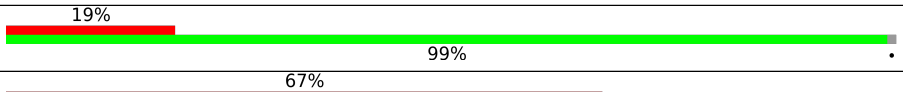
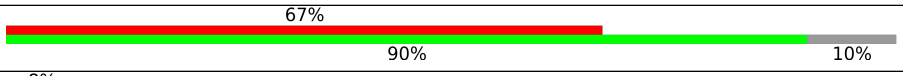
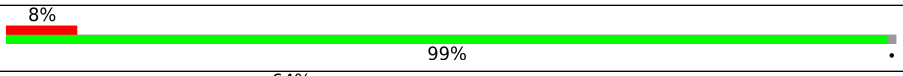
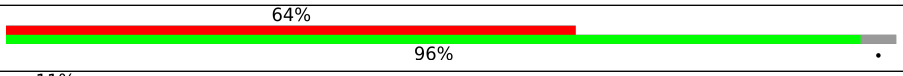
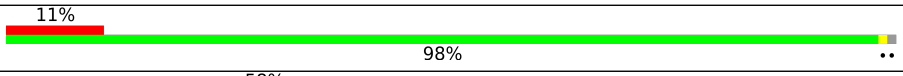
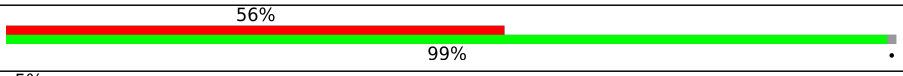
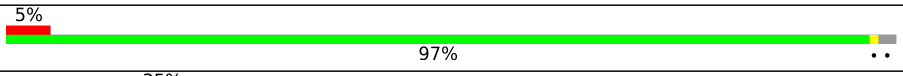
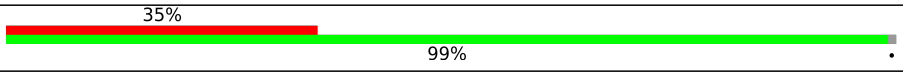
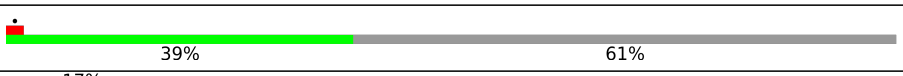
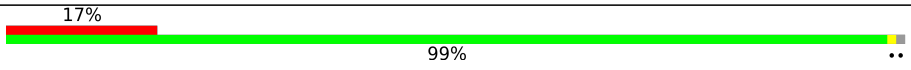
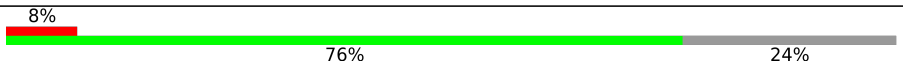
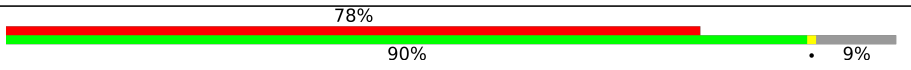
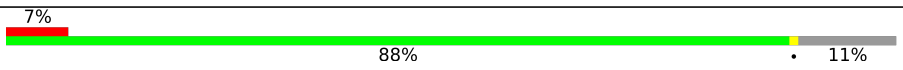
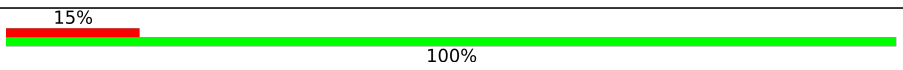
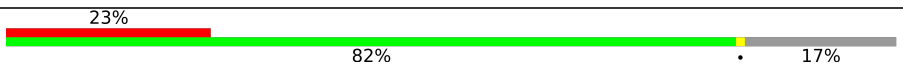
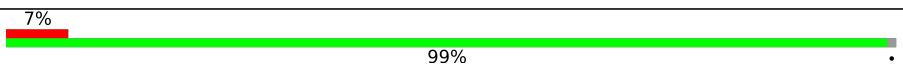
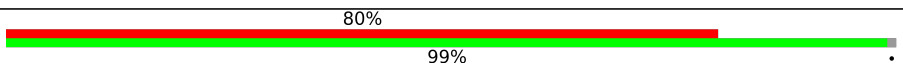
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | E1 | 392 | 98% |
| 10 | E2 | 262 | 60% 85% 15% |
| 11 | F1 | 361 | 5% 99% |
| 12 | F2 | 261 | 75% 98% |
| 13 | G1 | 301 | 28% 99% |
| 14 | G2 | 213 | 56% 95% 5% |
| 15 | H1 | 202 | 34% 96% |
| 16 | H2 | 239 | 79% 92% 7% |
| 17 | I1 | 248 | 10% 99% |
| 18 | I2 | 202 | 82% 92% 6% |
| 19 | J1 | 262 | 18% 90% 10% |
| 20 | J2 | 202 | 30% 91% 9% |
| 21 | K1 | 193 | 10% 98% |
| 22 | K2 | 190 | 60% 92% 8% |
| 23 | L1 | 221 | 15% 98% |
| 24 | L2 | 163 | 47% 55% 45% |
| 25 | M1 | 174 | 32% 94% 5% |
| 26 | M2 | 161 | 17% 81% 19% |
| 27 | N1 | 214 | 15% 99% |
| 28 | N2 | 147 | 79% 79% 21% |
| 29 | O1 | 142 | 15% 99% |
| 30 | O2 | 151 | 48% 99% |
| 31 | P1 | 203 | 100% |
| 32 | P2 | 150 | 25% 84% 16% |
| 33 | Q1 | 231 | 86% 14% |

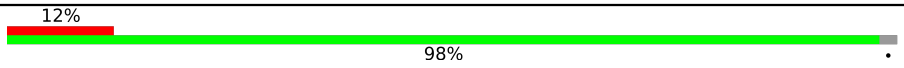
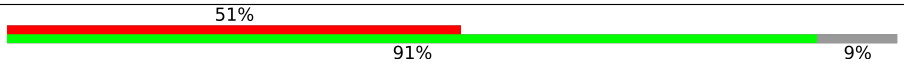
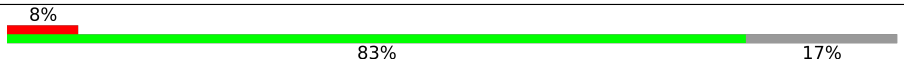
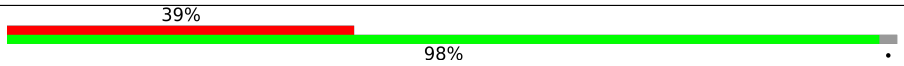
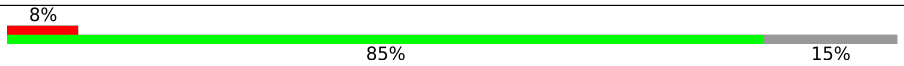
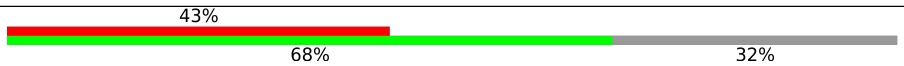
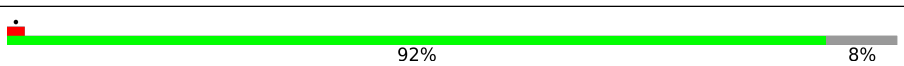
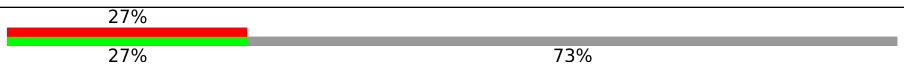
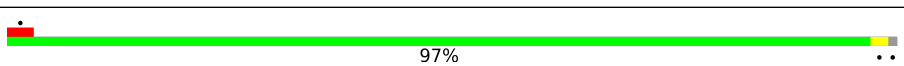
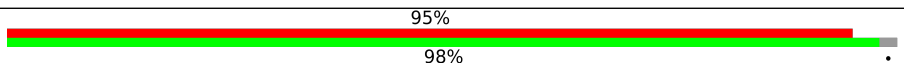
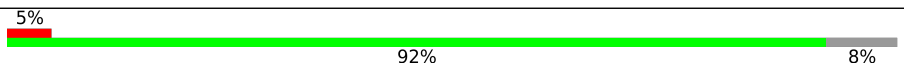
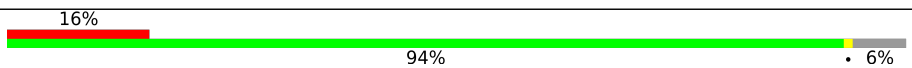
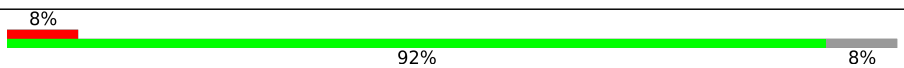
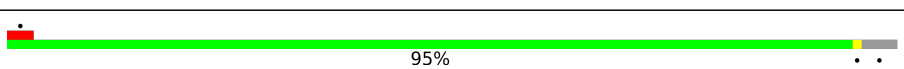
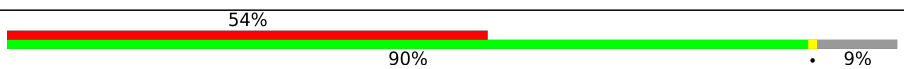
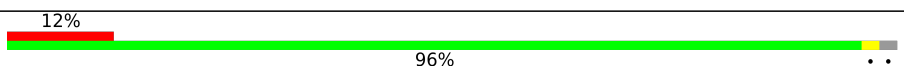
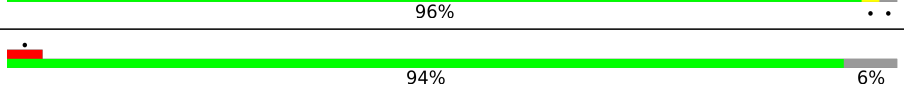
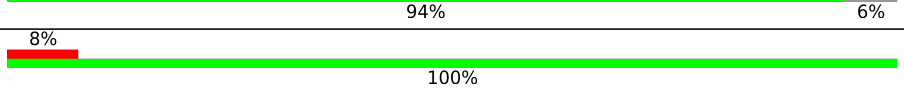
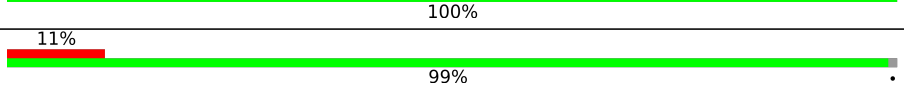
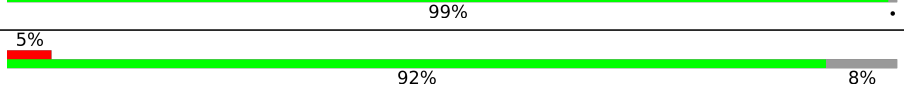
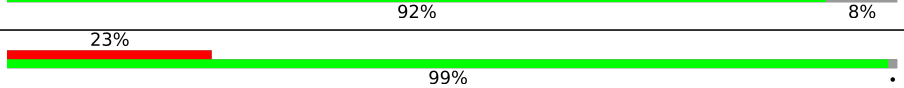
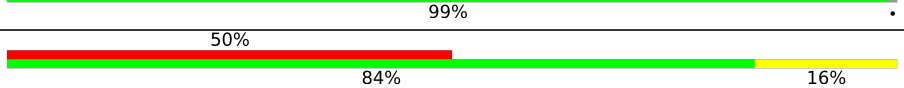
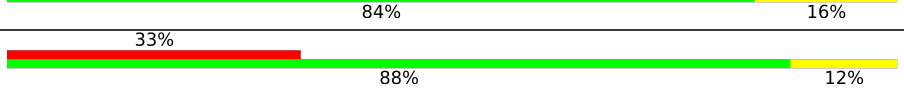
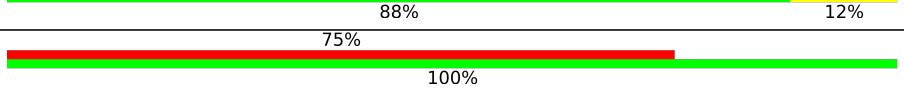
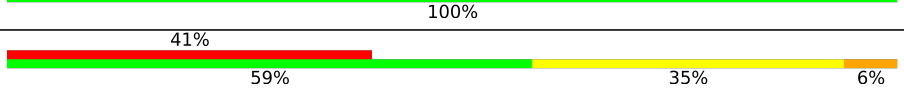
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | Q2 | 152 |   |
| 35 | R1 | 186 |   |
| 36 | R2 | 142 |   |
| 37 | S1 | 183 |   |
| 38 | S2 | 146 |   |
| 39 | T1 | 192 |   |
| 40 | T2 | 156 |   |
| 41 | U1 | 174 |   |
| 42 | U2 | 149 |   |
| 43 | V1 | 160 |   |
| 44 | V2 | 117 |   |
| 45 | W1 | 126 |   |
| 46 | W2 | 87 |   |
| 47 | X1 | 139 |   |
| 48 | X2 | 130 |   |
| 49 | Y1 | 156 |   |
| 50 | Y2 | 145 |   |
| 51 | Z1 | 156 |   |
| 52 | Z2 | 136 |   |
| 53 | a1 | 136 |   |
| 54 | a2 | 97 |   |
| 55 | b1 | 135 |   |
| 56 | b2 | 119 |   |
| 57 | c1 | 149 |   |
| 58 | c2 | 82 |   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 59 | d1 | 65 |   |
| 60 | d2 | 68 |   |
| 61 | e1 | 109 |   |
| 62 | e2 | 56 |   |
| 63 | f1 | 122 |   |
| 64 | f2 | 63 |   |
| 65 | g1 | 131 |   |
| 66 | g2 | 154 |   |
| 67 | h1 | 109 |   |
| 68 | h2 | 316 |   |
| 69 | i1 | 117 |   |
| 70 | j1 | 125 |   |
| 71 | k1 | 104 |   |
| 72 | l1 | 92 |   |
| 73 | m1 | 80 |   |
| 74 | n1 | 51 |   |
| 75 | o1 | 52 |   |
| 76 | p1 | 25 |   |
| 77 | q1 | 106 |   |
| 78 | r1 | 92 |   |
| 79 | s1 | 150 |   |
| 80 | t1 | 76 |   |
| 80 | u1 | 76 |   |
| 81 | v1 | 4 |   |
| 82 | w1 | 17 |   |

# 2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 202730 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 26S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | A1 | 3123 | 66761 | 29810 | 12043 | 21785 | 3123 | 0 | 0 |

- Molecule 2 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | A2 | 1769 | 37713 | 16852 | 6713 | 12379 | 1769 | 0 | 0 |

- Molecule 3 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 3 | B1 | 120 | 2554 | 1141 | 456 | 837 | 120 | 0 | 0 |

- Molecule 4 is a protein called 40S ribosomal protein S0.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | B2 | 209 | 1635 | 1045 | 289 | 294 | 7 | 0 | 0 |

- Molecule 5 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | C1 | 158 | 3360 | 1503 | 593 | 1106 | 158 | 0 | 0 |

- Molecule 6 is a protein called 40S ribosomal protein S1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | C2 | 212 | 1706 | 1082 | 314 | 306 | 4 | 0 | 0 |

- Molecule 7 is a protein called 60S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | D1 | 245 | Total | C | N | O | S | 0 | 0 |
| | | | 1855 | 1158 | 368 | 326 | 3 | | |

- Molecule 8 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | D2 | 210 | Total | C | N | O | S | 0 | 0 |
| | | | 1612 | 1036 | 282 | 291 | 3 | | |

- Molecule 9 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | E1 | 385 | Total | C | N | O | S | 0 | 0 |
| | | | 3058 | 1946 | 573 | 529 | 10 | | |

- Molecule 10 is a protein called Cytoplasmic ribosomal protein 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | E2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1750 | 1102 | 319 | 322 | 7 | | |

- Molecule 11 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | F1 | 360 | Total | C | N | O | S | 0 | 0 |
| | | | 2727 | 1711 | 524 | 487 | 5 | | |

- Molecule 12 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | F2 | 256 | Total | C | N | O | S | 0 | 0 |
| | | | 2048 | 1299 | 385 | 357 | 7 | | |

- Molecule 13 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | G1 | 300 | Total | C | N | O | S | 0 | 0 |
| | | | 2423 | 1527 | 426 | 467 | 3 | | |

- Molecule 14 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | G2 | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1586 | 987 | 298 | 294 | 7 | | |

- Molecule 15 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | H1 | 194 | Total | C | N | O | S | 0 | 0 |
| | | | 1521 | 969 | 277 | 274 | 1 | | |

- Molecule 16 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | H2 | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1782 | 1116 | 351 | 310 | 5 | | |

- Molecule 17 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | I1 | 247 | Total | C | N | O | S | 0 | 0 |
| | | | 2016 | 1291 | 369 | 352 | 4 | | |

- Molecule 18 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 18 | I2 | 189 | Total | C | N | O | 0 | 0 |
| | | | 1514 | 955 | 287 | 272 | | |

- Molecule 19 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | J1 | 236 | Total | C | N | O | S | 0 | 0 |
| | | | 1882 | 1206 | 347 | 323 | 6 | | |

- Molecule 20 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | J2 | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1464 | 910 | 293 | 259 | 2 | | |

- Molecule 21 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | K1 | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1504 | 952 | 275 | 273 | 4 | | |

- Molecule 22 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | K2 | 174 | Total | C | N | O | S | 0 | 0 |
| | | | 1420 | 900 | 284 | 234 | 2 | | |

- Molecule 23 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | L1 | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1751 | 1106 | 340 | 295 | 10 | | |

- Molecule 24 is a protein called Probable 40s ribosomal protein s10-b.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | L2 | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 490 | 125 | 135 | 3 | | |

- Molecule 25 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | M1 | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1341 | 839 | 260 | 236 | 6 | | |

- Molecule 26 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | M2 | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1068 | 682 | 206 | 177 | 3 | | |

- Molecule 27 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | N1 | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1675 | 1046 | 336 | 291 | 2 | | |

- Molecule 28 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | N2 | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 907 | 566 | 163 | 169 | 9 | | |

- Molecule 29 is a protein called Ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | O1 | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1109 | 702 | 212 | 194 | 1 | | |

- Molecule 30 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | O2 | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1179 | 750 | 218 | 208 | 3 | | |

- Molecule 31 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | P1 | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1702 | 1063 | 359 | 278 | 2 | | |

- Molecule 32 is a protein called 40S ribosomal protein S14 (uS11).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | P2 | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 938 | 574 | 186 | 173 | 5 | | |

- Molecule 33 is a protein called 60S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | Q1 | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1595 | 1022 | 301 | 267 | 5 | | |

- Molecule 34 is a protein called Ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | Q2 | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1007 | 639 | 189 | 175 | 4 | | |

- Molecule 35 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | R1 | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1322 | 819 | 269 | 231 | 3 | | |

- Molecule 36 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | R2 | 139 | Total | C | N | O | S | 0 | 0 |
| | | | 1089 | 700 | 200 | 187 | 2 | | |

- Molecule 37 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | S1 | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1445 | 912 | 291 | 240 | 2 | | |

- Molecule 38 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | S2 | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1005 | 636 | 182 | 185 | 2 | | |

- Molecule 39 is a protein called Ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | T1 | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1563 | 963 | 331 | 265 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | T2 | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1139 | 709 | 227 | 201 | 2 | | |

- Molecule 41 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | U1 | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1429 | 920 | 268 | 237 | 4 | | |

- Molecule 42 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | U2 | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1124 | 701 | 221 | 201 | 1 | | |

- Molecule 43 is a protein called Ribosomal protein Srp1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | V1 | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1276 | 807 | 246 | 221 | 2 | | |

- Molecule 44 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | V2 | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 786 | 498 | 145 | 140 | 3 | | |

- Molecule 45 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | W1 | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 530 | 141 | 144 | 1 | | |

- Molecule 46 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | W2 | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 668 | 408 | 127 | 130 | 3 | | |

- Molecule 47 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | X1 | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1007 | 638 | 186 | 176 | 7 | | |

- Molecule 48 is a protein called 40S ribosomal protein S22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | X2 | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1035 | 659 | 192 | 180 | 4 | | |

- Molecule 49 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | Y1 | 61 | Total | C | N | O | S | 0 | 0 |
| | | | 525 | 334 | 104 | 86 | 1 | | |

- Molecule 50 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | Y2 | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1113 | 701 | 218 | 192 | 2 | | |

- Molecule 51 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 51 | Z1 | 118 | Total | C | N | O | 0 | 0 |
| | | | 941 | 602 | 170 | 169 | | |

- Molecule 52 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | Z2 | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1003 | 630 | 197 | 174 | 2 | | |

- Molecule 53 is a protein called Ribosomal protein L26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | a1 | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 961 | 596 | 189 | 175 | 1 | | |

- Molecule 54 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | a2 | 71 | Total | C | N | O | S | 0 | 0 |
| | | | 565 | 356 | 105 | 102 | 2 | | |

- Molecule 55 is a protein called 60S ribosomal protein L27 (eL27).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | b1 | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1108 | 707 | 206 | 191 | 4 | | |

- Molecule 56 is a protein called 40S ribosomal protein S26E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | b2 | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 793 | 488 | 167 | 131 | 7 | | |

- Molecule 57 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | c1 | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1166 | 738 | 235 | 191 | 2 | | |

- Molecule 58 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 58 | c2 | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 611 | 386 | 110 | 108 | 7 | | |

- Molecule 59 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 59 | d1 | 64 | Total | C | N | O | 0 | 0 |
| | | | 518 | 315 | 113 | 90 | | |

- Molecule 60 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 60 | d2 | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 491 | 302 | 98 | 90 | 1 | | |

- Molecule 61 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | e1 | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 681 | 433 | 118 | 125 | 5 | | |

- Molecule 62 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | e2 | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 446 | 271 | 94 | 77 | 4 | | |

- Molecule 63 is a protein called 60s ribosomal protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 63 | f1 | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 854 | 540 | 166 | 145 | 3 | | |

- Molecule 64 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 64 | f2 | 43 | Total | C | N | O | 0 | 0 |
| | | | 346 | 216 | 72 | 58 | | |

- Molecule 65 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 65 | g1 | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 973 | 609 | 199 | 159 | 6 | | |

- Molecule 66 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 66 | g2 | 41 | Total | C | N | O | S | 0 | 0 |
| | | | 328 | 204 | 59 | 61 | 4 | | |

- Molecule 67 is a protein called 60S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 67 | h1 | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 853 | 541 | 167 | 144 | 1 | | |

- Molecule 68 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 68 | h2 | 310 | Total | C | N | O | S | 0 | 0 |
| | | | 2429 | 1528 | 424 | 468 | 9 | | |

- Molecule 69 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 69 | i1 | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 853 | 530 | 174 | 145 | 4 | | |

- Molecule 70 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 70 | j1 | 118 | Total<br>967 | C<br>613 | N<br>192 | O<br>162 | 0 | 0 |

- Molecule 71 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 71 | k1 | 96 | Total<br>760 | C<br>473 | N<br>162 | O<br>125 | 0 | 0 |

- Molecule 72 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | l1 | 88 | Total<br>691 | C<br>424 | N<br>147 | O<br>116 | S<br>4 | 0 | 0 |

- Molecule 73 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 73 | m1 | 73 | Total<br>585 | C<br>373 | N<br>107 | O<br>103 | S<br>2 | 0 | 0 |

- Molecule 74 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 74 | n1 | 50 | Total<br>435 | C<br>274 | N<br>97 | O<br>64 | 0 | 0 |

- Molecule 75 is a protein called 60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 75 | o1 | 49 | Total<br>395 | C<br>245 | N<br>83 | O<br>61 | S<br>6 | 0 | 0 |

- Molecule 76 is a protein called hypothetical protein NCU16635 (eL41).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 76 | p1 | 25 | Total<br>235 | C<br>143 | N<br>63 | O<br>27 | S<br>2 | 0 | 0 |

- Molecule 77 is a protein called 60S ribosomal protein L44.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 77 | q1 | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 827 | 522 | 163 | 137 | 5 | | |

- Molecule 78 is a protein called 60S ribosomal protein L43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 78 | r1 | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 129 | 112 | 5 | | |

- Molecule 79 is a protein called Ribosomal_L28e domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 79 | s1 | 149 | Total | C | N | O | 0 | 0 |
| | | | 1118 | 697 | 222 | 199 | | |

- Molecule 80 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 80 | t1 | 76 | Total | C | N | O | P | 0 | 0 |
| | | | 1621 | 723 | 291 | 531 | 76 | | |
| 80 | u1 | 76 | Total | C | N | O | P | 0 | 0 |
| | | | 1621 | 723 | 291 | 531 | 76 | | |

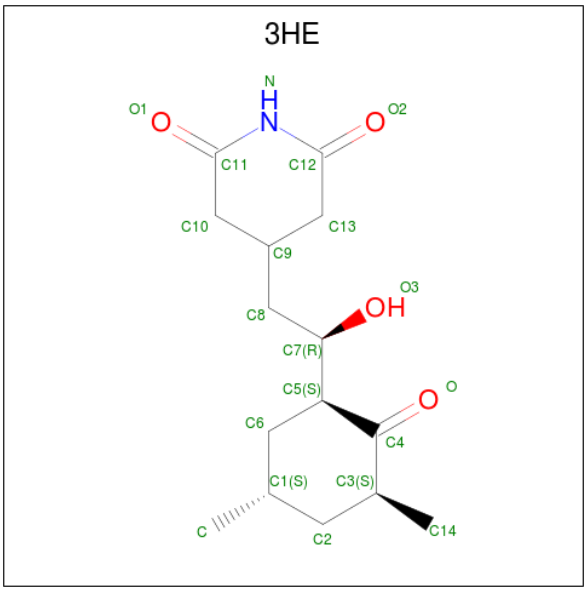
- Molecule 81 is a protein called Nascent peptide.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 81 | v1 | 4 | Total | C | N | O | 0 | 0 |
| | | | 20 | 12 | 4 | 4 | | |

- Molecule 82 is a RNA chain called mRNA.

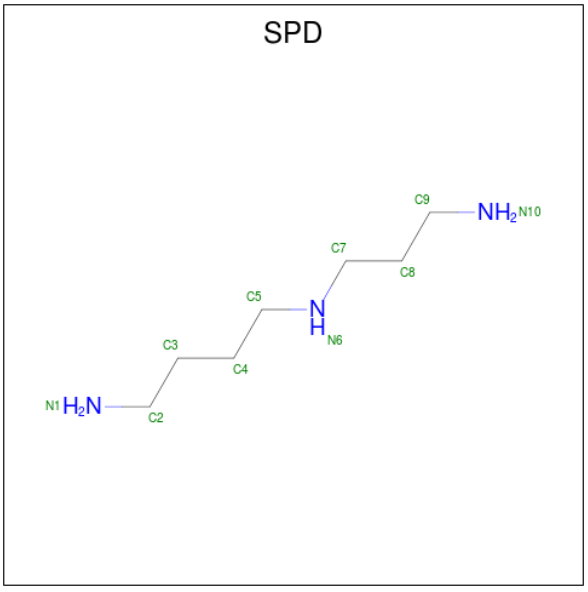
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 82 | w1 | 17 | Total | C | N | O | P | 0 | 0 |
| | | | 340 | 153 | 34 | 136 | 17 | | |

- Molecule 83 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: $C_{15}H_{23}NO_4$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 83 | A1 | 1 | Total | C | N | O | 0 |
| | | | 20 | 15 | 1 | 4 | |

- Molecule 84 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 84 | A1 | 1 | Total | C | N | 0 |
| | | | 10 | 7 | 3 | |

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

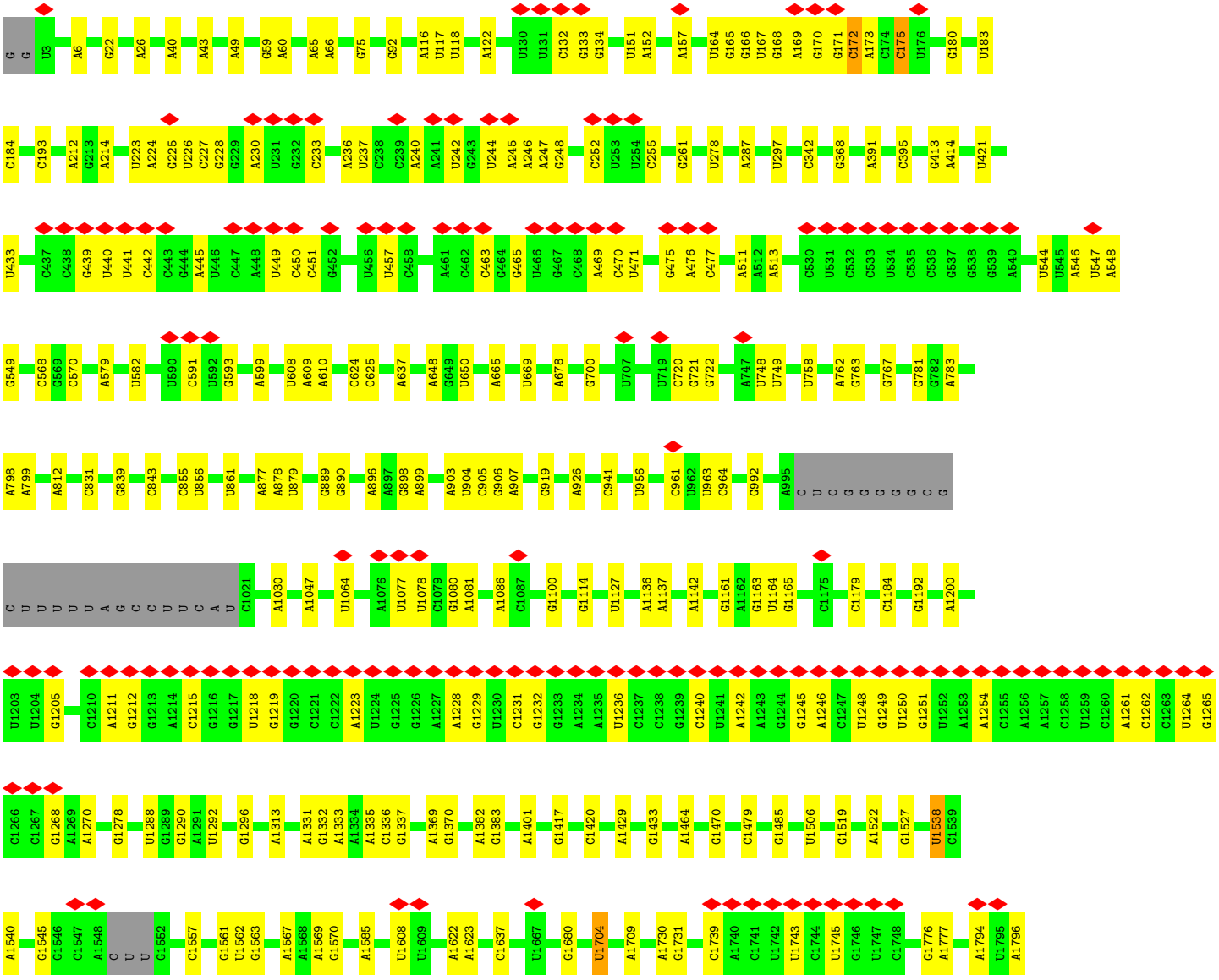
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 85 | A1 | 180 | Total Mg<br>180 180 | 0 |
| 85 | A2 | 74 | Total Mg<br>74 74 | 0 |
| 85 | F1 | 1 | Total Mg<br>1 1 | 0 |
| 85 | F2 | 1 | Total Mg<br>1 1 | 0 |
| 85 | V1 | 1 | Total Mg<br>1 1 | 0 |
| 85 | Y2 | 1 | Total Mg<br>1 1 | 0 |
| 85 | i1 | 1 | Total Mg<br>1 1 | 0 |
| 85 | u1 | 1 | Total Mg<br>1 1 | 0 |

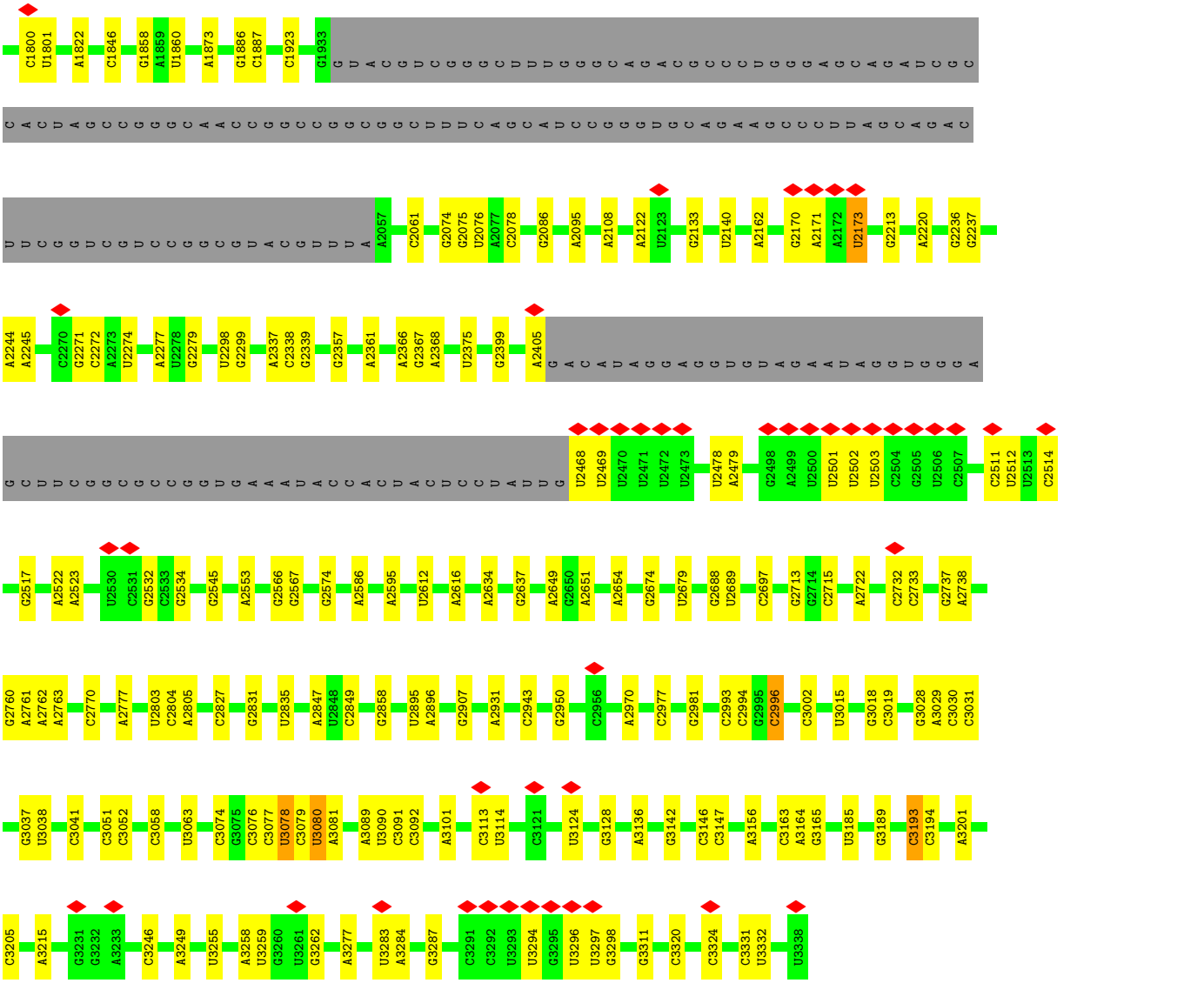
# 3 Residue-property plots (i)

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: 26S rRNA

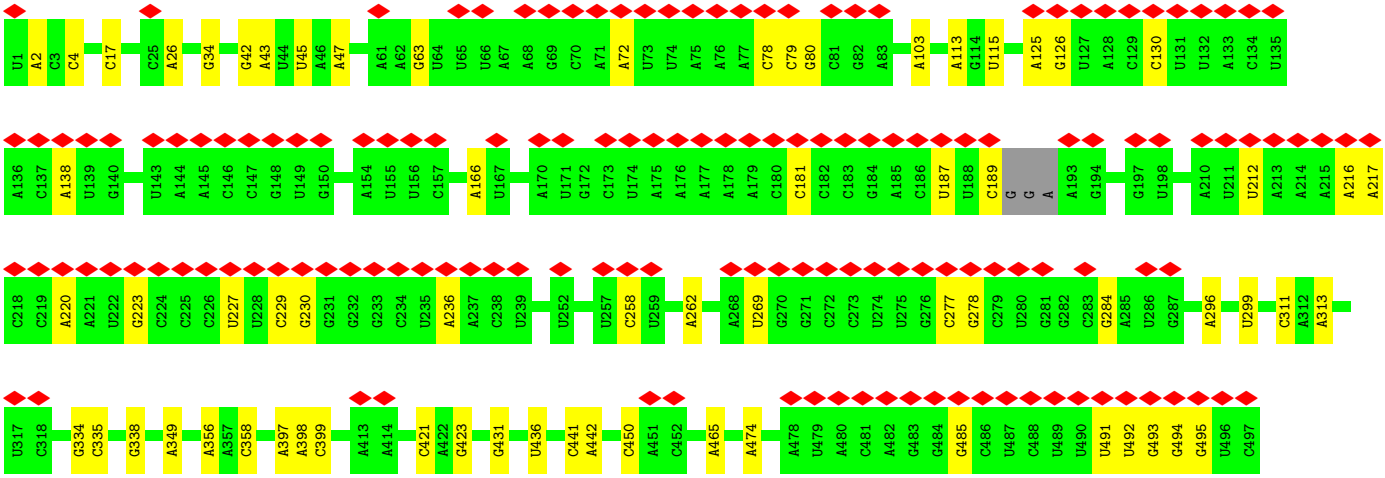
Chain A1:

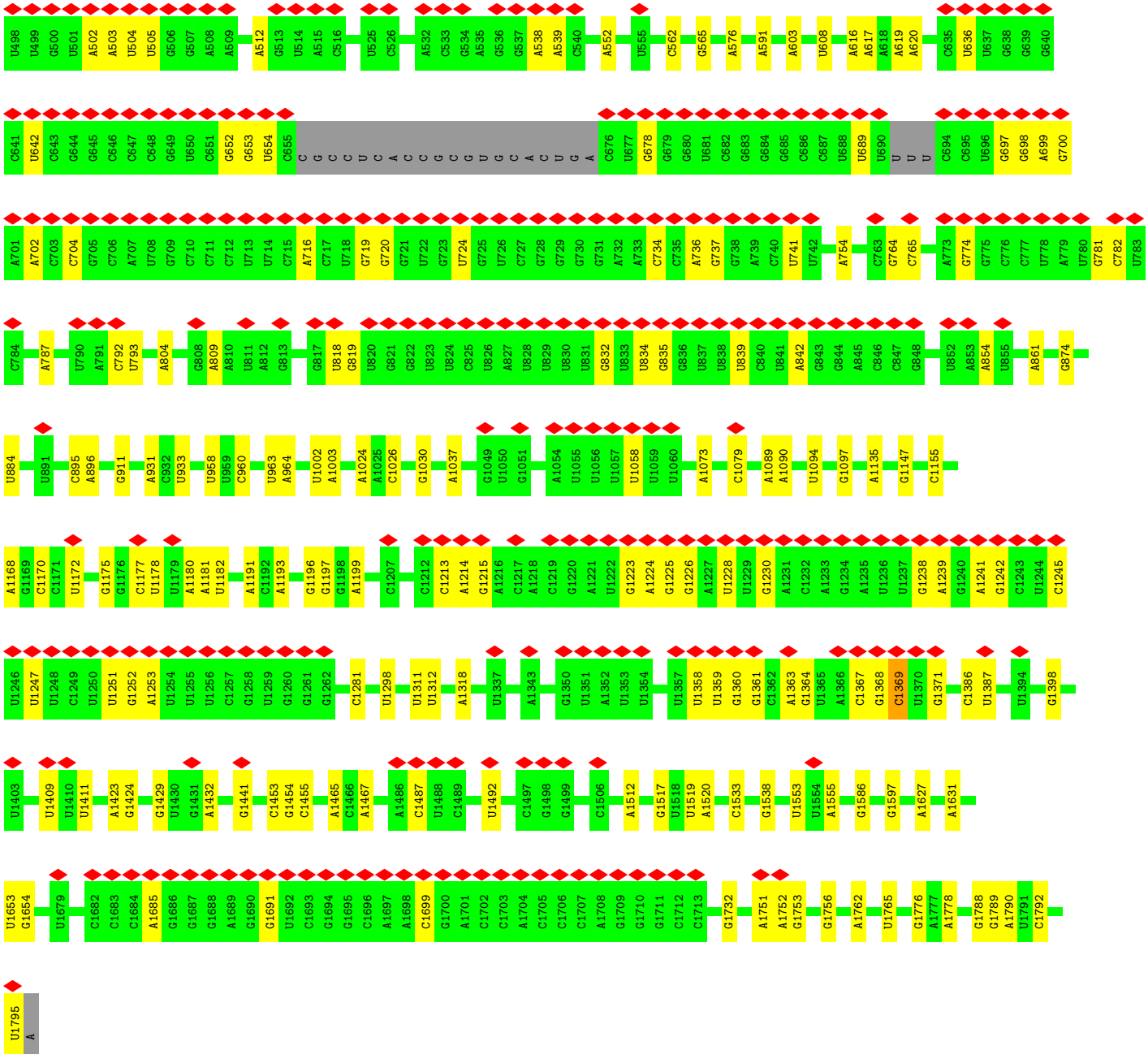





• Molecule 2: 18S rRNA

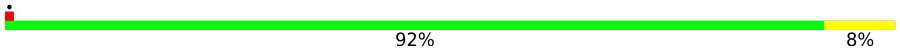
Chain A2:

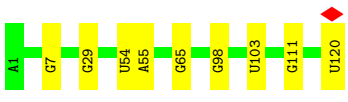






• Molecule 3: 5S rRNA

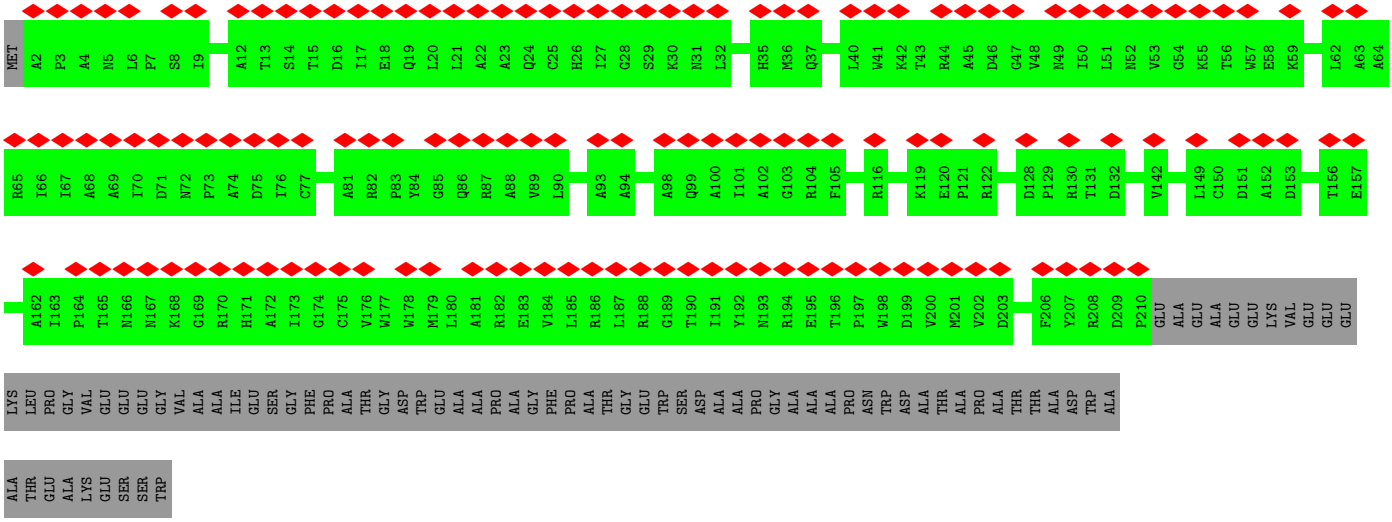
Chain B1:



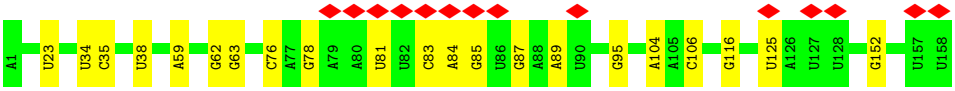

• Molecule 4: 40S ribosomal protein S0

Chain B2:



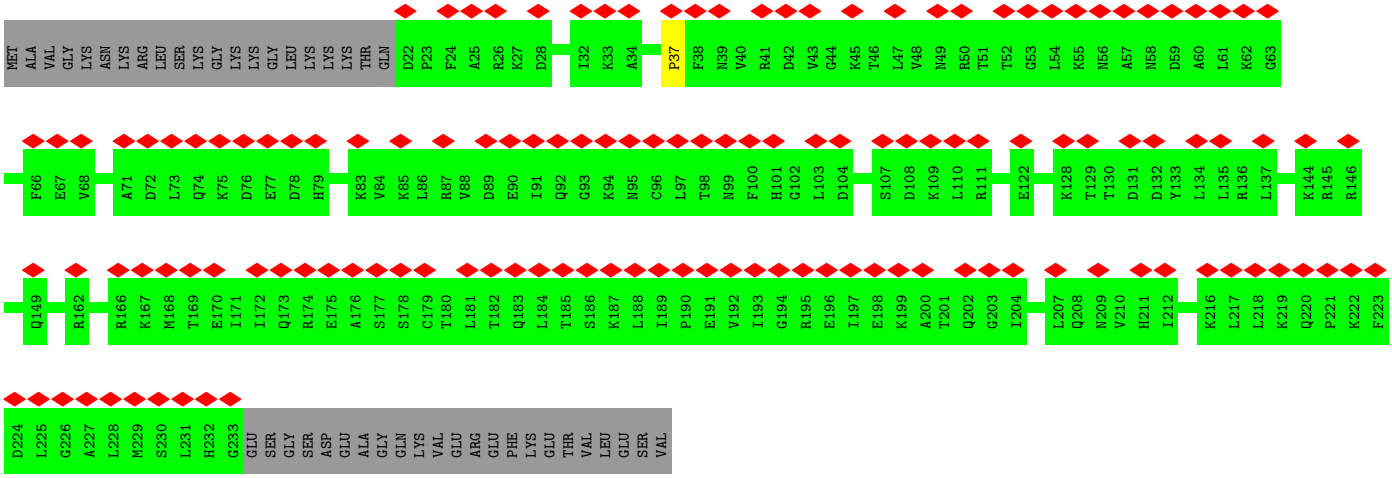

• Molecule 5: 5.8S rRNA

Chain C1:

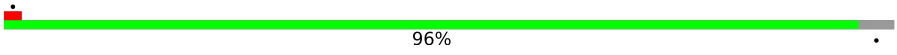

• Molecule 6: 40S ribosomal protein S1

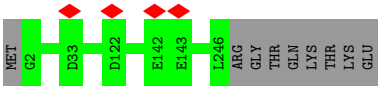
Chain C2:


• Molecule 7: 60S ribosomal protein L2

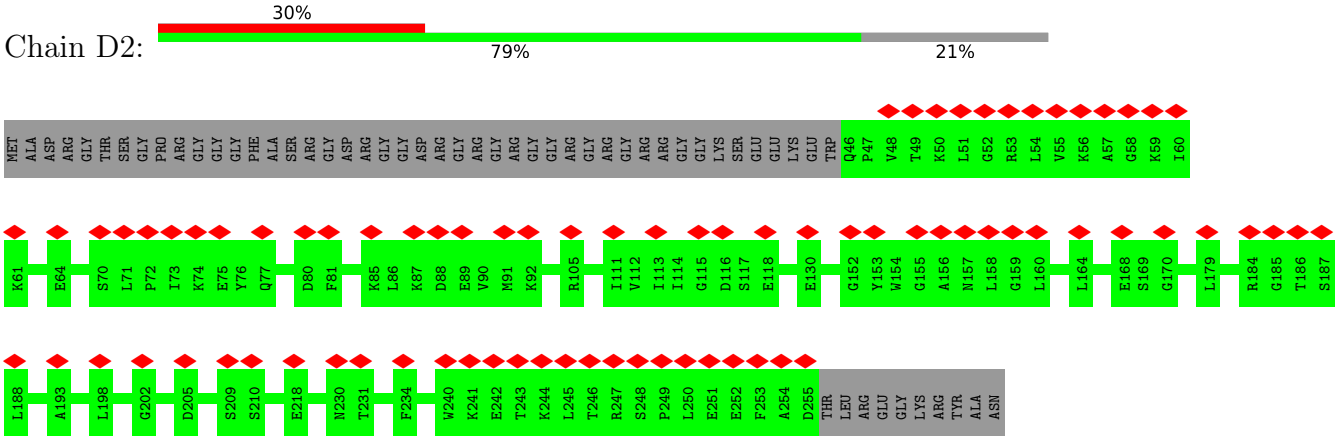
Chain D1:



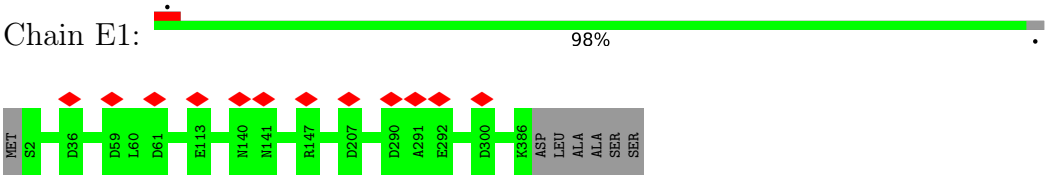

• Molecule 8: 40S ribosomal protein S2

Chain D2:



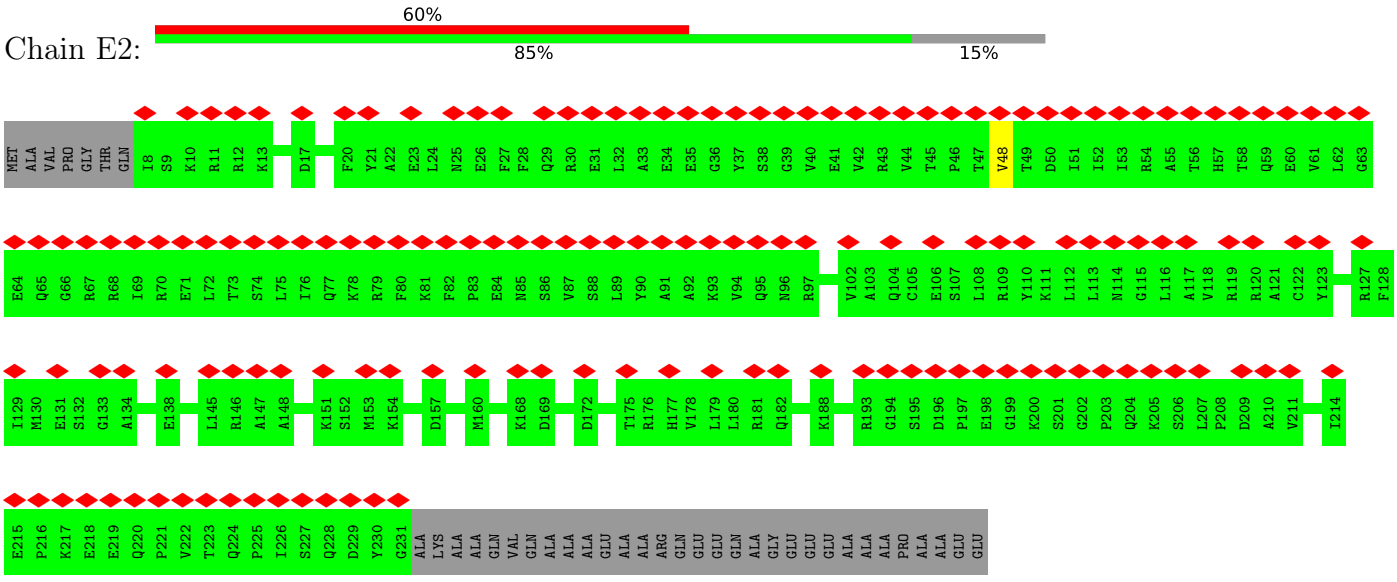

• Molecule 9: 60S ribosomal protein L3

Chain E1:



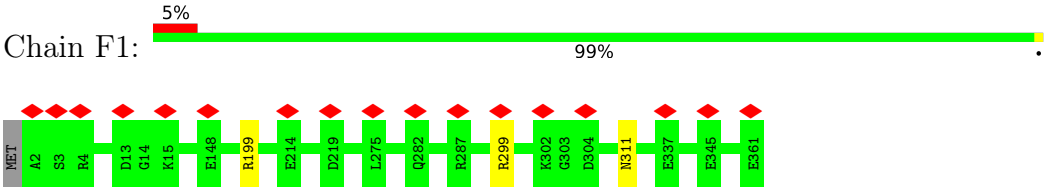

• Molecule 10: Cytoplasmic ribosomal protein 10

Chain E2:



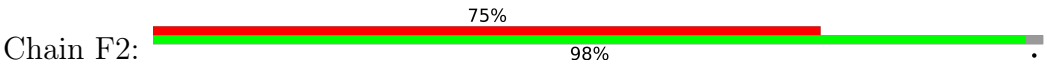

• Molecule 11: 60S ribosomal protein L4-A

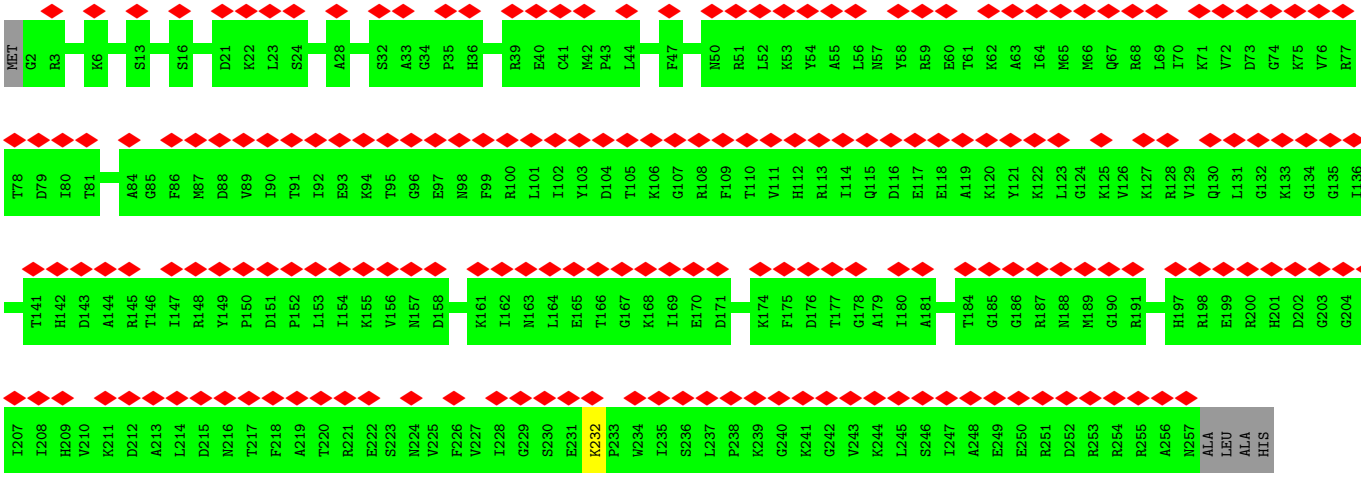
Chain F1:




• Molecule 12: 40S ribosomal protein S4

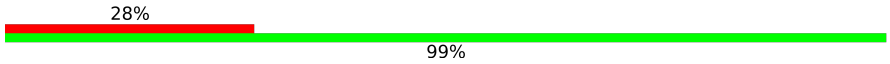
Chain F2:

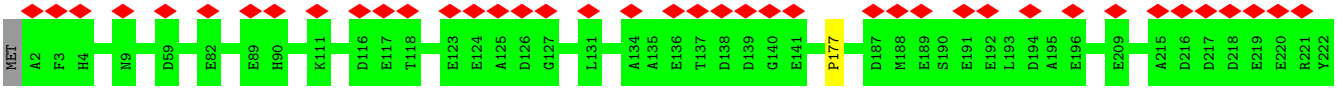


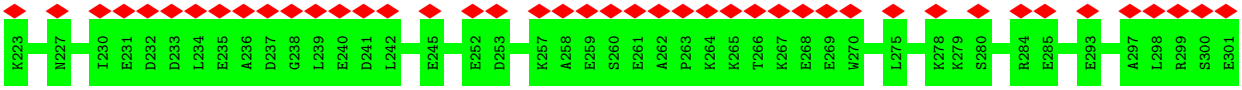



• Molecule 13: 60S ribosomal protein L5

Chain G1:

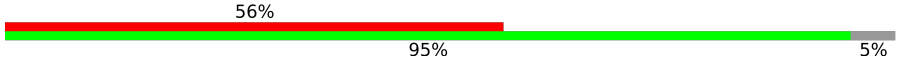


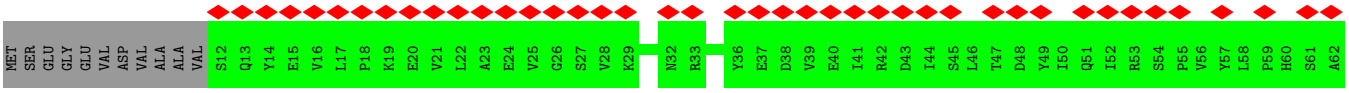



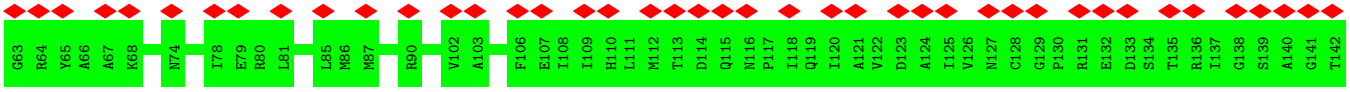



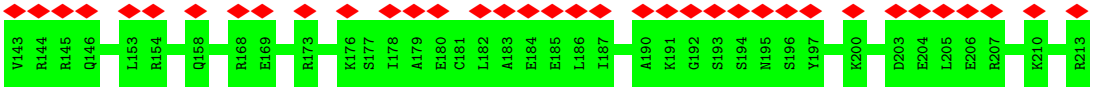

• Molecule 14: 40S ribosomal protein S5

Chain G2:



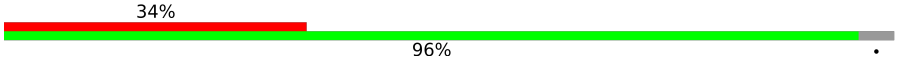



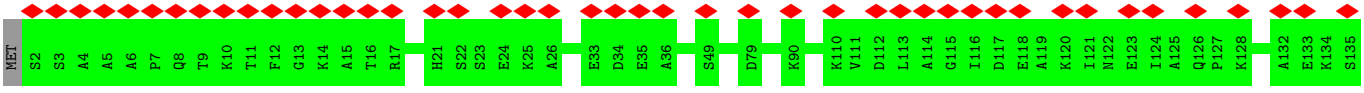



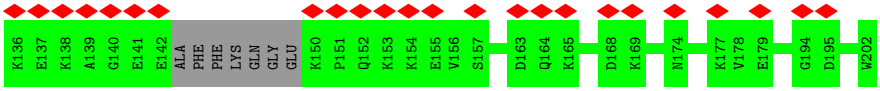




• Molecule 15: 60S ribosomal protein L6

Chain H1:

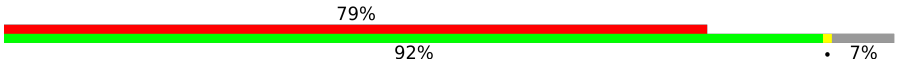


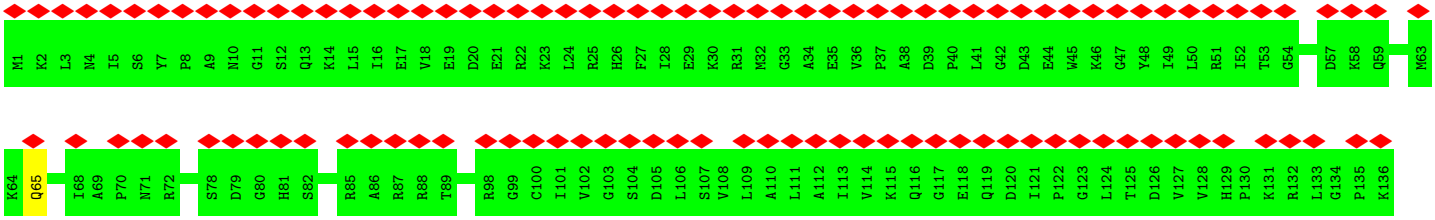






• Molecule 16: 40S ribosomal protein S6

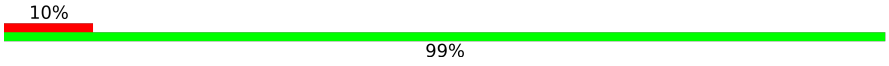
Chain H2:

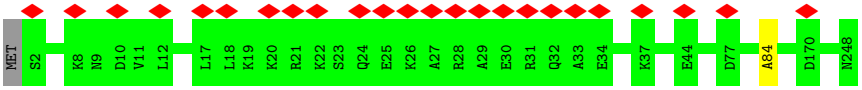



• Molecule 17: 60S ribosomal protein L7

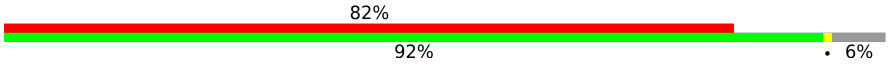
Chain I1:

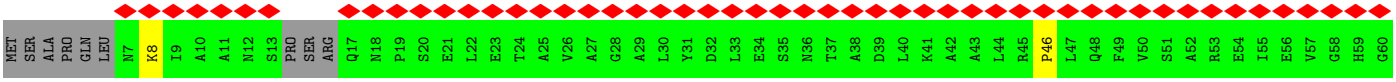


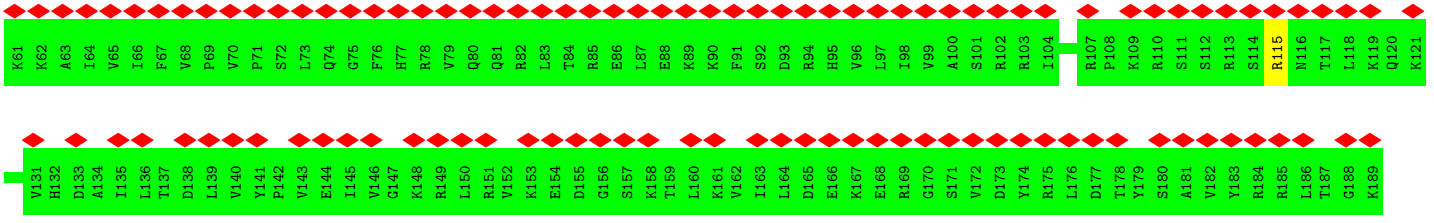




• Molecule 18: 40S ribosomal protein S7

Chain I2:

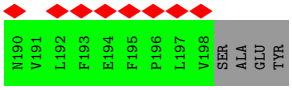


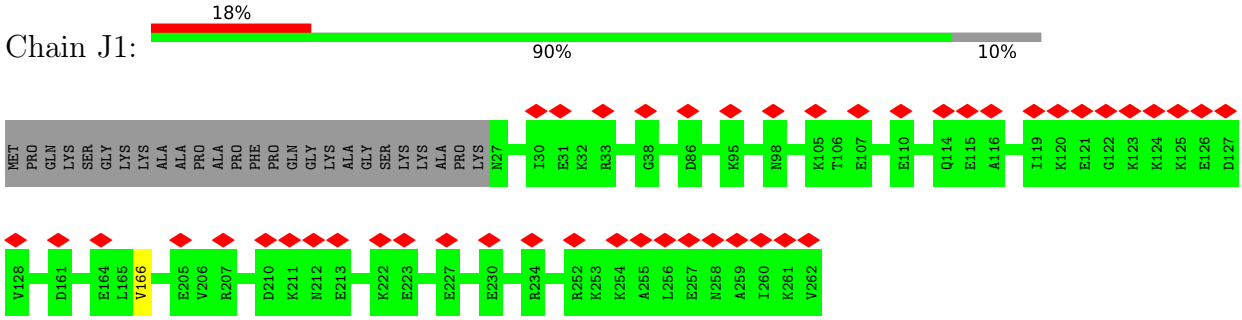






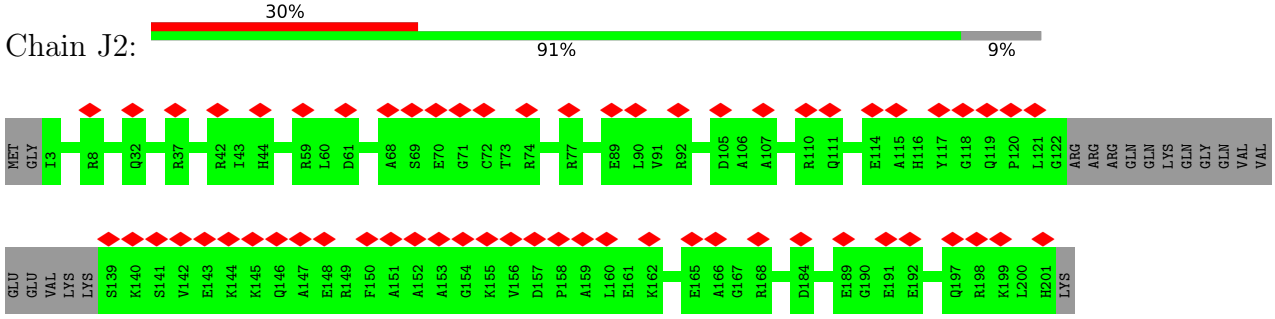

• Molecule 19: 60S ribosomal protein L8

Chain J1:



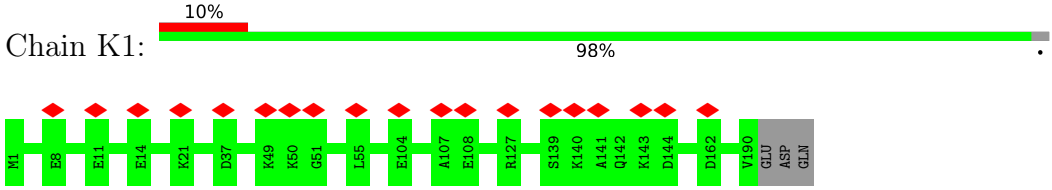

• Molecule 20: 40S ribosomal protein S8

Chain J2:



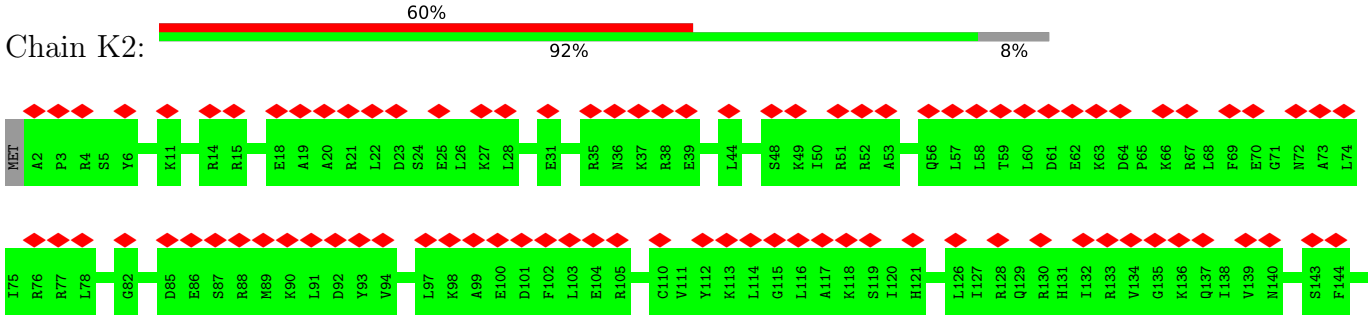

• Molecule 21: 60S ribosomal protein L9

Chain K1:



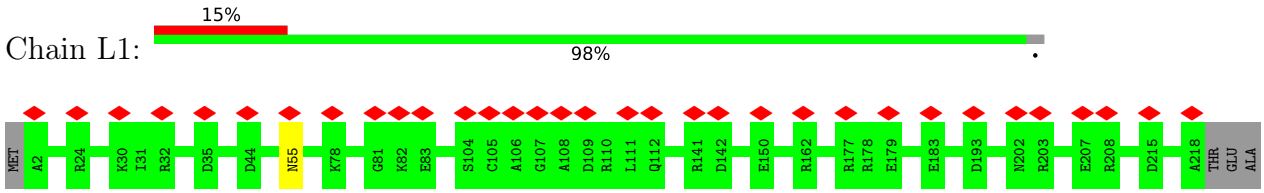

• Molecule 22: 40S ribosomal protein S9

Chain K2:



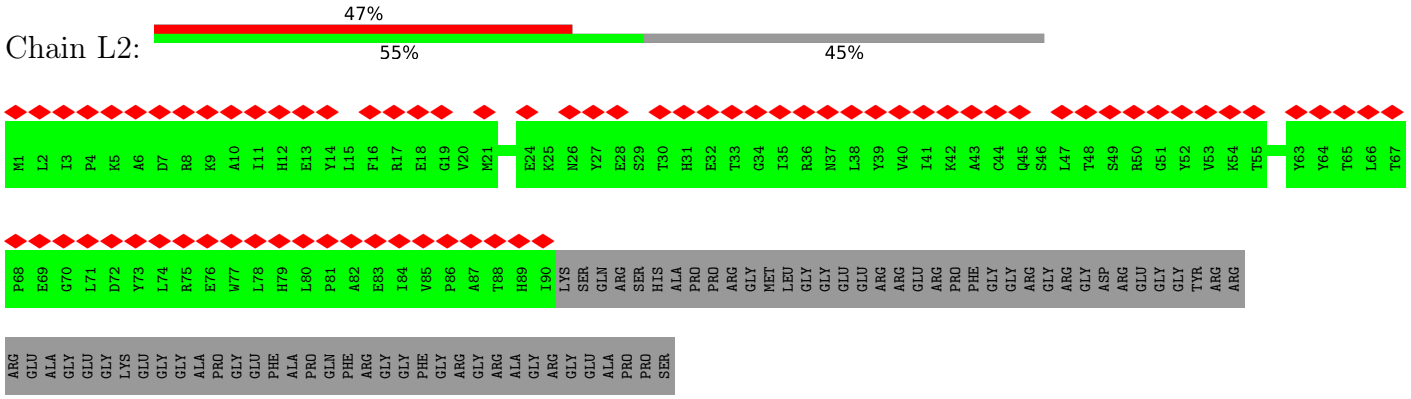

• Molecule 23: 60S ribosomal protein L10

Chain L1:



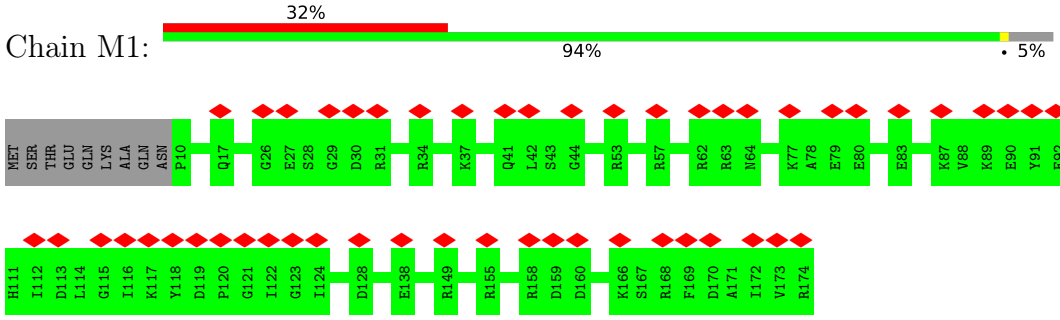
• Molecule 24: Probable 40s ribosomal protein s10-b

Chain L2:



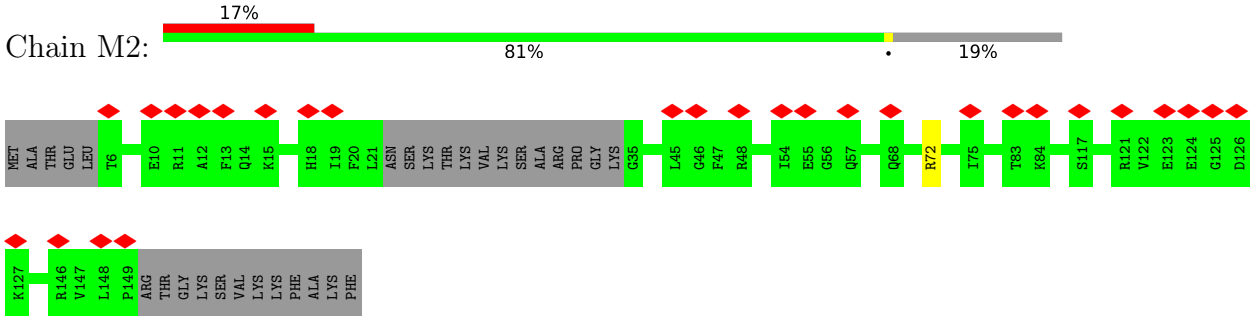

• Molecule 25: 60S ribosomal protein L11

Chain M1:



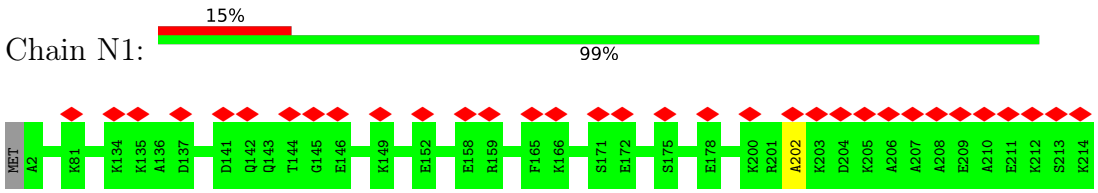

• Molecule 26: 40S ribosomal protein S11

Chain M2:



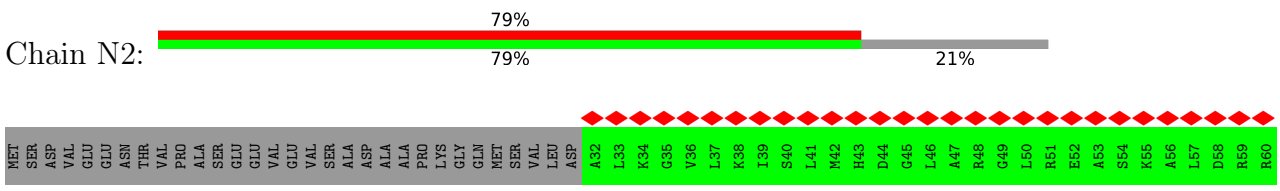

• Molecule 27: 60S ribosomal protein L13

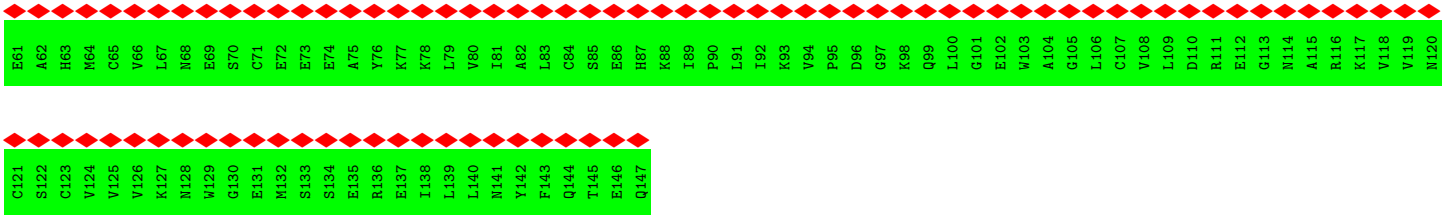
Chain N1:




• Molecule 28: 40S ribosomal protein S12

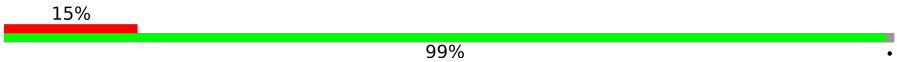
Chain N2:

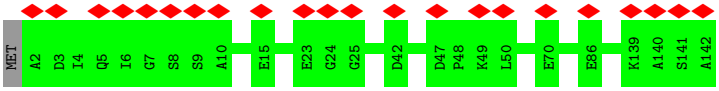





• Molecule 29: Ribosomal protein L14

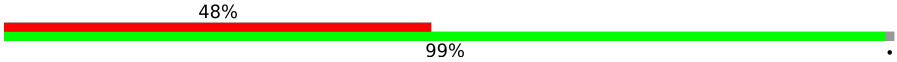
Chain O1:

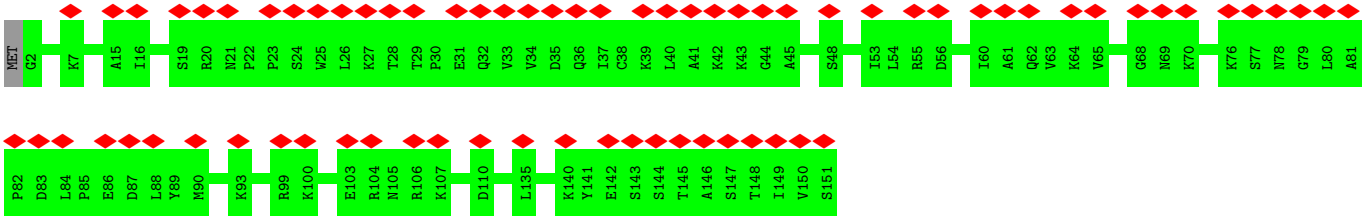



• Molecule 30: 40S ribosomal protein S13

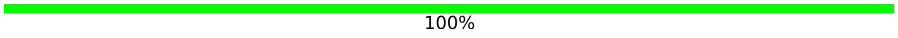
Chain O2:

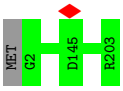



• Molecule 31: 60S ribosomal protein L15

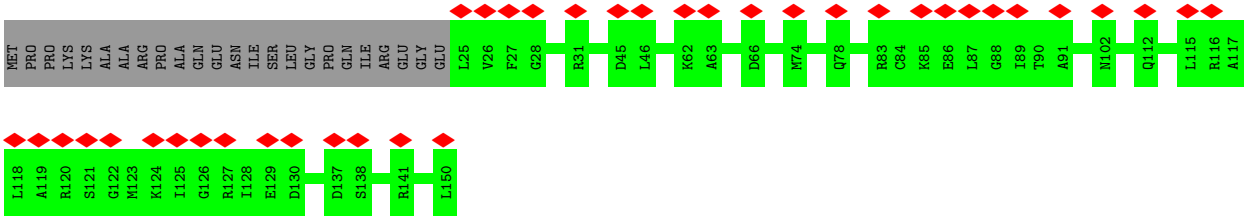
Chain P1:



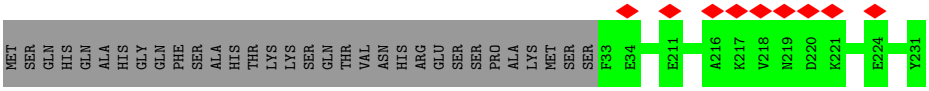

• Molecule 32: 40S ribosomal protein S14 (uS11)

Chain P2:

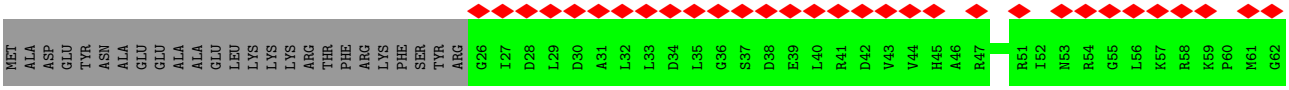

• Molecule 33: 60S ribosomal protein L16

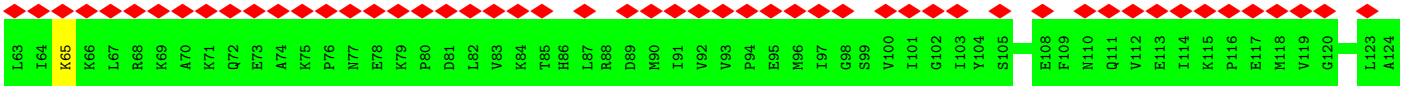
Chain Q1:

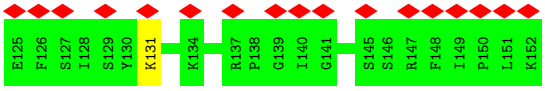



• Molecule 34: Ribosomal protein S12

Chain Q2:

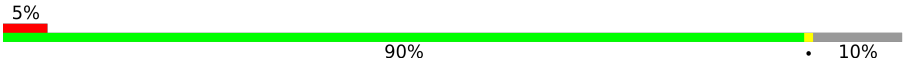



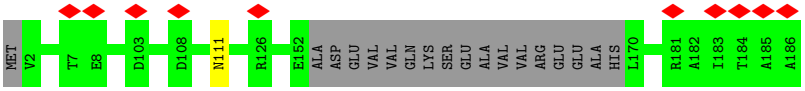




• Molecule 35: 60S ribosomal protein L17

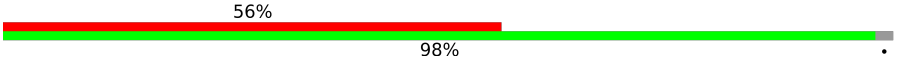
Chain R1:

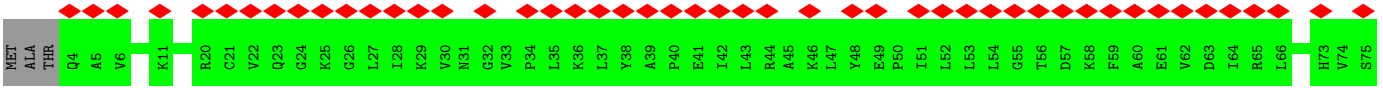


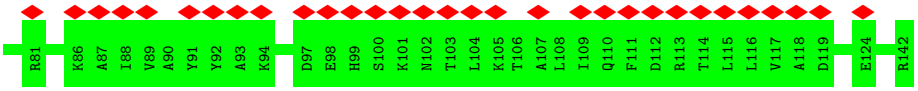




• Molecule 36: 40S ribosomal protein S16

Chain R2:

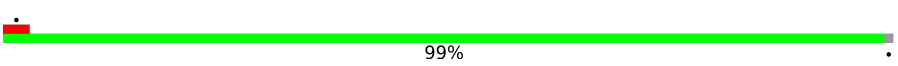


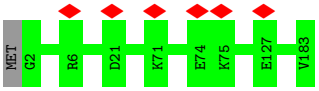




• Molecule 37: 60S ribosomal protein L18

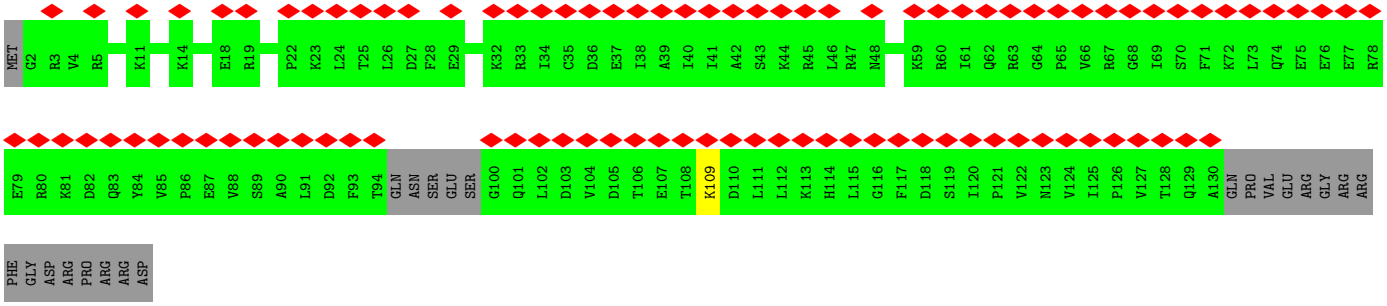
Chain S1:



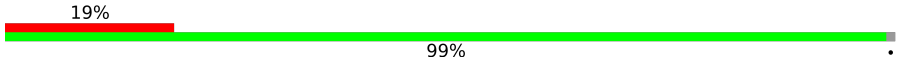

• Molecule 38: 40S ribosomal protein S17

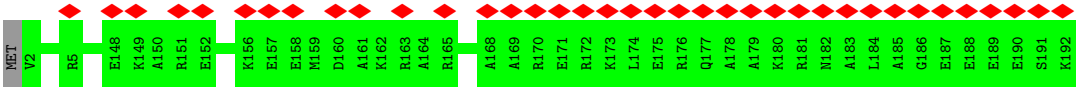
Chain S2:




• Molecule 39: Ribosomal protein L19

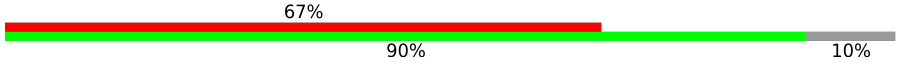
Chain T1:

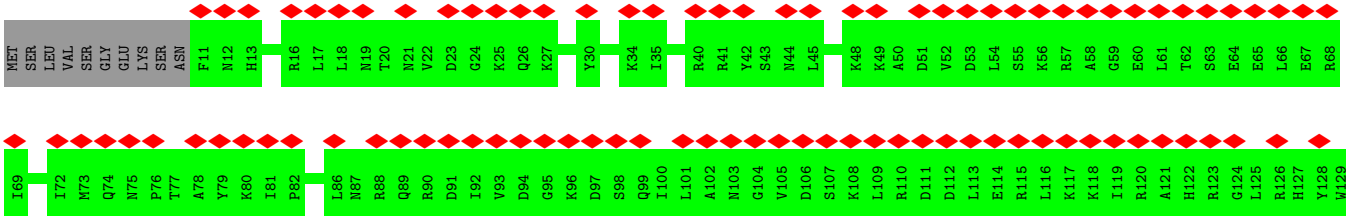



• Molecule 40: 40S ribosomal protein S18

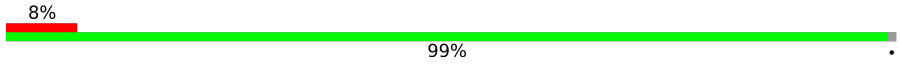
Chain T2:

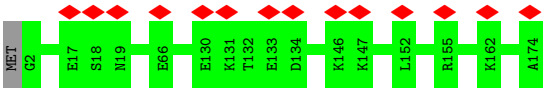



• Molecule 41: 60S ribosomal protein L20

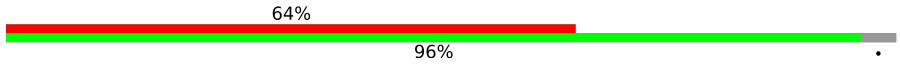
Chain U1:

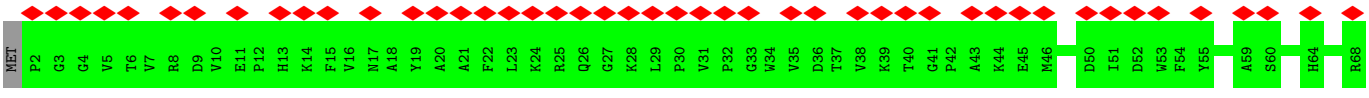


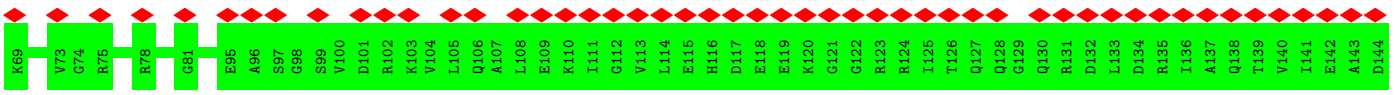




• Molecule 42: 40S ribosomal protein S19

Chain U2:

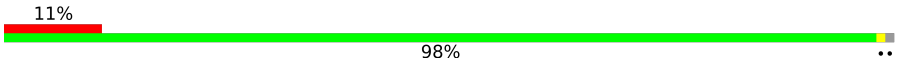


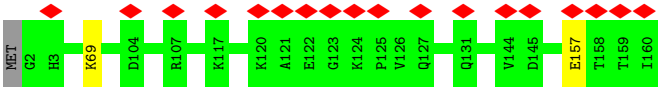




• Molecule 43: Ribosomal protein Srp1

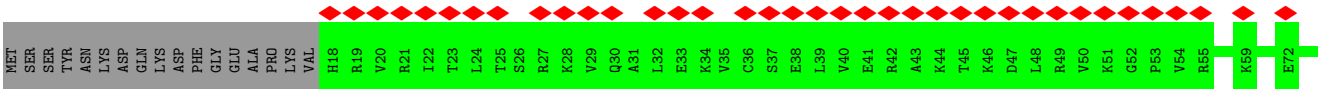
Chain V1:

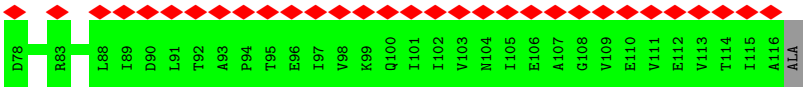



• Molecule 44: 40S ribosomal protein S20

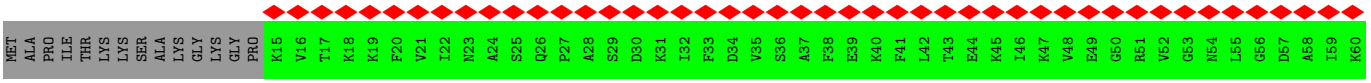
Chain V2:

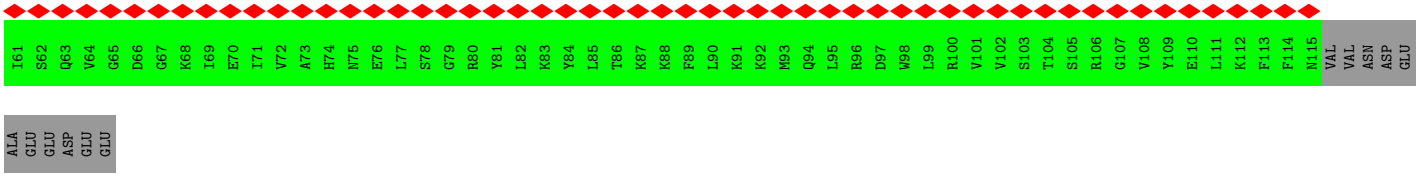




• Molecule 45: 60S ribosomal protein L22

Chain W1:

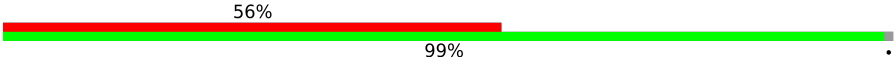



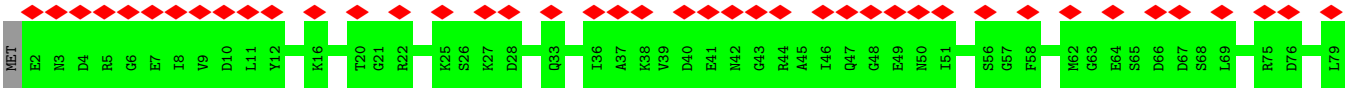


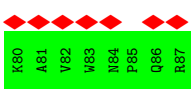


• Molecule 46: 40S ribosomal protein S21

Chain W2:

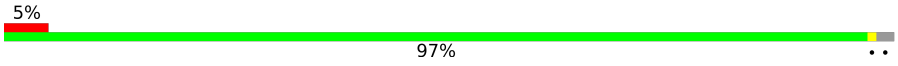


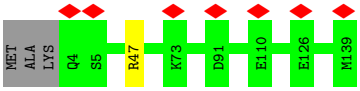




• Molecule 47: 60S ribosomal protein L23

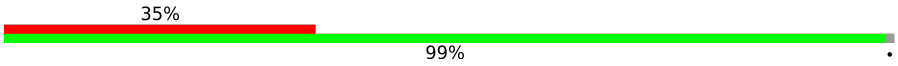
Chain X1:

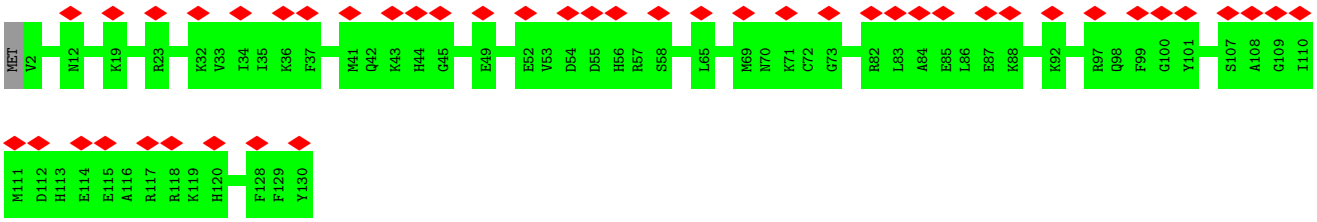





• Molecule 48: 40S ribosomal protein S22

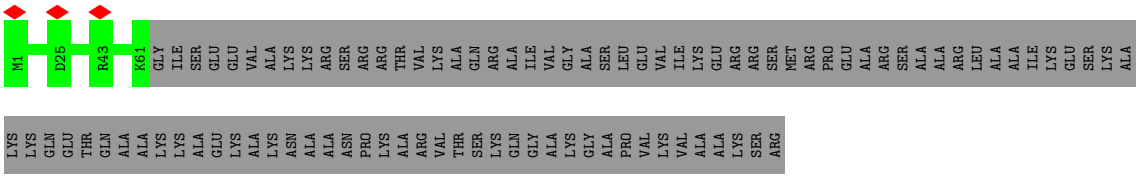
Chain X2:



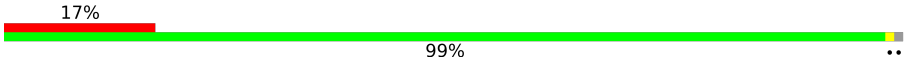

• Molecule 49: 60S ribosomal protein L24

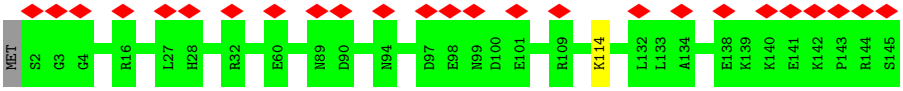
Chain Y1:


• Molecule 50: 40S ribosomal protein S23

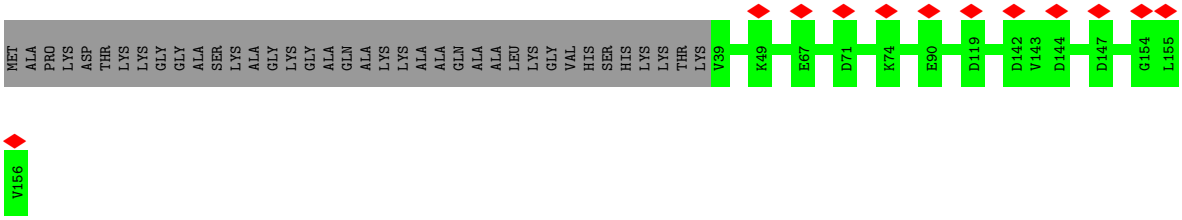
Chain Y2:



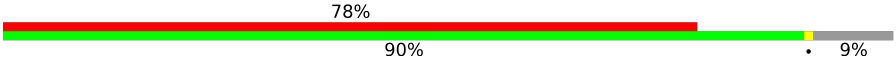

• Molecule 51: 60S ribosomal protein L25

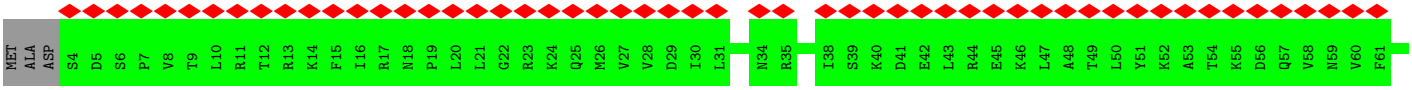
Chain Z1:

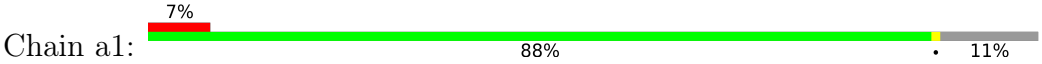

• Molecule 52: 40S ribosomal protein S24

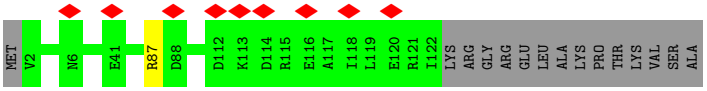
Chain Z2:




• Molecule 53: Ribosomal protein L26

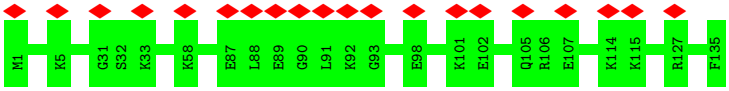


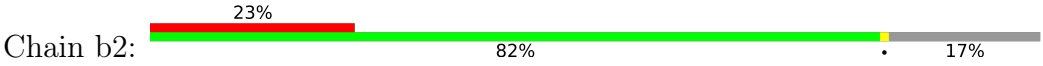

• Molecule 54: 40S ribosomal protein S25

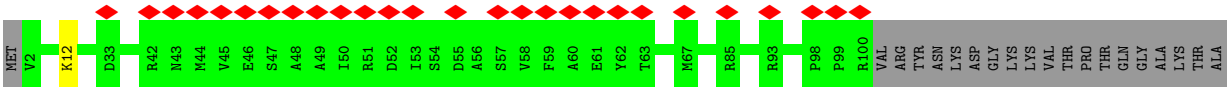


• Molecule 55: 60S ribosomal protein L27 (eL27)

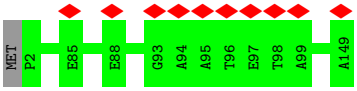




• Molecule 56: 40S ribosomal protein S26E



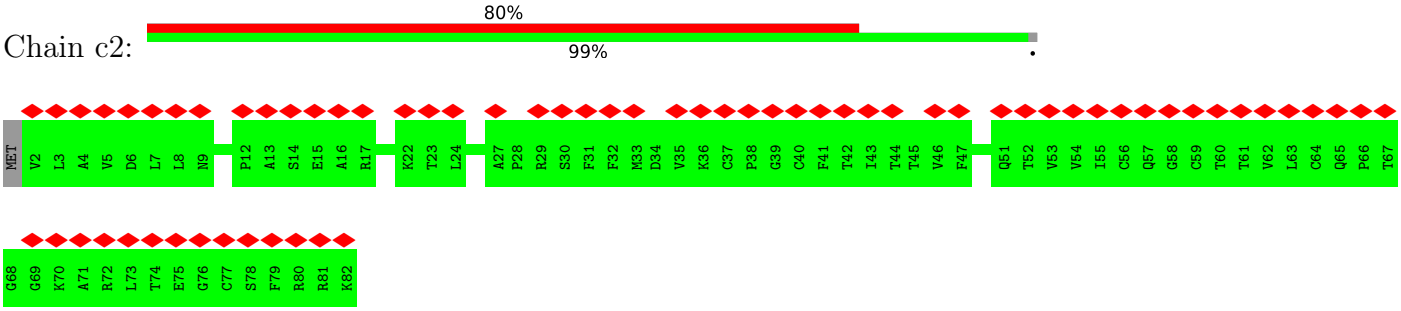




• Molecule 57: 60S ribosomal protein L28

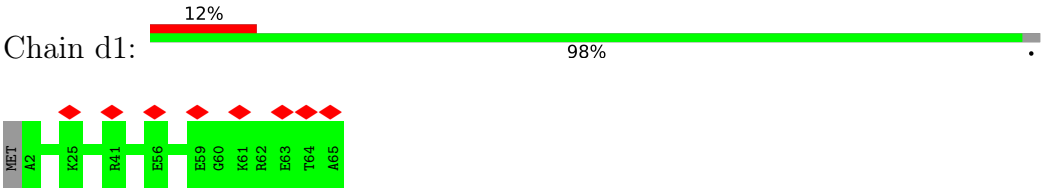

• Molecule 58: 40S ribosomal protein S27

Chain c2:



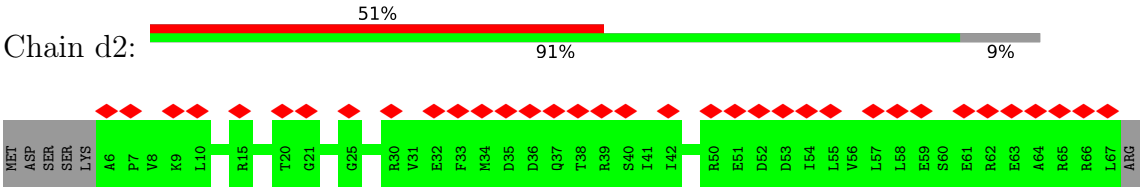

• Molecule 59: 60S ribosomal protein L29

Chain d1:



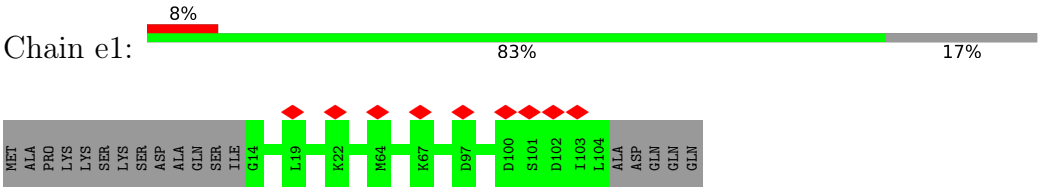

• Molecule 60: 40S ribosomal protein S28

Chain d2:



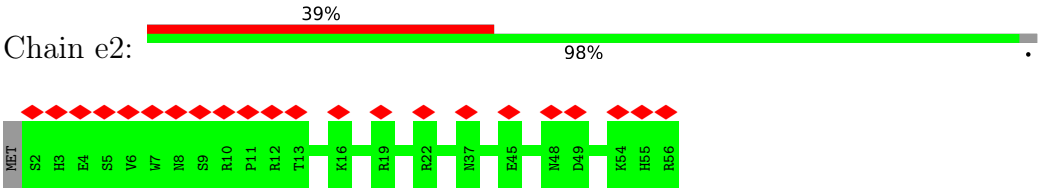

• Molecule 61: 60S ribosomal protein L30

Chain e1:



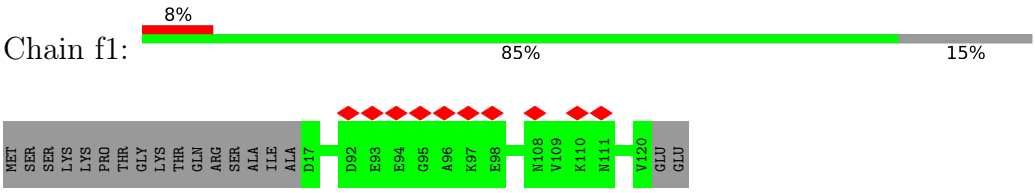

• Molecule 62: 40S ribosomal protein S29

Chain e2:



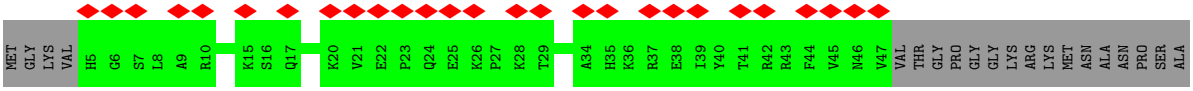

• Molecule 63: 60s ribosomal protein

Chain f1:



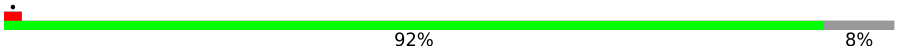

• Molecule 64: 40S ribosomal protein S30

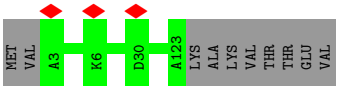
Chain f2:




• Molecule 65: 60S ribosomal protein L32

Chain g1:

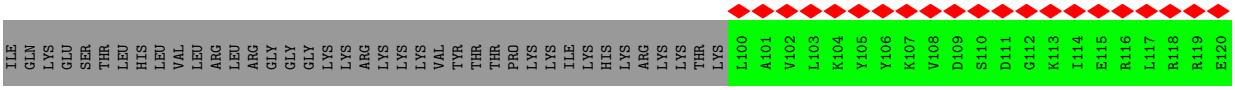


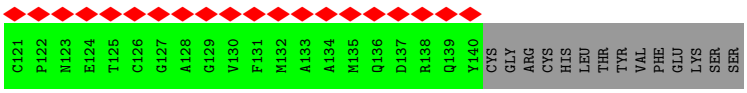




• Molecule 66: Ubiquitin-40S ribosomal protein S27a

Chain g2:

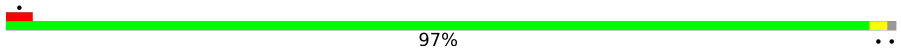


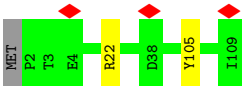



• Molecule 67: 60S ribosomal protein L33

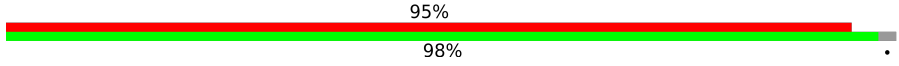
Chain h1:

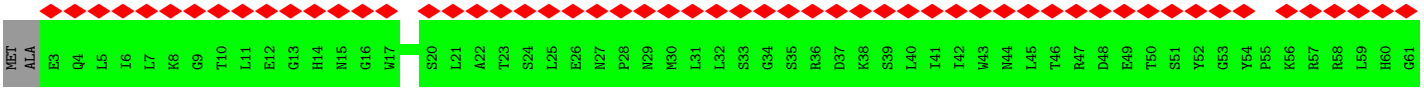


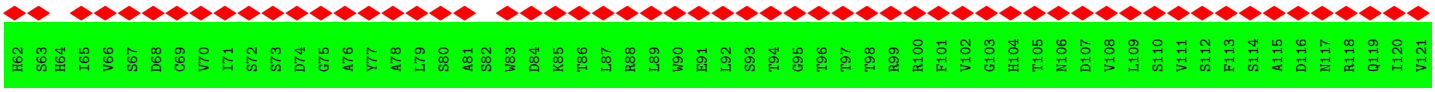



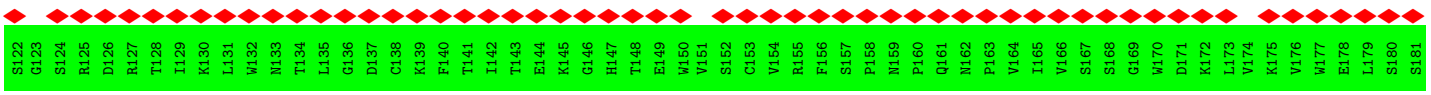

• Molecule 68: Guanine nucleotide-binding protein subunit beta-like protein

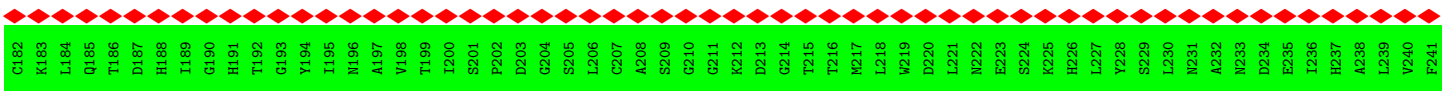
Chain h2:

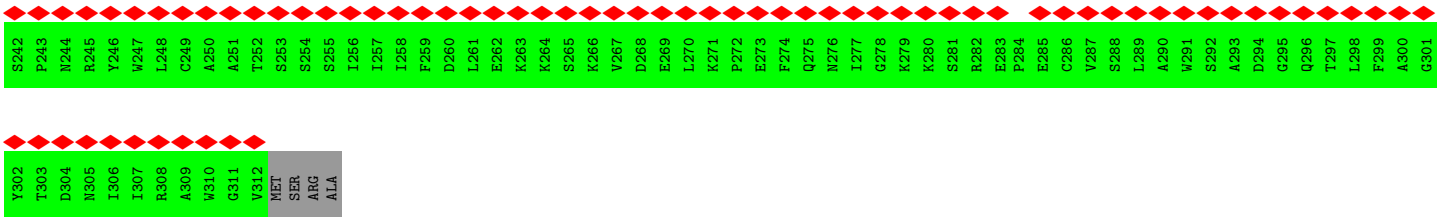


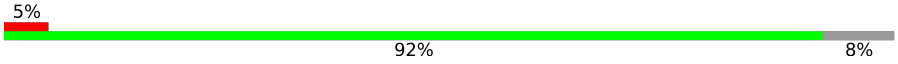



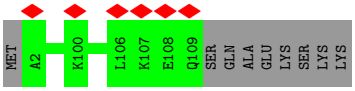






• Molecule 69: 60S ribosomal protein L34

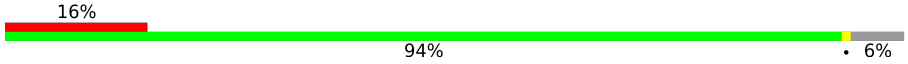
Chain i1:

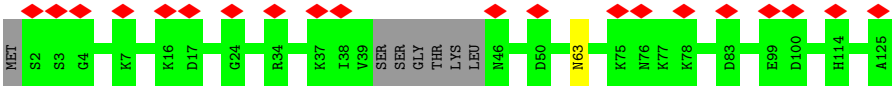



• Molecule 70: 60S ribosomal protein L35

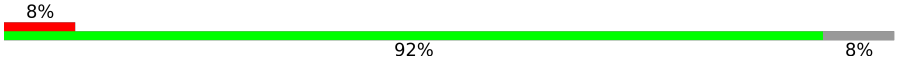
Chain j1:

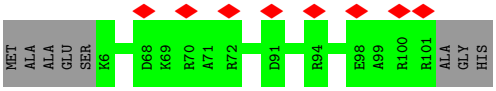



• Molecule 71: 60S ribosomal protein L36

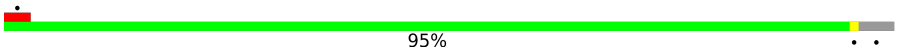
Chain k1:

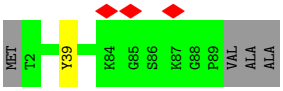



• Molecule 72: Ribosomal protein L37

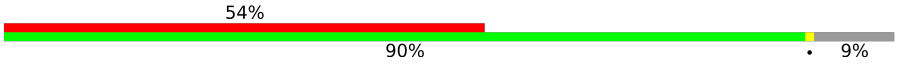
Chain l1:

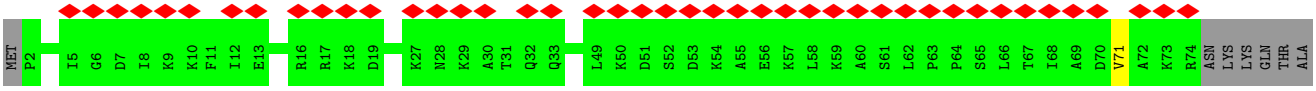



• Molecule 73: 60S ribosomal protein L38

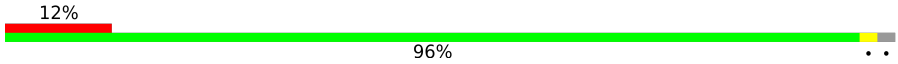
Chain m1:

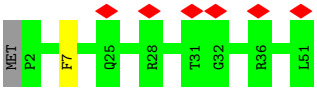



• Molecule 74: 60S ribosomal protein L39

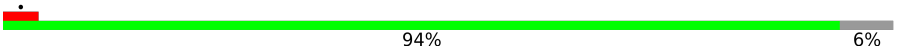
Chain n1:

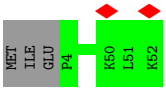





• Molecule 75: 60S ribosomal protein L40

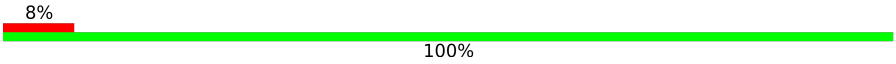
Chain o1:

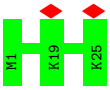



• Molecule 76: hypothetical protein NCU16635 (eL41)

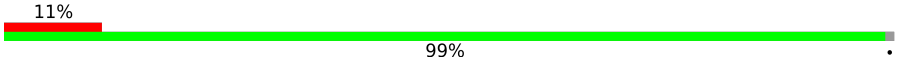
Chain p1:

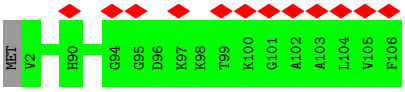



• Molecule 77: 60S ribosomal protein L44

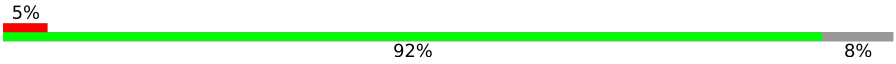
Chain q1:

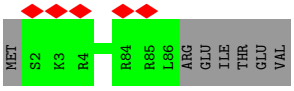



• Molecule 78: 60S ribosomal protein L43

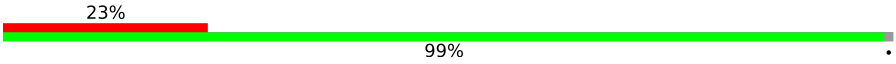
Chain r1:

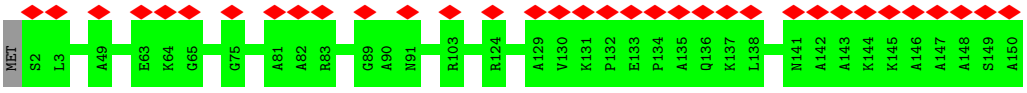



• Molecule 79: Ribosomal_L28e domain-containing protein

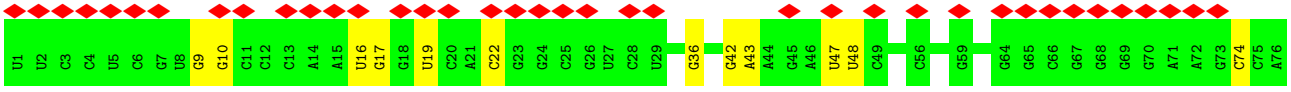
Chain s1:



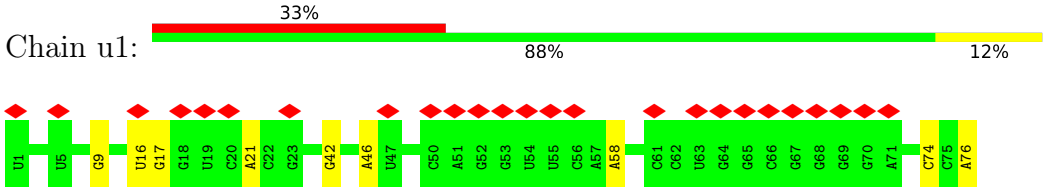

• Molecule 80: tRNA

Chain t1:

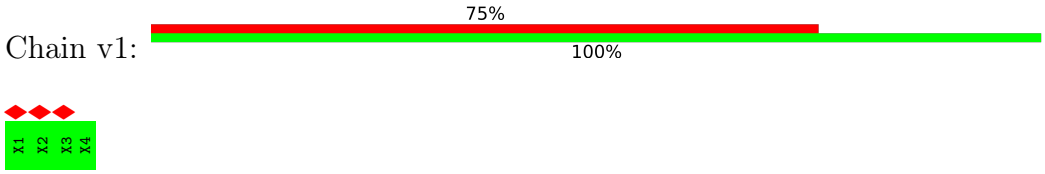

• Molecule 80: tRNA

Chain u1:



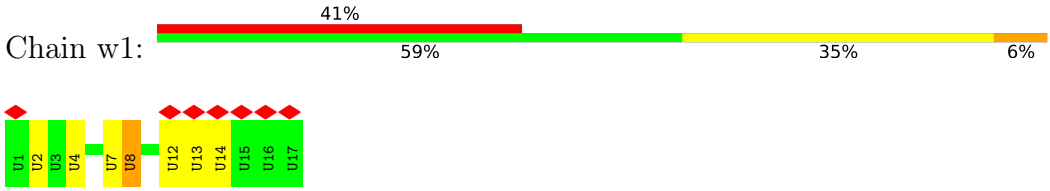

• Molecule 81: Nascent peptide

Chain v1:




• Molecule 82: mRNA

Chain w1:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 196154 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 32 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 4.040 | Depositor |
| Minimum map value | -2.001 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.132 | Depositor |
| Recommended contour level | 0.5 | Depositor |
| Map size (Å) | 407.03998, 407.03998, 407.03998 | wwPDB |
| Map dimensions | 384, 384, 384 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.06, 1.06, 1.06 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, 3HE, MG

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 | A1 | 0.36 | 0/74705 | 0.81 | 43/116467 (0.0%) |
| 2 | A2 | 0.24 | 0/42178 | 0.76 | 8/65727 (0.0%) |
| 3 | B1 | 0.28 | 0/2854 | 0.77 | 0/4445 |
| 4 | B2 | 0.25 | 0/1675 | 0.49 | 0/2288 |
| 5 | C1 | 0.32 | 0/3756 | 0.76 | 0/5849 |
| 6 | C2 | 0.26 | 0/1733 | 0.55 | 1/2332 (0.0%) |
| 7 | D1 | 0.29 | 0/1890 | 0.55 | 0/2540 |
| 8 | D2 | 0.26 | 0/1641 | 0.49 | 0/2218 |
| 9 | E1 | 0.28 | 0/3127 | 0.51 | 0/4201 |
| 10 | E2 | 0.25 | 0/1777 | 0.53 | 0/2387 |
| 11 | F1 | 0.27 | 0/2776 | 0.51 | 0/3744 |
| 12 | F2 | 0.26 | 0/2088 | 0.56 | 0/2806 |
| 13 | G1 | 0.26 | 0/2469 | 0.50 | 0/3311 |
| 14 | G2 | 0.25 | 0/1608 | 0.51 | 0/2167 |
| 15 | H1 | 0.25 | 0/1549 | 0.49 | 0/2084 |
| 16 | H2 | 0.25 | 0/1810 | 0.55 | 0/2420 |
| 17 | I1 | 0.27 | 0/2052 | 0.50 | 0/2751 |
| 18 | I2 | 0.25 | 0/1536 | 0.56 | 0/2069 |
| 19 | J1 | 0.26 | 0/1909 | 0.49 | 0/2557 |
| 20 | J2 | 0.27 | 0/1494 | 0.54 | 0/2004 |
| 21 | K1 | 0.26 | 0/1523 | 0.50 | 0/2048 |
| 22 | K2 | 0.24 | 0/1442 | 0.56 | 0/1932 |
| 23 | L1 | 0.27 | 0/1788 | 0.54 | 0/2398 |
| 24 | L2 | 0.24 | 0/775 | 0.47 | 0/1053 |
| 25 | M1 | 0.25 | 0/1363 | 0.56 | 0/1821 |
| 26 | M2 | 0.27 | 0/1092 | 0.57 | 0/1468 |
| 27 | N1 | 0.26 | 0/1703 | 0.54 | 1/2281 (0.0%) |
| 28 | N2 | 0.24 | 0/918 | 0.53 | 0/1230 |
| 29 | O1 | 0.24 | 0/1125 | 0.49 | 0/1508 |
| 30 | O2 | 0.24 | 0/1201 | 0.47 | 0/1618 |
| 31 | P1 | 0.29 | 0/1738 | 0.58 | 0/2327 |
| 32 | P2 | 0.27 | 0/949 | 0.57 | 0/1272 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | Q1 | 0.28 | 0/1627 | 0.51 | 0/2176 |
| 34 | Q2 | 0.25 | 0/1025 | 0.54 | 0/1371 |
| 35 | R1 | 0.26 | 0/1342 | 0.55 | 0/1799 |
| 36 | R2 | 0.25 | 0/1107 | 0.50 | 0/1485 |
| 37 | S1 | 0.27 | 0/1469 | 0.57 | 0/1966 |
| 38 | S2 | 0.25 | 0/1018 | 0.51 | 0/1367 |
| 39 | T1 | 0.25 | 0/1582 | 0.53 | 0/2102 |
| 40 | T2 | 0.25 | 0/1154 | 0.56 | 0/1547 |
| 41 | U1 | 0.27 | 0/1464 | 0.53 | 0/1970 |
| 42 | U2 | 0.23 | 0/1147 | 0.50 | 0/1548 |
| 43 | V1 | 0.29 | 0/1296 | 0.52 | 0/1736 |
| 44 | V2 | 0.23 | 0/794 | 0.53 | 0/1069 |
| 45 | W1 | 0.25 | 0/829 | 0.46 | 0/1107 |
| 46 | W2 | 0.25 | 0/675 | 0.52 | 0/905 |
| 47 | X1 | 0.28 | 0/1025 | 0.51 | 0/1377 |
| 48 | X2 | 0.25 | 0/1053 | 0.53 | 0/1412 |
| 49 | Y1 | 0.29 | 0/537 | 0.56 | 0/714 |
| 50 | Y2 | 0.25 | 0/1131 | 0.50 | 0/1507 |
| 51 | Z1 | 0.25 | 0/957 | 0.49 | 0/1292 |
| 52 | Z2 | 0.25 | 0/1018 | 0.54 | 0/1361 |
| 53 | a1 | 0.26 | 0/972 | 0.56 | 0/1304 |
| 54 | a2 | 0.25 | 0/569 | 0.49 | 0/760 |
| 55 | b1 | 0.27 | 0/1130 | 0.52 | 0/1511 |
| 56 | b2 | 0.27 | 0/805 | 0.59 | 0/1073 |
| 57 | c1 | 0.28 | 0/1197 | 0.52 | 0/1608 |
| 58 | c2 | 0.25 | 0/623 | 0.51 | 0/842 |
| 59 | d1 | 0.24 | 0/528 | 0.50 | 0/697 |
| 60 | d2 | 0.24 | 0/493 | 0.60 | 0/661 |
| 61 | e1 | 0.26 | 0/689 | 0.47 | 0/925 |
| 62 | e2 | 0.26 | 0/455 | 0.53 | 0/605 |
| 63 | f1 | 0.27 | 0/869 | 0.53 | 0/1164 |
| 64 | f2 | 0.25 | 0/353 | 0.50 | 0/471 |
| 65 | g1 | 0.27 | 0/990 | 0.54 | 0/1319 |
| 66 | g2 | 0.24 | 0/332 | 0.56 | 0/443 |
| 67 | h1 | 0.30 | 0/874 | 0.56 | 0/1176 |
| 68 | h2 | 0.25 | 0/2486 | 0.51 | 0/3378 |
| 69 | i1 | 0.28 | 0/865 | 0.55 | 0/1158 |
| 70 | j1 | 0.23 | 0/976 | 0.49 | 0/1295 |
| 71 | k1 | 0.24 | 0/766 | 0.55 | 0/1016 |
| 72 | l1 | 0.28 | 0/704 | 0.58 | 0/933 |
| 73 | m1 | 0.26 | 0/591 | 0.49 | 0/786 |
| 74 | n1 | 0.24 | 0/445 | 0.59 | 0/592 |
| 75 | o1 | 0.25 | 0/401 | 0.55 | 0/528 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 76 | p1 | 0.24 | 0/236 | 0.68 | 0/300 |
| 77 | q1 | 0.27 | 0/841 | 0.51 | 0/1113 |
| 78 | r1 | 0.29 | 0/655 | 0.55 | 0/873 |
| 79 | s1 | 0.26 | 0/1134 | 0.51 | 0/1523 |
| 80 | t1 | 0.21 | 0/1811 | 0.76 | 0/2821 |
| 80 | u1 | 0.21 | 0/1811 | 0.74 | 0/2821 |
| 82 | w1 | 0.25 | 0/373 | 0.99 | 4/574 (0.7%) |
| All | All | 0.29 | 0/217468 | 0.70 | 57/319404 (0.0%) |

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 |
|---|---|---|---|
| 13 | G1 | 0 | 1 |
| 18 | I2 | 0 | 1 |
| 67 | h1 | 0 | 1 |
| 72 | l1 | 0 | 1 |
| All | All | 0 | 4 |

There are no bond length outliers.

All (57) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A1 | 470 | C | C2-N1-C1' | 8.87 | 128.56 | 118.80 |
| 1 | A1 | 470 | C | N1-C2-O2 | 8.49 | 124.00 | 118.90 |
| 1 | A1 | 175 | C | N3-C2-O2 | -7.79 | 116.44 | 121.90 |
| 82 | w1 | 8 | U | C2-N1-C1' | 7.38 | 126.55 | 117.70 |
| 1 | A1 | 2173 | U | C2-N1-C1' | 6.91 | 126.00 | 117.70 |
| 1 | A1 | 904 | U | C2-N1-C1' | 6.80 | 125.86 | 117.70 |
| 1 | A1 | 470 | C | N3-C2-O2 | -6.68 | 117.22 | 121.90 |
| 82 | w1 | 8 | U | N3-C2-O2 | -6.55 | 117.62 | 122.20 |
| 2 | A2 | 963 | U | C2-N1-C1' | 6.44 | 125.42 | 117.70 |
| 2 | A2 | 1386 | C | C2-N1-C1' | 6.38 | 125.82 | 118.80 |
| 1 | A1 | 470 | C | C6-N1-C1' | -6.33 | 113.20 | 120.80 |
| 1 | A1 | 2173 | U | N1-C2-O2 | 6.14 | 127.10 | 122.80 |
| 1 | A1 | 3002 | C | C2-N1-C1' | 6.01 | 125.41 | 118.80 |
| 27 | N1 | 202 | ALA | C-N-CA | 5.95 | 136.57 | 121.70 |
| 82 | w1 | 8 | U | N1-C2-O2 | 5.90 | 126.93 | 122.80 |
| 1 | A1 | 1479 | C | C2-N1-C1' | 5.86 | 125.24 | 118.80 |
| 1 | A1 | 1538 | U | N3-C2-O2 | -5.74 | 118.18 | 122.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A1 | 451 | C | C2-N1-C1' | 5.73 | 125.10 | 118.80 |
| 1 | A1 | 2173 | U | N3-C2-O2 | -5.71 | 118.20 | 122.20 |
| 2 | A2 | 450 | C | C2-N1-C1' | 5.70 | 125.07 | 118.80 |
| 1 | A1 | 3019 | C | C2-N1-C1' | 5.67 | 125.03 | 118.80 |
| 1 | A1 | 570 | C | C2-N1-C1' | 5.66 | 125.02 | 118.80 |
| 1 | A1 | 2994 | C | C2-N1-C1' | 5.58 | 124.94 | 118.80 |
| 2 | A2 | 450 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 1 | A1 | 172 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 1 | A1 | 2993 | C | C2-N1-C1' | 5.57 | 124.92 | 118.80 |
| 1 | A1 | 3194 | C | C2-N1-C1' | 5.52 | 124.87 | 118.80 |
| 82 | w1 | 7 | U | OP2-P-O3' | 5.50 | 117.31 | 105.20 |
| 1 | A1 | 1538 | U | N1-C2-O2 | 5.50 | 126.65 | 122.80 |
| 1 | A1 | 3041 | C | C2-N1-C1' | 5.50 | 124.85 | 118.80 |
| 1 | A1 | 450 | C | C2-N1-C1' | 5.42 | 124.77 | 118.80 |
| 6 | C2 | 37 | PRO | CA-N-CD | -5.42 | 103.92 | 111.50 |
| 1 | A1 | 1704 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 1 | A1 | 3078 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 1 | A1 | 3076 | C | C2-N1-C1' | 5.27 | 124.59 | 118.80 |
| 1 | A1 | 3091 | C | C6-N1-C2 | -5.26 | 118.19 | 120.30 |
| 1 | A1 | 3091 | C | C2-N1-C1' | 5.26 | 124.59 | 118.80 |
| 1 | A1 | 3092 | C | C2-N1-C1' | 5.25 | 124.58 | 118.80 |
| 1 | A1 | 470 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 2 | A2 | 1369 | C | N3-C2-O2 | -5.23 | 118.24 | 121.90 |
| 1 | A1 | 451 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 2 | A2 | 960 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 1 | A1 | 3091 | C | N3-C2-O2 | -5.15 | 118.29 | 121.90 |
| 1 | A1 | 2996 | C | N1-C2-O2 | 5.14 | 121.99 | 118.90 |
| 1 | A1 | 175 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 1 | A1 | 3080 | U | P-O3'-C3' | 5.14 | 125.86 | 119.70 |
| 2 | A2 | 960 | C | N3-C2-O2 | -5.14 | 118.30 | 121.90 |
| 1 | A1 | 3193 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 1 | A1 | 3041 | C | N3-C2-O2 | -5.11 | 118.33 | 121.90 |
| 1 | A1 | 2977 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 1 | A1 | 3078 | U | N1-C2-O2 | 5.09 | 126.36 | 122.80 |
| 1 | A1 | 904 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 1 | A1 | 172 | C | N3-C2-O2 | -5.05 | 118.36 | 121.90 |
| 1 | A1 | 1557 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 1 | A1 | 3193 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 1 | A1 | 2994 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 2 | A2 | 1454 | G | C4-N9-C1' | 5.00 | 133.00 | 126.50 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 13 | G1 | 177 | PRO | Peptide |
| 18 | I2 | 46 | PRO | Peptide |
| 67 | h1 | 105 | TYR | Peptide |
| 72 | l1 | 39 | TYR | Peptide |

## 5.2 Too-close contacts (i)

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

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 4 | B2 | 207/290 (71%) | 200 (97%) | 7 (3%) | 0 | 100 | 100 |
| 6 | C2 | 210/256 (82%) | 201 (96%) | 9 (4%) | 0 | 100 | 100 |
| 7 | D1 | 243/254 (96%) | 226 (93%) | 17 (7%) | 0 | 100 | 100 |
| 8 | D2 | 208/265 (78%) | 197 (95%) | 11 (5%) | 0 | 100 | 100 |
| 9 | E1 | 383/392 (98%) | 370 (97%) | 13 (3%) | 0 | 100 | 100 |
| 10 | E2 | 222/262 (85%) | 213 (96%) | 8 (4%) | 1 (0%) | 29 | 54 |
| 11 | F1 | 358/361 (99%) | 340 (95%) | 18 (5%) | 0 | 100 | 100 |
| 12 | F2 | 254/261 (97%) | 240 (94%) | 14 (6%) | 0 | 100 | 100 |
| 13 | G1 | 298/301 (99%) | 287 (96%) | 11 (4%) | 0 | 100 | 100 |
| 14 | G2 | 200/213 (94%) | 192 (96%) | 8 (4%) | 0 | 100 | 100 |
| 15 | H1 | 190/202 (94%) | 170 (90%) | 20 (10%) | 0 | 100 | 100 |
| 16 | H2 | 220/239 (92%) | 208 (94%) | 12 (6%) | 0 | 100 | 100 |
| 17 | I1 | 245/248 (99%) | 226 (92%) | 18 (7%) | 1 (0%) | 34 | 60 |
| 18 | I2 | 185/202 (92%) | 177 (96%) | 8 (4%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 19 | J1 | 234/262 (89%) | 221 (94%) | 12 (5%) | 1 (0%) | 34 60 |
| 20 | J2 | 179/202 (89%) | 176 (98%) | 3 (2%) | 0 | 100 100 |
| 21 | K1 | 188/193 (97%) | 174 (93%) | 14 (7%) | 0 | 100 100 |
| 22 | K2 | 172/190 (90%) | 167 (97%) | 5 (3%) | 0 | 100 100 |
| 23 | L1 | 215/221 (97%) | 205 (95%) | 10 (5%) | 0 | 100 100 |
| 24 | L2 | 88/163 (54%) | 87 (99%) | 1 (1%) | 0 | 100 100 |
| 25 | M1 | 163/174 (94%) | 159 (98%) | 4 (2%) | 0 | 100 100 |
| 26 | M2 | 127/161 (79%) | 119 (94%) | 8 (6%) | 0 | 100 100 |
| 27 | N1 | 211/214 (99%) | 206 (98%) | 5 (2%) | 0 | 100 100 |
| 28 | N2 | 114/147 (78%) | 113 (99%) | 1 (1%) | 0 | 100 100 |
| 29 | O1 | 139/142 (98%) | 134 (96%) | 5 (4%) | 0 | 100 100 |
| 30 | O2 | 148/151 (98%) | 143 (97%) | 5 (3%) | 0 | 100 100 |
| 31 | P1 | 200/203 (98%) | 187 (94%) | 13 (6%) | 0 | 100 100 |
| 32 | P2 | 124/150 (83%) | 120 (97%) | 4 (3%) | 0 | 100 100 |
| 33 | Q1 | 197/231 (85%) | 193 (98%) | 4 (2%) | 0 | 100 100 |
| 34 | Q2 | 125/152 (82%) | 119 (95%) | 5 (4%) | 1 (1%) | 19 43 |
| 35 | R1 | 164/186 (88%) | 155 (94%) | 9 (6%) | 0 | 100 100 |
| 36 | R2 | 137/142 (96%) | 133 (97%) | 4 (3%) | 0 | 100 100 |
| 37 | S1 | 180/183 (98%) | 174 (97%) | 6 (3%) | 0 | 100 100 |
| 38 | S2 | 120/146 (82%) | 115 (96%) | 5 (4%) | 0 | 100 100 |
| 39 | T1 | 189/192 (98%) | 187 (99%) | 2 (1%) | 0 | 100 100 |
| 40 | T2 | 139/156 (89%) | 127 (91%) | 12 (9%) | 0 | 100 100 |
| 41 | U1 | 171/174 (98%) | 163 (95%) | 8 (5%) | 0 | 100 100 |
| 42 | U2 | 141/149 (95%) | 137 (97%) | 4 (3%) | 0 | 100 100 |
| 43 | V1 | 157/160 (98%) | 153 (98%) | 2 (1%) | 2 (1%) | 12 30 |
| 44 | V2 | 97/117 (83%) | 95 (98%) | 2 (2%) | 0 | 100 100 |
| 45 | W1 | 99/126 (79%) | 99 (100%) | 0 | 0 | 100 100 |
| 46 | W2 | 84/87 (97%) | 80 (95%) | 4 (5%) | 0 | 100 100 |
| 47 | X1 | 134/139 (96%) | 125 (93%) | 9 (7%) | 0 | 100 100 |
| 48 | X2 | 127/130 (98%) | 119 (94%) | 8 (6%) | 0 | 100 100 |
| 49 | Y1 | 59/156 (38%) | 56 (95%) | 3 (5%) | 0 | 100 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 50 | Y2 | 142/145 (98%) | 139 (98%) | 3 (2%) | 0 | 100 | 100 |
| 51 | Z1 | 116/156 (74%) | 111 (96%) | 5 (4%) | 0 | 100 | 100 |
| 52 | Z2 | 122/136 (90%) | 117 (96%) | 5 (4%) | 0 | 100 | 100 |
| 53 | a1 | 119/136 (88%) | 114 (96%) | 5 (4%) | 0 | 100 | 100 |
| 54 | a2 | 69/97 (71%) | 68 (99%) | 1 (1%) | 0 | 100 | 100 |
| 55 | b1 | 133/135 (98%) | 127 (96%) | 6 (4%) | 0 | 100 | 100 |
| 56 | b2 | 97/119 (82%) | 92 (95%) | 5 (5%) | 0 | 100 | 100 |
| 57 | c1 | 146/149 (98%) | 130 (89%) | 16 (11%) | 0 | 100 | 100 |
| 58 | c2 | 79/82 (96%) | 73 (92%) | 6 (8%) | 0 | 100 | 100 |
| 59 | d1 | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 60 | d2 | 60/68 (88%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 61 | e1 | 89/109 (82%) | 89 (100%) | 0 | 0 | 100 | 100 |
| 62 | e2 | 53/56 (95%) | 52 (98%) | 1 (2%) | 0 | 100 | 100 |
| 63 | f1 | 102/122 (84%) | 97 (95%) | 5 (5%) | 0 | 100 | 100 |
| 64 | f2 | 41/63 (65%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |
| 65 | g1 | 119/131 (91%) | 113 (95%) | 6 (5%) | 0 | 100 | 100 |
| 66 | g2 | 39/154 (25%) | 37 (95%) | 2 (5%) | 0 | 100 | 100 |
| 67 | h1 | 106/109 (97%) | 100 (94%) | 5 (5%) | 1 (1%) | 17 | 40 |
| 68 | h2 | 308/316 (98%) | 292 (95%) | 16 (5%) | 0 | 100 | 100 |
| 69 | i1 | 106/117 (91%) | 103 (97%) | 3 (3%) | 0 | 100 | 100 |
| 70 | j1 | 114/125 (91%) | 110 (96%) | 4 (4%) | 0 | 100 | 100 |
| 71 | k1 | 94/104 (90%) | 91 (97%) | 3 (3%) | 0 | 100 | 100 |
| 72 | l1 | 86/92 (94%) | 78 (91%) | 8 (9%) | 0 | 100 | 100 |
| 73 | m1 | 71/80 (89%) | 67 (94%) | 3 (4%) | 1 (1%) | 11 | 28 |
| 74 | n1 | 48/51 (94%) | 45 (94%) | 2 (4%) | 1 (2%) | 7 | 18 |
| 75 | o1 | 47/52 (90%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 76 | p1 | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 77 | q1 | 103/106 (97%) | 97 (94%) | 6 (6%) | 0 | 100 | 100 |
| 78 | r1 | 83/92 (90%) | 79 (95%) | 4 (5%) | 0 | 100 | 100 |
| 79 | s1 | 147/150 (98%) | 139 (95%) | 8 (5%) | 0 | 100 | 100 |
| All | All | 10969/12287 (89%) | 10478 (96%) | 482 (4%) | 9 (0%) | 54 | 78 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 43 | V1 | 69 | LYS |
| 43 | V1 | 157 | GLU |
| 67 | h1 | 22 | ARG |
| 10 | E2 | 48 | VAL |
| 73 | m1 | 71 | VAL |
| 17 | I1 | 84 | ALA |
| 74 | n1 | 7 | PHE |
| 19 | J1 | 166 | VAL |
| 34 | Q2 | 131 | LYS |

### 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 | |
|---|---|---|---|---|---|---|
| 4 | B2 | 172/225 (76%) | 172 (100%) | 0 | 100 | 100 |
| 6 | C2 | 187/224 (84%) | 187 (100%) | 0 | 100 | 100 |
| 7 | D1 | 188/196 (96%) | 188 (100%) | 0 | 100 | 100 |
| 8 | D2 | 176/211 (83%) | 176 (100%) | 0 | 100 | 100 |
| 9 | E1 | 323/328 (98%) | 323 (100%) | 0 | 100 | 100 |
| 10 | E2 | 188/209 (90%) | 188 (100%) | 0 | 100 | 100 |
| 11 | F1 | 281/282 (100%) | 278 (99%) | 3 (1%) | 73 | 90 |
| 12 | F2 | 219/222 (99%) | 218 (100%) | 1 (0%) | 88 | 96 |
| 13 | G1 | 244/245 (100%) | 244 (100%) | 0 | 100 | 100 |
| 14 | G2 | 171/179 (96%) | 171 (100%) | 0 | 100 | 100 |
| 15 | H1 | 162/168 (96%) | 162 (100%) | 0 | 100 | 100 |
| 16 | H2 | 188/202 (93%) | 186 (99%) | 2 (1%) | 73 | 90 |
| 17 | I1 | 216/217 (100%) | 216 (100%) | 0 | 100 | 100 |
| 18 | I2 | 167/178 (94%) | 165 (99%) | 2 (1%) | 71 | 88 |
| 19 | J1 | 201/219 (92%) | 201 (100%) | 0 | 100 | 100 |
| 20 | J2 | 146/163 (90%) | 146 (100%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 21 | K1 | 168/171 (98%) | 168 (100%) | 0 | 100 | 100 |
| 22 | K2 | 151/161 (94%) | 151 (100%) | 0 | 100 | 100 |
| 23 | L1 | 181/184 (98%) | 180 (99%) | 1 (1%) | 86 | 95 |
| 24 | L2 | 80/127 (63%) | 80 (100%) | 0 | 100 | 100 |
| 25 | M1 | 143/151 (95%) | 142 (99%) | 1 (1%) | 84 | 94 |
| 26 | M2 | 114/139 (82%) | 113 (99%) | 1 (1%) | 78 | 92 |
| 27 | N1 | 172/173 (99%) | 172 (100%) | 0 | 100 | 100 |
| 28 | N2 | 99/125 (79%) | 99 (100%) | 0 | 100 | 100 |
| 29 | O1 | 115/116 (99%) | 115 (100%) | 0 | 100 | 100 |
| 30 | O2 | 131/132 (99%) | 131 (100%) | 0 | 100 | 100 |
| 31 | P1 | 178/179 (99%) | 178 (100%) | 0 | 100 | 100 |
| 32 | P2 | 96/115 (84%) | 96 (100%) | 0 | 100 | 100 |
| 33 | Q1 | 164/192 (85%) | 164 (100%) | 0 | 100 | 100 |
| 34 | Q2 | 109/130 (84%) | 108 (99%) | 1 (1%) | 78 | 92 |
| 35 | R1 | 131/146 (90%) | 130 (99%) | 1 (1%) | 81 | 93 |
| 36 | R2 | 112/114 (98%) | 112 (100%) | 0 | 100 | 100 |
| 37 | S1 | 152/153 (99%) | 152 (100%) | 0 | 100 | 100 |
| 38 | S2 | 112/132 (85%) | 111 (99%) | 1 (1%) | 78 | 92 |
| 39 | T1 | 159/160 (99%) | 159 (100%) | 0 | 100 | 100 |
| 40 | T2 | 123/136 (90%) | 123 (100%) | 0 | 100 | 100 |
| 41 | U1 | 153/154 (99%) | 153 (100%) | 0 | 100 | 100 |
| 42 | U2 | 117/123 (95%) | 117 (100%) | 0 | 100 | 100 |
| 43 | V1 | 134/135 (99%) | 134 (100%) | 0 | 100 | 100 |
| 44 | V2 | 90/105 (86%) | 90 (100%) | 0 | 100 | 100 |
| 45 | W1 | 89/109 (82%) | 89 (100%) | 0 | 100 | 100 |
| 46 | W2 | 71/72 (99%) | 71 (100%) | 0 | 100 | 100 |
| 47 | X1 | 104/106 (98%) | 103 (99%) | 1 (1%) | 76 | 91 |
| 48 | X2 | 112/113 (99%) | 112 (100%) | 0 | 100 | 100 |
| 49 | Y1 | 55/125 (44%) | 55 (100%) | 0 | 100 | 100 |
| 50 | Y2 | 116/117 (99%) | 115 (99%) | 1 (1%) | 78 | 92 |
| 51 | Z1 | 104/128 (81%) | 104 (100%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 52 | Z2 | 109/118 (92%) | 108 (99%) | 1 (1%) | 78 92 |
| 53 | a1 | 110/122 (90%) | 109 (99%) | 1 (1%) | 78 92 |
| 54 | a2 | 63/81 (78%) | 63 (100%) | 0 | 100 100 |
| 55 | b1 | 122/122 (100%) | 122 (100%) | 0 | 100 100 |
| 56 | b2 | 87/103 (84%) | 86 (99%) | 1 (1%) | 73 90 |
| 57 | c1 | 116/117 (99%) | 116 (100%) | 0 | 100 100 |
| 58 | c2 | 70/71 (99%) | 70 (100%) | 0 | 100 100 |
| 59 | d1 | 54/55 (98%) | 54 (100%) | 0 | 100 100 |
| 60 | d2 | 55/61 (90%) | 55 (100%) | 0 | 100 100 |
| 61 | e1 | 74/89 (83%) | 74 (100%) | 0 | 100 100 |
| 62 | e2 | 48/49 (98%) | 48 (100%) | 0 | 100 100 |
| 63 | f1 | 90/105 (86%) | 90 (100%) | 0 | 100 100 |
| 64 | f2 | 37/51 (72%) | 37 (100%) | 0 | 100 100 |
| 65 | g1 | 104/113 (92%) | 104 (100%) | 0 | 100 100 |
| 66 | g2 | 34/138 (25%) | 34 (100%) | 0 | 100 100 |
| 67 | h1 | 88/89 (99%) | 88 (100%) | 0 | 100 100 |
| 68 | h2 | 272/276 (99%) | 272 (100%) | 0 | 100 100 |
| 69 | i1 | 93/101 (92%) | 93 (100%) | 0 | 100 100 |
| 70 | j1 | 103/109 (94%) | 102 (99%) | 1 (1%) | 76 91 |
| 71 | k1 | 78/82 (95%) | 78 (100%) | 0 | 100 100 |
| 72 | l1 | 73/75 (97%) | 73 (100%) | 0 | 100 100 |
| 73 | m1 | 64/70 (91%) | 64 (100%) | 0 | 100 100 |
| 74 | n1 | 45/46 (98%) | 45 (100%) | 0 | 100 100 |
| 75 | o1 | 44/47 (94%) | 44 (100%) | 0 | 100 100 |
| 76 | p1 | 23/23 (100%) | 23 (100%) | 0 | 100 100 |
| 77 | q1 | 87/88 (99%) | 87 (100%) | 0 | 100 100 |
| 78 | r1 | 68/75 (91%) | 68 (100%) | 0 | 100 100 |
| 79 | s1 | 112/113 (99%) | 112 (100%) | 0 | 100 100 |
| All | All | 9387/10280 (91%) | 9367 (100%) | 20 (0%) | 93 98 |

All (20) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | F1 | 199 | ARG |
| 11 | F1 | 299 | ARG |
| 11 | F1 | 311 | ASN |
| 12 | F2 | 232 | LYS |
| 16 | H2 | 65 | GLN |
| 16 | H2 | 217 | LYS |
| 18 | I2 | 8 | LYS |
| 18 | I2 | 115 | ARG |
| 23 | L1 | 55 | ASN |
| 25 | M1 | 103 | ASN |
| 26 | M2 | 72 | ARG |
| 34 | Q2 | 65 | LYS |
| 35 | R1 | 111 | ASN |
| 38 | S2 | 109 | LYS |
| 47 | X1 | 47 | ARG |
| 50 | Y2 | 114 | LYS |
| 52 | Z2 | 66 | GLN |
| 53 | a1 | 87 | ARG |
| 56 | b2 | 12 | LYS |
| 70 | j1 | 63 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | B2 | 52 | ASN |
| 9 | E1 | 3 | HIS |
| 11 | F1 | 311 | ASN |
| 16 | H2 | 116 | GLN |
| 19 | J1 | 41 | GLN |
| 46 | W2 | 50 | ASN |
| 48 | X2 | 42 | GLN |
| 51 | Z1 | 110 | GLN |
| 52 | Z2 | 32 | HIS |
| 54 | a2 | 43 | GLN |
| 54 | a2 | 76 | GLN |
| 74 | n1 | 17 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | A1 | 3119/3338 (93%) | 419 (13%) | 12 (0%) |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 2 | A2 | 1765/1796 (98%) | 244 (13%) | 0 |
| 3 | B1 | 119/120 (99%) | 9 (7%) | 0 |
| 5 | C1 | 157/158 (99%) | 21 (13%) | 1 (0%) |
| 80 | t1 | 75/76 (98%) | 12 (16%) | 0 |
| 80 | u1 | 75/76 (98%) | 9 (12%) | 0 |
| 82 | w1 | 16/17 (94%) | 6 (37%) | 0 |
| All | All | 5326/5581 (95%) | 720 (13%) | 13 (0%) |

All (720) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 6 | A |
| 1 | A1 | 22 | G |
| 1 | A1 | 26 | A |
| 1 | A1 | 40 | A |
| 1 | A1 | 43 | A |
| 1 | A1 | 49 | A |
| 1 | A1 | 59 | G |
| 1 | A1 | 60 | A |
| 1 | A1 | 65 | A |
| 1 | A1 | 66 | A |
| 1 | A1 | 75 | G |
| 1 | A1 | 92 | G |
| 1 | A1 | 116 | A |
| 1 | A1 | 117 | U |
| 1 | A1 | 118 | U |
| 1 | A1 | 122 | A |
| 1 | A1 | 132 | C |
| 1 | A1 | 133 | G |
| 1 | A1 | 134 | G |
| 1 | A1 | 151 | U |
| 1 | A1 | 152 | A |
| 1 | A1 | 157 | A |
| 1 | A1 | 164 | U |
| 1 | A1 | 165 | G |
| 1 | A1 | 166 | G |
| 1 | A1 | 167 | U |
| 1 | A1 | 168 | G |
| 1 | A1 | 169 | A |
| 1 | A1 | 170 | G |
| 1 | A1 | 171 | G |
| 1 | A1 | 172 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 173 | A |
| 1 | A1 | 175 | C |
| 1 | A1 | 180 | G |
| 1 | A1 | 183 | U |
| 1 | A1 | 184 | C |
| 1 | A1 | 193 | C |
| 1 | A1 | 212 | A |
| 1 | A1 | 214 | A |
| 1 | A1 | 223 | U |
| 1 | A1 | 224 | A |
| 1 | A1 | 225 | G |
| 1 | A1 | 226 | U |
| 1 | A1 | 227 | C |
| 1 | A1 | 228 | G |
| 1 | A1 | 230 | A |
| 1 | A1 | 233 | C |
| 1 | A1 | 236 | A |
| 1 | A1 | 237 | U |
| 1 | A1 | 240 | A |
| 1 | A1 | 242 | U |
| 1 | A1 | 244 | U |
| 1 | A1 | 245 | A |
| 1 | A1 | 246 | A |
| 1 | A1 | 247 | A |
| 1 | A1 | 248 | G |
| 1 | A1 | 252 | C |
| 1 | A1 | 255 | C |
| 1 | A1 | 261 | G |
| 1 | A1 | 278 | U |
| 1 | A1 | 287 | A |
| 1 | A1 | 297 | U |
| 1 | A1 | 342 | C |
| 1 | A1 | 368 | G |
| 1 | A1 | 391 | A |
| 1 | A1 | 395 | C |
| 1 | A1 | 413 | G |
| 1 | A1 | 414 | A |
| 1 | A1 | 421 | U |
| 1 | A1 | 433 | U |
| 1 | A1 | 440 | U |
| 1 | A1 | 441 | U |
| 1 | A1 | 442 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 445 | A |
| 1 | A1 | 449 | U |
| 1 | A1 | 457 | U |
| 1 | A1 | 463 | C |
| 1 | A1 | 465 | G |
| 1 | A1 | 469 | A |
| 1 | A1 | 471 | U |
| 1 | A1 | 475 | G |
| 1 | A1 | 476 | A |
| 1 | A1 | 477 | C |
| 1 | A1 | 511 | A |
| 1 | A1 | 513 | A |
| 1 | A1 | 544 | U |
| 1 | A1 | 546 | A |
| 1 | A1 | 547 | U |
| 1 | A1 | 548 | A |
| 1 | A1 | 549 | G |
| 1 | A1 | 568 | C |
| 1 | A1 | 579 | A |
| 1 | A1 | 582 | U |
| 1 | A1 | 591 | C |
| 1 | A1 | 593 | G |
| 1 | A1 | 599 | A |
| 1 | A1 | 608 | U |
| 1 | A1 | 609 | A |
| 1 | A1 | 610 | A |
| 1 | A1 | 624 | C |
| 1 | A1 | 625 | C |
| 1 | A1 | 637 | A |
| 1 | A1 | 648 | A |
| 1 | A1 | 650 | U |
| 1 | A1 | 665 | A |
| 1 | A1 | 669 | U |
| 1 | A1 | 678 | A |
| 1 | A1 | 700 | G |
| 1 | A1 | 720 | C |
| 1 | A1 | 721 | G |
| 1 | A1 | 722 | G |
| 1 | A1 | 748 | U |
| 1 | A1 | 749 | U |
| 1 | A1 | 758 | U |
| 1 | A1 | 762 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 763 | G |
| 1 | A1 | 767 | G |
| 1 | A1 | 781 | G |
| 1 | A1 | 783 | A |
| 1 | A1 | 798 | A |
| 1 | A1 | 799 | A |
| 1 | A1 | 812 | A |
| 1 | A1 | 831 | C |
| 1 | A1 | 839 | G |
| 1 | A1 | 843 | C |
| 1 | A1 | 856 | U |
| 1 | A1 | 861 | U |
| 1 | A1 | 877 | A |
| 1 | A1 | 878 | A |
| 1 | A1 | 879 | U |
| 1 | A1 | 889 | G |
| 1 | A1 | 890 | G |
| 1 | A1 | 896 | A |
| 1 | A1 | 898 | G |
| 1 | A1 | 899 | A |
| 1 | A1 | 903 | A |
| 1 | A1 | 905 | C |
| 1 | A1 | 906 | G |
| 1 | A1 | 907 | A |
| 1 | A1 | 919 | G |
| 1 | A1 | 926 | A |
| 1 | A1 | 941 | C |
| 1 | A1 | 956 | U |
| 1 | A1 | 961 | C |
| 1 | A1 | 963 | U |
| 1 | A1 | 964 | C |
| 1 | A1 | 992 | G |
| 1 | A1 | 1030 | A |
| 1 | A1 | 1047 | A |
| 1 | A1 | 1064 | U |
| 1 | A1 | 1077 | U |
| 1 | A1 | 1078 | U |
| 1 | A1 | 1080 | G |
| 1 | A1 | 1081 | A |
| 1 | A1 | 1086 | A |
| 1 | A1 | 1100 | G |
| 1 | A1 | 1114 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 1127 | U |
| 1 | A1 | 1136 | A |
| 1 | A1 | 1137 | A |
| 1 | A1 | 1142 | A |
| 1 | A1 | 1161 | G |
| 1 | A1 | 1163 | G |
| 1 | A1 | 1164 | U |
| 1 | A1 | 1165 | G |
| 1 | A1 | 1179 | C |
| 1 | A1 | 1184 | C |
| 1 | A1 | 1192 | G |
| 1 | A1 | 1200 | A |
| 1 | A1 | 1205 | G |
| 1 | A1 | 1211 | A |
| 1 | A1 | 1212 | G |
| 1 | A1 | 1215 | C |
| 1 | A1 | 1218 | U |
| 1 | A1 | 1219 | G |
| 1 | A1 | 1223 | A |
| 1 | A1 | 1228 | A |
| 1 | A1 | 1229 | G |
| 1 | A1 | 1231 | C |
| 1 | A1 | 1232 | G |
| 1 | A1 | 1236 | U |
| 1 | A1 | 1240 | C |
| 1 | A1 | 1242 | A |
| 1 | A1 | 1245 | G |
| 1 | A1 | 1246 | A |
| 1 | A1 | 1248 | U |
| 1 | A1 | 1249 | G |
| 1 | A1 | 1250 | U |
| 1 | A1 | 1251 | G |
| 1 | A1 | 1254 | A |
| 1 | A1 | 1261 | A |
| 1 | A1 | 1262 | C |
| 1 | A1 | 1264 | U |
| 1 | A1 | 1265 | G |
| 1 | A1 | 1268 | G |
| 1 | A1 | 1270 | A |
| 1 | A1 | 1278 | G |
| 1 | A1 | 1288 | U |
| 1 | A1 | 1290 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 1292 | U |
| 1 | A1 | 1296 | G |
| 1 | A1 | 1313 | A |
| 1 | A1 | 1331 | A |
| 1 | A1 | 1332 | G |
| 1 | A1 | 1333 | A |
| 1 | A1 | 1335 | A |
| 1 | A1 | 1336 | C |
| 1 | A1 | 1337 | G |
| 1 | A1 | 1369 | A |
| 1 | A1 | 1370 | G |
| 1 | A1 | 1382 | A |
| 1 | A1 | 1383 | G |
| 1 | A1 | 1401 | A |
| 1 | A1 | 1417 | G |
| 1 | A1 | 1420 | C |
| 1 | A1 | 1429 | A |
| 1 | A1 | 1433 | G |
| 1 | A1 | 1464 | A |
| 1 | A1 | 1470 | G |
| 1 | A1 | 1485 | G |
| 1 | A1 | 1506 | U |
| 1 | A1 | 1519 | G |
| 1 | A1 | 1522 | A |
| 1 | A1 | 1527 | G |
| 1 | A1 | 1538 | U |
| 1 | A1 | 1540 | A |
| 1 | A1 | 1545 | G |
| 1 | A1 | 1561 | G |
| 1 | A1 | 1562 | U |
| 1 | A1 | 1563 | G |
| 1 | A1 | 1567 | A |
| 1 | A1 | 1569 | A |
| 1 | A1 | 1570 | G |
| 1 | A1 | 1585 | A |
| 1 | A1 | 1608 | U |
| 1 | A1 | 1622 | A |
| 1 | A1 | 1623 | A |
| 1 | A1 | 1637 | C |
| 1 | A1 | 1680 | G |
| 1 | A1 | 1704 | U |
| 1 | A1 | 1709 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 1730 | A |
| 1 | A1 | 1731 | G |
| 1 | A1 | 1739 | C |
| 1 | A1 | 1743 | U |
| 1 | A1 | 1745 | U |
| 1 | A1 | 1776 | G |
| 1 | A1 | 1777 | A |
| 1 | A1 | 1794 | A |
| 1 | A1 | 1796 | A |
| 1 | A1 | 1800 | C |
| 1 | A1 | 1801 | U |
| 1 | A1 | 1822 | A |
| 1 | A1 | 1846 | C |
| 1 | A1 | 1858 | G |
| 1 | A1 | 1860 | U |
| 1 | A1 | 1873 | A |
| 1 | A1 | 1886 | G |
| 1 | A1 | 1887 | C |
| 1 | A1 | 1923 | C |
| 1 | A1 | 2061 | C |
| 1 | A1 | 2074 | G |
| 1 | A1 | 2075 | G |
| 1 | A1 | 2076 | U |
| 1 | A1 | 2078 | C |
| 1 | A1 | 2086 | G |
| 1 | A1 | 2095 | A |
| 1 | A1 | 2108 | A |
| 1 | A1 | 2122 | A |
| 1 | A1 | 2133 | G |
| 1 | A1 | 2140 | U |
| 1 | A1 | 2162 | A |
| 1 | A1 | 2170 | G |
| 1 | A1 | 2171 | A |
| 1 | A1 | 2173 | U |
| 1 | A1 | 2213 | G |
| 1 | A1 | 2220 | A |
| 1 | A1 | 2236 | G |
| 1 | A1 | 2237 | G |
| 1 | A1 | 2244 | A |
| 1 | A1 | 2245 | A |
| 1 | A1 | 2271 | G |
| 1 | A1 | 2272 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 2274 | U |
| 1 | A1 | 2277 | A |
| 1 | A1 | 2279 | G |
| 1 | A1 | 2298 | U |
| 1 | A1 | 2299 | G |
| 1 | A1 | 2337 | A |
| 1 | A1 | 2338 | C |
| 1 | A1 | 2339 | G |
| 1 | A1 | 2357 | G |
| 1 | A1 | 2361 | A |
| 1 | A1 | 2366 | A |
| 1 | A1 | 2367 | G |
| 1 | A1 | 2368 | A |
| 1 | A1 | 2375 | U |
| 1 | A1 | 2399 | G |
| 1 | A1 | 2405 | A |
| 1 | A1 | 2469 | U |
| 1 | A1 | 2478 | U |
| 1 | A1 | 2479 | A |
| 1 | A1 | 2501 | U |
| 1 | A1 | 2502 | U |
| 1 | A1 | 2503 | U |
| 1 | A1 | 2511 | C |
| 1 | A1 | 2512 | U |
| 1 | A1 | 2514 | C |
| 1 | A1 | 2517 | G |
| 1 | A1 | 2522 | A |
| 1 | A1 | 2523 | A |
| 1 | A1 | 2532 | G |
| 1 | A1 | 2534 | G |
| 1 | A1 | 2545 | G |
| 1 | A1 | 2553 | A |
| 1 | A1 | 2566 | G |
| 1 | A1 | 2567 | G |
| 1 | A1 | 2574 | G |
| 1 | A1 | 2586 | A |
| 1 | A1 | 2595 | A |
| 1 | A1 | 2612 | U |
| 1 | A1 | 2616 | A |
| 1 | A1 | 2634 | A |
| 1 | A1 | 2637 | G |
| 1 | A1 | 2649 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 2651 | A |
| 1 | A1 | 2654 | A |
| 1 | A1 | 2674 | G |
| 1 | A1 | 2679 | U |
| 1 | A1 | 2688 | G |
| 1 | A1 | 2689 | U |
| 1 | A1 | 2697 | C |
| 1 | A1 | 2713 | G |
| 1 | A1 | 2715 | C |
| 1 | A1 | 2722 | A |
| 1 | A1 | 2732 | C |
| 1 | A1 | 2733 | C |
| 1 | A1 | 2737 | G |
| 1 | A1 | 2738 | A |
| 1 | A1 | 2760 | G |
| 1 | A1 | 2761 | A |
| 1 | A1 | 2762 | A |
| 1 | A1 | 2763 | A |
| 1 | A1 | 2770 | C |
| 1 | A1 | 2777 | A |
| 1 | A1 | 2804 | C |
| 1 | A1 | 2805 | A |
| 1 | A1 | 2827 | C |
| 1 | A1 | 2831 | G |
| 1 | A1 | 2835 | U |
| 1 | A1 | 2847 | A |
| 1 | A1 | 2849 | C |
| 1 | A1 | 2858 | G |
| 1 | A1 | 2895 | U |
| 1 | A1 | 2896 | A |
| 1 | A1 | 2907 | G |
| 1 | A1 | 2931 | A |
| 1 | A1 | 2943 | C |
| 1 | A1 | 2950 | G |
| 1 | A1 | 2970 | A |
| 1 | A1 | 2981 | G |
| 1 | A1 | 2996 | C |
| 1 | A1 | 3015 | U |
| 1 | A1 | 3018 | G |
| 1 | A1 | 3028 | G |
| 1 | A1 | 3029 | A |
| 1 | A1 | 3030 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 3031 | C |
| 1 | A1 | 3037 | G |
| 1 | A1 | 3038 | U |
| 1 | A1 | 3051 | C |
| 1 | A1 | 3052 | C |
| 1 | A1 | 3058 | C |
| 1 | A1 | 3063 | U |
| 1 | A1 | 3074 | C |
| 1 | A1 | 3077 | C |
| 1 | A1 | 3078 | U |
| 1 | A1 | 3079 | C |
| 1 | A1 | 3081 | A |
| 1 | A1 | 3089 | A |
| 1 | A1 | 3090 | U |
| 1 | A1 | 3101 | A |
| 1 | A1 | 3113 | C |
| 1 | A1 | 3114 | U |
| 1 | A1 | 3124 | U |
| 1 | A1 | 3128 | G |
| 1 | A1 | 3136 | A |
| 1 | A1 | 3142 | G |
| 1 | A1 | 3146 | C |
| 1 | A1 | 3147 | C |
| 1 | A1 | 3156 | A |
| 1 | A1 | 3163 | C |
| 1 | A1 | 3164 | A |
| 1 | A1 | 3165 | G |
| 1 | A1 | 3185 | U |
| 1 | A1 | 3189 | G |
| 1 | A1 | 3193 | C |
| 1 | A1 | 3201 | A |
| 1 | A1 | 3205 | C |
| 1 | A1 | 3215 | A |
| 1 | A1 | 3246 | C |
| 1 | A1 | 3249 | A |
| 1 | A1 | 3255 | U |
| 1 | A1 | 3258 | A |
| 1 | A1 | 3259 | U |
| 1 | A1 | 3262 | G |
| 1 | A1 | 3277 | A |
| 1 | A1 | 3283 | U |
| 1 | A1 | 3284 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 3287 | G |
| 1 | A1 | 3294 | U |
| 1 | A1 | 3296 | U |
| 1 | A1 | 3297 | U |
| 1 | A1 | 3298 | G |
| 1 | A1 | 3311 | G |
| 1 | A1 | 3320 | C |
| 1 | A1 | 3324 | C |
| 1 | A1 | 3331 | C |
| 1 | A1 | 3332 | U |
| 2 | A2 | 2 | A |
| 2 | A2 | 4 | C |
| 2 | A2 | 17 | C |
| 2 | A2 | 26 | A |
| 2 | A2 | 34 | G |
| 2 | A2 | 42 | G |
| 2 | A2 | 43 | A |
| 2 | A2 | 45 | U |
| 2 | A2 | 47 | A |
| 2 | A2 | 63 | G |
| 2 | A2 | 72 | A |
| 2 | A2 | 78 | C |
| 2 | A2 | 79 | C |
| 2 | A2 | 80 | G |
| 2 | A2 | 103 | A |
| 2 | A2 | 113 | A |
| 2 | A2 | 115 | U |
| 2 | A2 | 125 | A |
| 2 | A2 | 126 | G |
| 2 | A2 | 130 | C |
| 2 | A2 | 138 | A |
| 2 | A2 | 166 | A |
| 2 | A2 | 181 | C |
| 2 | A2 | 187 | U |
| 2 | A2 | 189 | C |
| 2 | A2 | 212 | U |
| 2 | A2 | 216 | A |
| 2 | A2 | 217 | A |
| 2 | A2 | 220 | A |
| 2 | A2 | 223 | G |
| 2 | A2 | 227 | U |
| 2 | A2 | 229 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A2 | 230 | G |
| 2 | A2 | 236 | A |
| 2 | A2 | 258 | C |
| 2 | A2 | 262 | A |
| 2 | A2 | 269 | U |
| 2 | A2 | 277 | C |
| 2 | A2 | 278 | G |
| 2 | A2 | 284 | G |
| 2 | A2 | 296 | A |
| 2 | A2 | 299 | U |
| 2 | A2 | 311 | C |
| 2 | A2 | 313 | A |
| 2 | A2 | 334 | G |
| 2 | A2 | 335 | C |
| 2 | A2 | 338 | G |
| 2 | A2 | 349 | A |
| 2 | A2 | 356 | A |
| 2 | A2 | 358 | C |
| 2 | A2 | 397 | A |
| 2 | A2 | 398 | A |
| 2 | A2 | 399 | C |
| 2 | A2 | 421 | C |
| 2 | A2 | 423 | G |
| 2 | A2 | 431 | G |
| 2 | A2 | 436 | U |
| 2 | A2 | 441 | C |
| 2 | A2 | 442 | A |
| 2 | A2 | 465 | A |
| 2 | A2 | 474 | A |
| 2 | A2 | 485 | G |
| 2 | A2 | 491 | U |
| 2 | A2 | 492 | U |
| 2 | A2 | 493 | G |
| 2 | A2 | 494 | G |
| 2 | A2 | 495 | G |
| 2 | A2 | 502 | A |
| 2 | A2 | 503 | A |
| 2 | A2 | 504 | U |
| 2 | A2 | 505 | U |
| 2 | A2 | 512 | A |
| 2 | A2 | 538 | A |
| 2 | A2 | 539 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A2 | 552 | A |
| 2 | A2 | 562 | C |
| 2 | A2 | 565 | G |
| 2 | A2 | 576 | A |
| 2 | A2 | 591 | A |
| 2 | A2 | 603 | A |
| 2 | A2 | 608 | U |
| 2 | A2 | 616 | A |
| 2 | A2 | 617 | A |
| 2 | A2 | 619 | A |
| 2 | A2 | 620 | A |
| 2 | A2 | 636 | U |
| 2 | A2 | 642 | U |
| 2 | A2 | 652 | G |
| 2 | A2 | 653 | G |
| 2 | A2 | 654 | U |
| 2 | A2 | 678 | G |
| 2 | A2 | 689 | U |
| 2 | A2 | 697 | G |
| 2 | A2 | 698 | G |
| 2 | A2 | 699 | A |
| 2 | A2 | 700 | G |
| 2 | A2 | 702 | A |
| 2 | A2 | 704 | C |
| 2 | A2 | 716 | A |
| 2 | A2 | 719 | G |
| 2 | A2 | 720 | G |
| 2 | A2 | 724 | U |
| 2 | A2 | 734 | C |
| 2 | A2 | 736 | A |
| 2 | A2 | 737 | G |
| 2 | A2 | 741 | U |
| 2 | A2 | 754 | A |
| 2 | A2 | 764 | G |
| 2 | A2 | 765 | C |
| 2 | A2 | 774 | G |
| 2 | A2 | 781 | G |
| 2 | A2 | 782 | C |
| 2 | A2 | 787 | A |
| 2 | A2 | 792 | C |
| 2 | A2 | 793 | U |
| 2 | A2 | 804 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A2 | 809 | A |
| 2 | A2 | 818 | U |
| 2 | A2 | 819 | G |
| 2 | A2 | 832 | G |
| 2 | A2 | 834 | U |
| 2 | A2 | 835 | G |
| 2 | A2 | 839 | U |
| 2 | A2 | 842 | A |
| 2 | A2 | 854 | A |
| 2 | A2 | 861 | A |
| 2 | A2 | 874 | G |
| 2 | A2 | 884 | U |
| 2 | A2 | 895 | C |
| 2 | A2 | 896 | A |
| 2 | A2 | 911 | G |
| 2 | A2 | 931 | A |
| 2 | A2 | 933 | U |
| 2 | A2 | 958 | U |
| 2 | A2 | 964 | A |
| 2 | A2 | 1002 | U |
| 2 | A2 | 1003 | A |
| 2 | A2 | 1024 | A |
| 2 | A2 | 1026 | C |
| 2 | A2 | 1030 | G |
| 2 | A2 | 1037 | A |
| 2 | A2 | 1058 | U |
| 2 | A2 | 1073 | A |
| 2 | A2 | 1079 | C |
| 2 | A2 | 1089 | A |
| 2 | A2 | 1090 | A |
| 2 | A2 | 1094 | U |
| 2 | A2 | 1097 | G |
| 2 | A2 | 1135 | A |
| 2 | A2 | 1147 | G |
| 2 | A2 | 1155 | C |
| 2 | A2 | 1168 | A |
| 2 | A2 | 1170 | C |
| 2 | A2 | 1172 | U |
| 2 | A2 | 1175 | G |
| 2 | A2 | 1177 | C |
| 2 | A2 | 1178 | U |
| 2 | A2 | 1180 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A2 | 1181 | A |
| 2 | A2 | 1182 | U |
| 2 | A2 | 1191 | A |
| 2 | A2 | 1193 | A |
| 2 | A2 | 1196 | G |
| 2 | A2 | 1197 | G |
| 2 | A2 | 1199 | A |
| 2 | A2 | 1213 | C |
| 2 | A2 | 1214 | A |
| 2 | A2 | 1215 | G |
| 2 | A2 | 1223 | G |
| 2 | A2 | 1224 | A |
| 2 | A2 | 1225 | G |
| 2 | A2 | 1226 | G |
| 2 | A2 | 1228 | U |
| 2 | A2 | 1230 | G |
| 2 | A2 | 1238 | G |
| 2 | A2 | 1239 | A |
| 2 | A2 | 1241 | A |
| 2 | A2 | 1242 | G |
| 2 | A2 | 1245 | C |
| 2 | A2 | 1247 | U |
| 2 | A2 | 1251 | U |
| 2 | A2 | 1252 | G |
| 2 | A2 | 1253 | A |
| 2 | A2 | 1281 | C |
| 2 | A2 | 1298 | U |
| 2 | A2 | 1311 | U |
| 2 | A2 | 1312 | U |
| 2 | A2 | 1318 | A |
| 2 | A2 | 1358 | U |
| 2 | A2 | 1359 | U |
| 2 | A2 | 1360 | G |
| 2 | A2 | 1361 | G |
| 2 | A2 | 1363 | A |
| 2 | A2 | 1364 | G |
| 2 | A2 | 1367 | C |
| 2 | A2 | 1368 | G |
| 2 | A2 | 1369 | C |
| 2 | A2 | 1371 | G |
| 2 | A2 | 1387 | U |
| 2 | A2 | 1398 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A2 | 1409 | U |
| 2 | A2 | 1411 | U |
| 2 | A2 | 1423 | A |
| 2 | A2 | 1424 | G |
| 2 | A2 | 1429 | G |
| 2 | A2 | 1432 | A |
| 2 | A2 | 1441 | G |
| 2 | A2 | 1453 | C |
| 2 | A2 | 1455 | C |
| 2 | A2 | 1465 | A |
| 2 | A2 | 1467 | A |
| 2 | A2 | 1487 | C |
| 2 | A2 | 1492 | U |
| 2 | A2 | 1512 | A |
| 2 | A2 | 1517 | G |
| 2 | A2 | 1519 | U |
| 2 | A2 | 1520 | A |
| 2 | A2 | 1533 | C |
| 2 | A2 | 1538 | G |
| 2 | A2 | 1553 | U |
| 2 | A2 | 1555 | A |
| 2 | A2 | 1586 | G |
| 2 | A2 | 1597 | G |
| 2 | A2 | 1627 | A |
| 2 | A2 | 1631 | A |
| 2 | A2 | 1653 | U |
| 2 | A2 | 1654 | G |
| 2 | A2 | 1685 | A |
| 2 | A2 | 1691 | G |
| 2 | A2 | 1699 | C |
| 2 | A2 | 1732 | G |
| 2 | A2 | 1751 | A |
| 2 | A2 | 1752 | A |
| 2 | A2 | 1753 | G |
| 2 | A2 | 1756 | G |
| 2 | A2 | 1762 | A |
| 2 | A2 | 1765 | U |
| 2 | A2 | 1776 | G |
| 2 | A2 | 1778 | A |
| 2 | A2 | 1788 | G |
| 2 | A2 | 1789 | G |
| 2 | A2 | 1790 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A2 | 1792 | C |
| 2 | A2 | 1795 | U |
| 3 | B1 | 7 | G |
| 3 | B1 | 29 | G |
| 3 | B1 | 54 | U |
| 3 | B1 | 55 | A |
| 3 | B1 | 65 | G |
| 3 | B1 | 98 | G |
| 3 | B1 | 103 | U |
| 3 | B1 | 111 | G |
| 3 | B1 | 120 | U |
| 5 | C1 | 23 | U |
| 5 | C1 | 34 | U |
| 5 | C1 | 35 | C |
| 5 | C1 | 38 | U |
| 5 | C1 | 59 | A |
| 5 | C1 | 62 | G |
| 5 | C1 | 63 | G |
| 5 | C1 | 76 | C |
| 5 | C1 | 78 | G |
| 5 | C1 | 81 | U |
| 5 | C1 | 83 | C |
| 5 | C1 | 84 | A |
| 5 | C1 | 85 | G |
| 5 | C1 | 87 | G |
| 5 | C1 | 89 | A |
| 5 | C1 | 95 | G |
| 5 | C1 | 104 | A |
| 5 | C1 | 106 | C |
| 5 | C1 | 116 | G |
| 5 | C1 | 125 | U |
| 5 | C1 | 152 | G |
| 80 | t1 | 9 | G |
| 80 | t1 | 10 | G |
| 80 | t1 | 16 | U |
| 80 | t1 | 17 | G |
| 80 | t1 | 19 | U |
| 80 | t1 | 22 | C |
| 80 | t1 | 36 | G |
| 80 | t1 | 42 | G |
| 80 | t1 | 43 | A |
| 80 | t1 | 47 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 80 | t1 | 48 | U |
| 80 | t1 | 74 | C |
| 80 | u1 | 9 | G |
| 80 | u1 | 16 | U |
| 80 | u1 | 17 | G |
| 80 | u1 | 21 | A |
| 80 | u1 | 42 | G |
| 80 | u1 | 46 | A |
| 80 | u1 | 58 | A |
| 80 | u1 | 74 | C |
| 80 | u1 | 76 | A |
| 82 | w1 | 2 | U |
| 82 | w1 | 4 | U |
| 82 | w1 | 8 | U |
| 82 | w1 | 12 | U |
| 82 | w1 | 13 | U |
| 82 | w1 | 14 | U |

All (13) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 166 | G |
| 1 | A1 | 169 | A |
| 1 | A1 | 170 | G |
| 1 | A1 | 246 | A |
| 1 | A1 | 439 | G |
| 1 | A1 | 855 | C |
| 1 | A1 | 898 | G |
| 1 | A1 | 1136 | A |
| 1 | A1 | 1211 | A |
| 1 | A1 | 2468 | U |
| 1 | A1 | 2803 | U |
| 1 | A1 | 3080 | U |
| 5 | C1 | 84 | A |

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 262 ligands modelled in this entry, 260 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | SPD | A1 | 8002 | - | 9,9,9 | 0.31 | 0 | 8,8,8 | 0.58 | 0 |
| 83 | 3HE | A1 | 8001 | - | 21,21,21 | 4.31 | 8 (38%) | 19,30,30 | 5.20 | 11 (57%) |

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 |
|---|---|---|---|---|---|---|---|
| 84 | SPD | A1 | 8002 | - | - | 2/7/7/7 | - |
| 83 | 3HE | A1 | 8001 | - | - | 5/8/36/36 | 0/2/2/2 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 83 | A1 | 8001 | 3HE | O-C4 | 11.63 | 1.40 | 1.21 |
| 83 | A1 | 8001 | 3HE | O1-C11 | 8.04 | 1.39 | 1.23 |
| 83 | A1 | 8001 | 3HE | O2-C12 | 7.74 | 1.39 | 1.23 |
| 83 | A1 | 8001 | 3HE | C12-N | 7.65 | 1.50 | 1.37 |
| 83 | A1 | 8001 | 3HE | C11-N | 6.58 | 1.48 | 1.37 |
| 83 | A1 | 8001 | 3HE | C8-C9 | 3.21 | 1.58 | 1.53 |
| 83 | A1 | 8001 | 3HE | C13-C9 | -2.38 | 1.49 | 1.53 |
| 83 | A1 | 8001 | 3HE | C10-C9 | -2.00 | 1.50 | 1.53 |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | A1 | 8001 | 3HE | C11-N-C12 | -10.78 | 112.71 | 125.78 |
| 83 | A1 | 8001 | 3HE | O-C4-C5 | -8.93 | 110.28 | 123.28 |
| 83 | A1 | 8001 | 3HE | O-C4-C3 | -8.02 | 110.20 | 122.15 |
| 83 | A1 | 8001 | 3HE | O2-C12-N | -7.94 | 107.69 | 120.28 |
| 83 | A1 | 8001 | 3HE | O2-C12-C13 | -7.34 | 108.33 | 122.62 |
| 83 | A1 | 8001 | 3HE | O1-C11-N | -7.11 | 109.01 | 120.28 |
| 83 | A1 | 8001 | 3HE | O1-C11-C10 | -7.04 | 108.92 | 122.62 |
| 83 | A1 | 8001 | 3HE | C10-C11-N | -3.31 | 111.89 | 115.95 |
| 83 | A1 | 8001 | 3HE | C9-C8-C7 | -2.40 | 110.89 | 116.82 |
| 83 | A1 | 8001 | 3HE | C6-C1-C2 | 2.10 | 113.19 | 110.10 |
| 83 | A1 | 8001 | 3HE | C13-C12-N | -2.10 | 113.38 | 115.95 |

There are no chirality outliers.

All (7) torsion outliers are listed below:

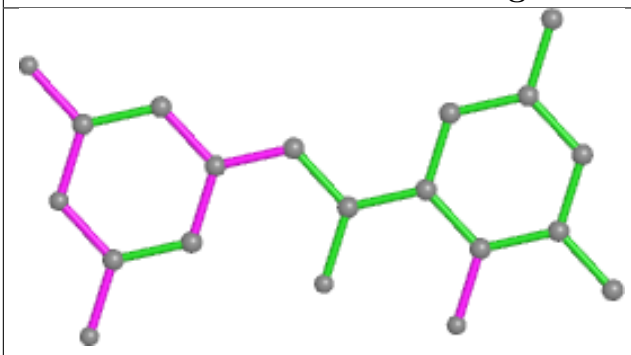
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 83 | A1 | 8001 | 3HE | C6-C5-C7-C8 |
| 83 | A1 | 8001 | 3HE | C6-C5-C7-O3 |
| 83 | A1 | 8001 | 3HE | C7-C8-C9-C10 |
| 83 | A1 | 8001 | 3HE | C7-C8-C9-C13 |
| 84 | A1 | 8002 | SPD | C3-C4-C5-N6 |
| 84 | A1 | 8002 | SPD | C2-C3-C4-C5 |
| 83 | A1 | 8001 | 3HE | C4-C5-C7-O3 |

There are no ring outliers.

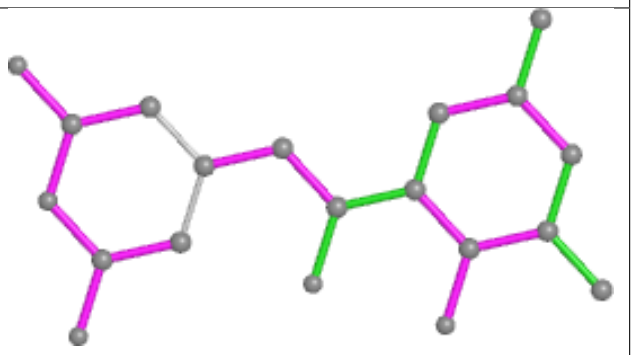
No monomer is involved in short contacts.

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

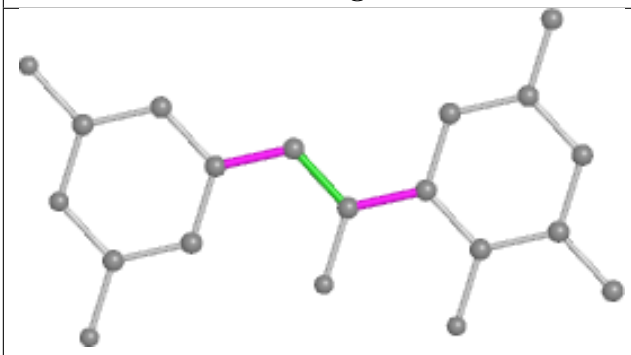
**Ligand 3HE A1 8001**



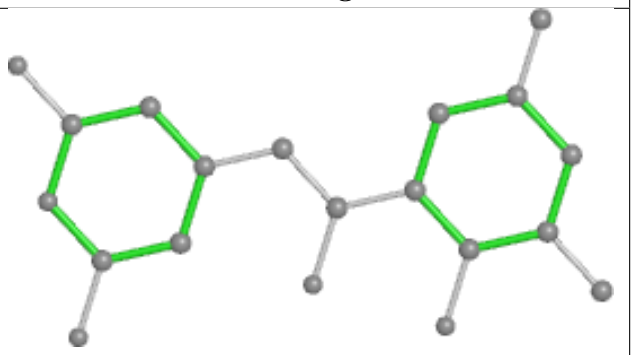
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

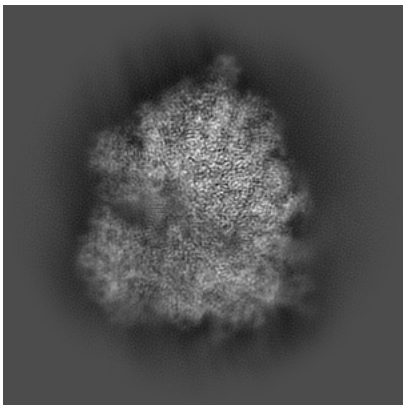
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24307. These allow visual inspection of the internal detail of the map and identification of artifacts.

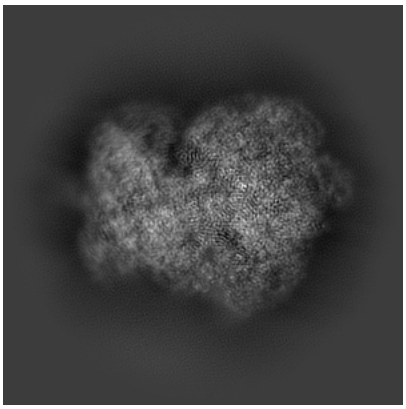
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

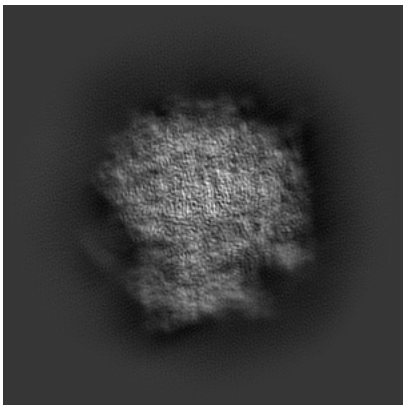
### 6.1.1 Primary map



X

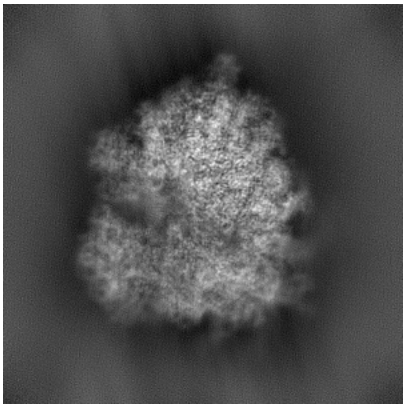


Y

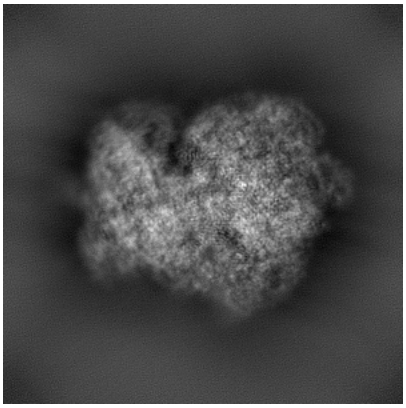


Z

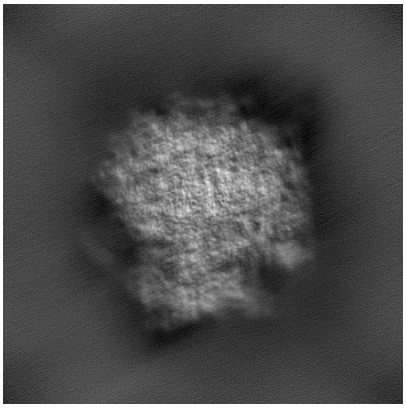
### 6.1.2 Raw map



X



Y

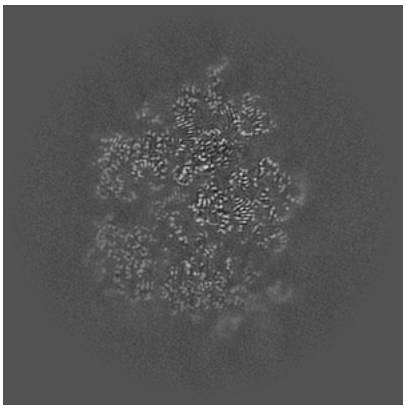


Z

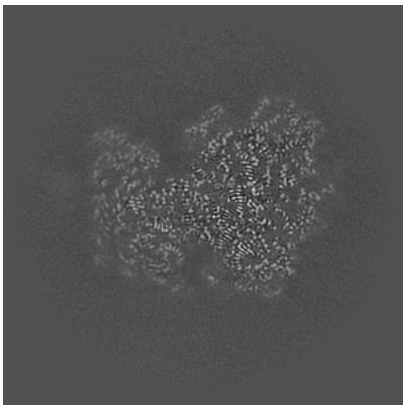
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

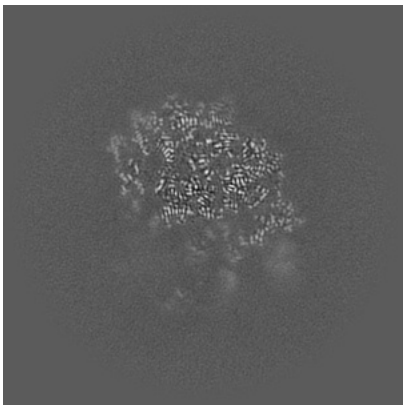
### 6.2.1 Primary map



X Index: 192

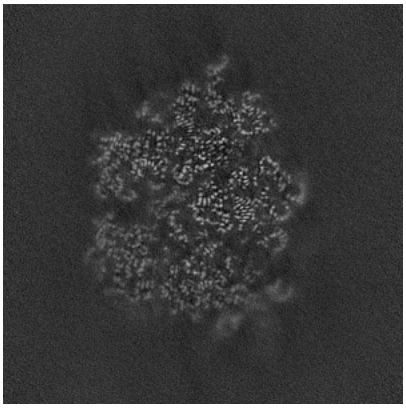


Y Index: 192

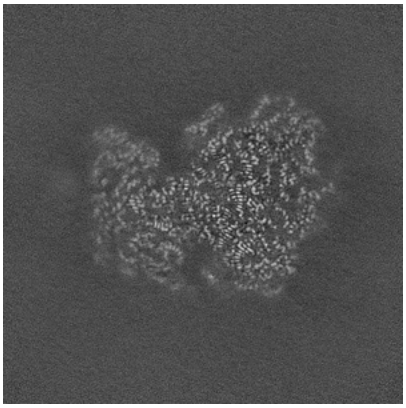


Z Index: 192

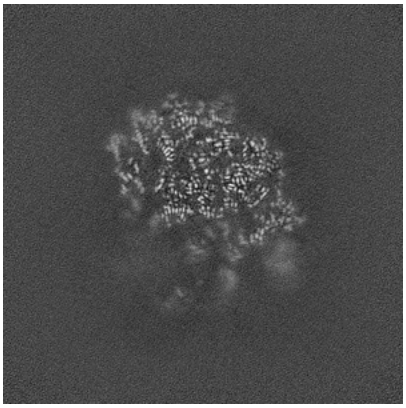
### 6.2.2 Raw map



X Index: 192



Y Index: 192

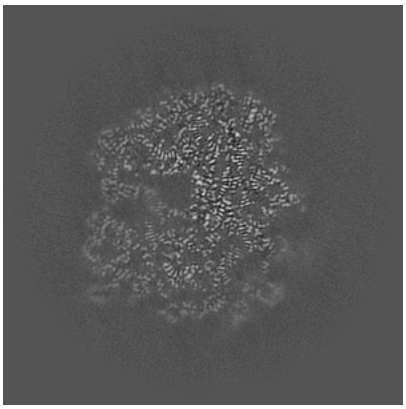


Z Index: 192

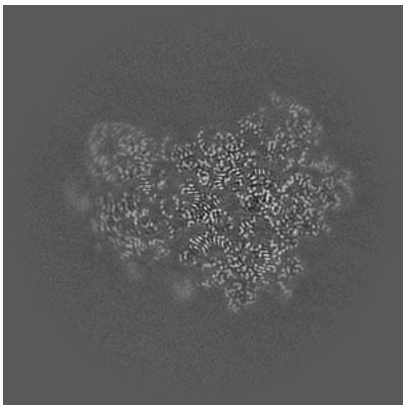
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

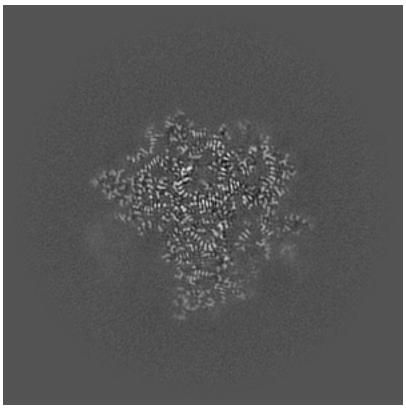
### 6.3.1 Primary map



X Index: 180

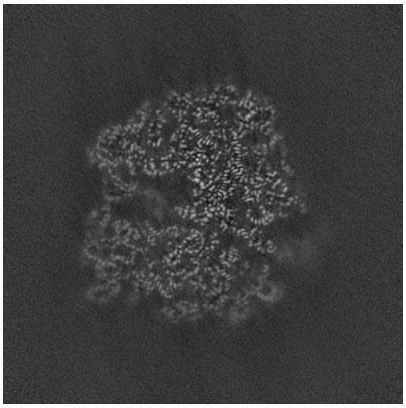


Y Index: 207

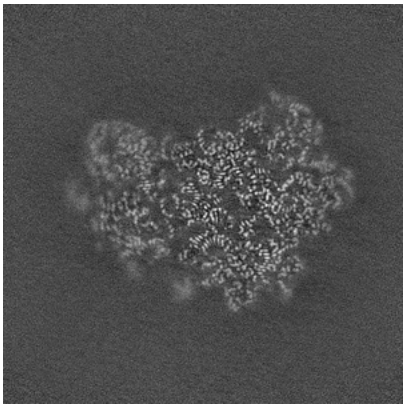


Z Index: 228

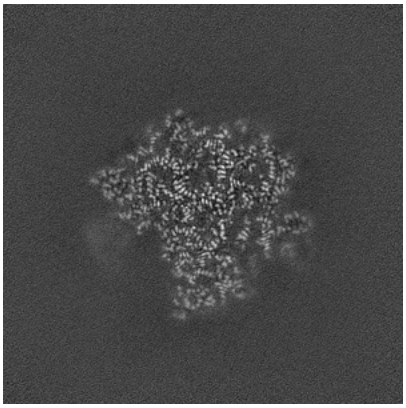
### 6.3.2 Raw map



X Index: 177



Y Index: 207

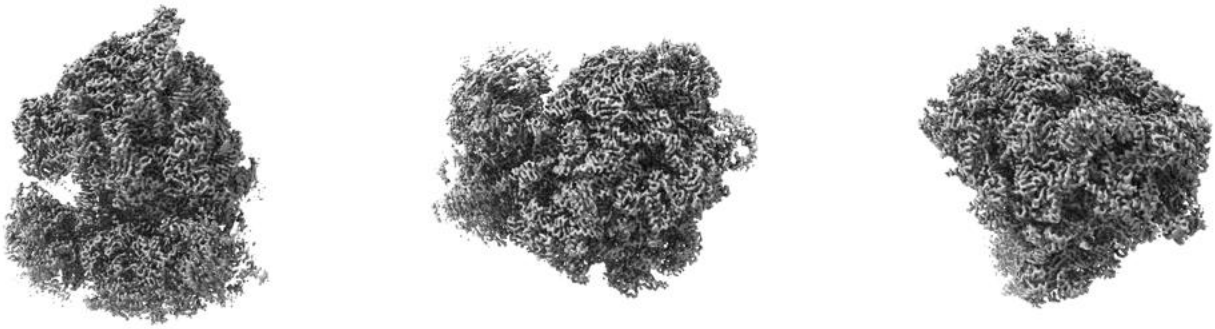


Z Index: 229

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

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map

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.

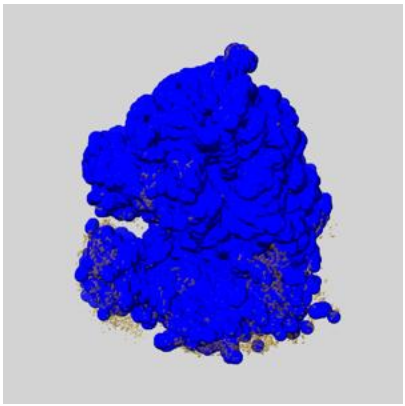
## 6.5 Mask visualisation (i)

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

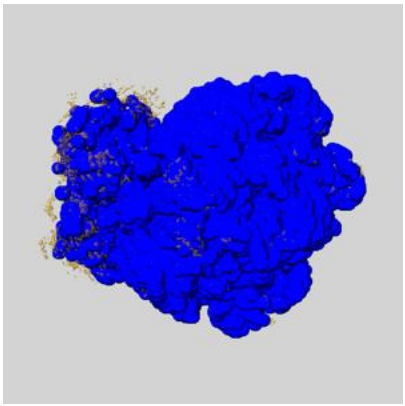
A mask typically either:

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

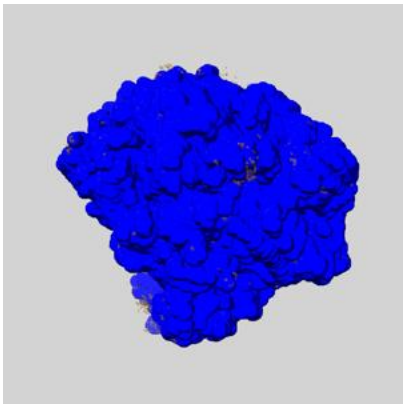
### 6.5.1 emd_24307_msk_1.map (i)



X



Y

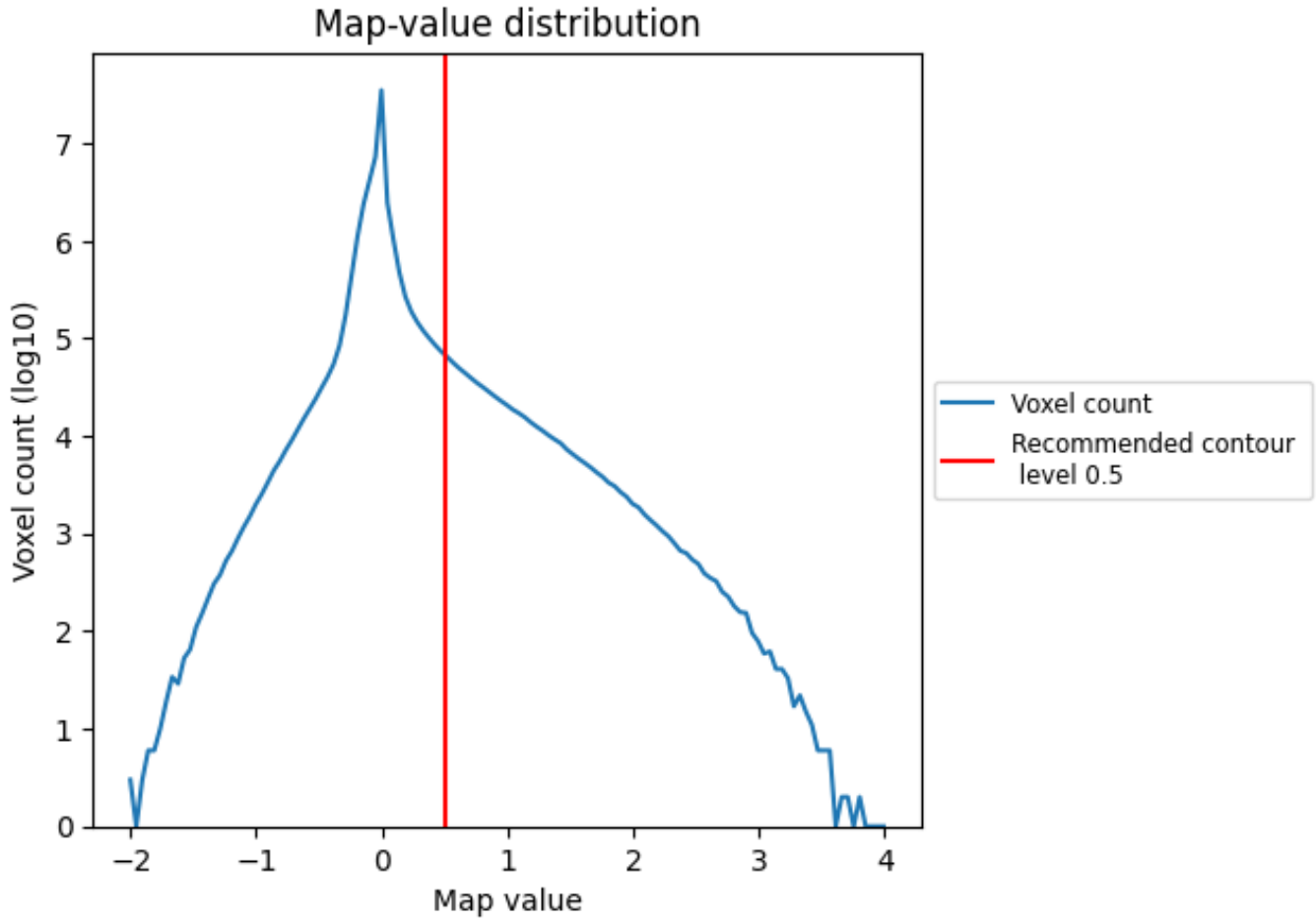


Z

# 7 Map analysis

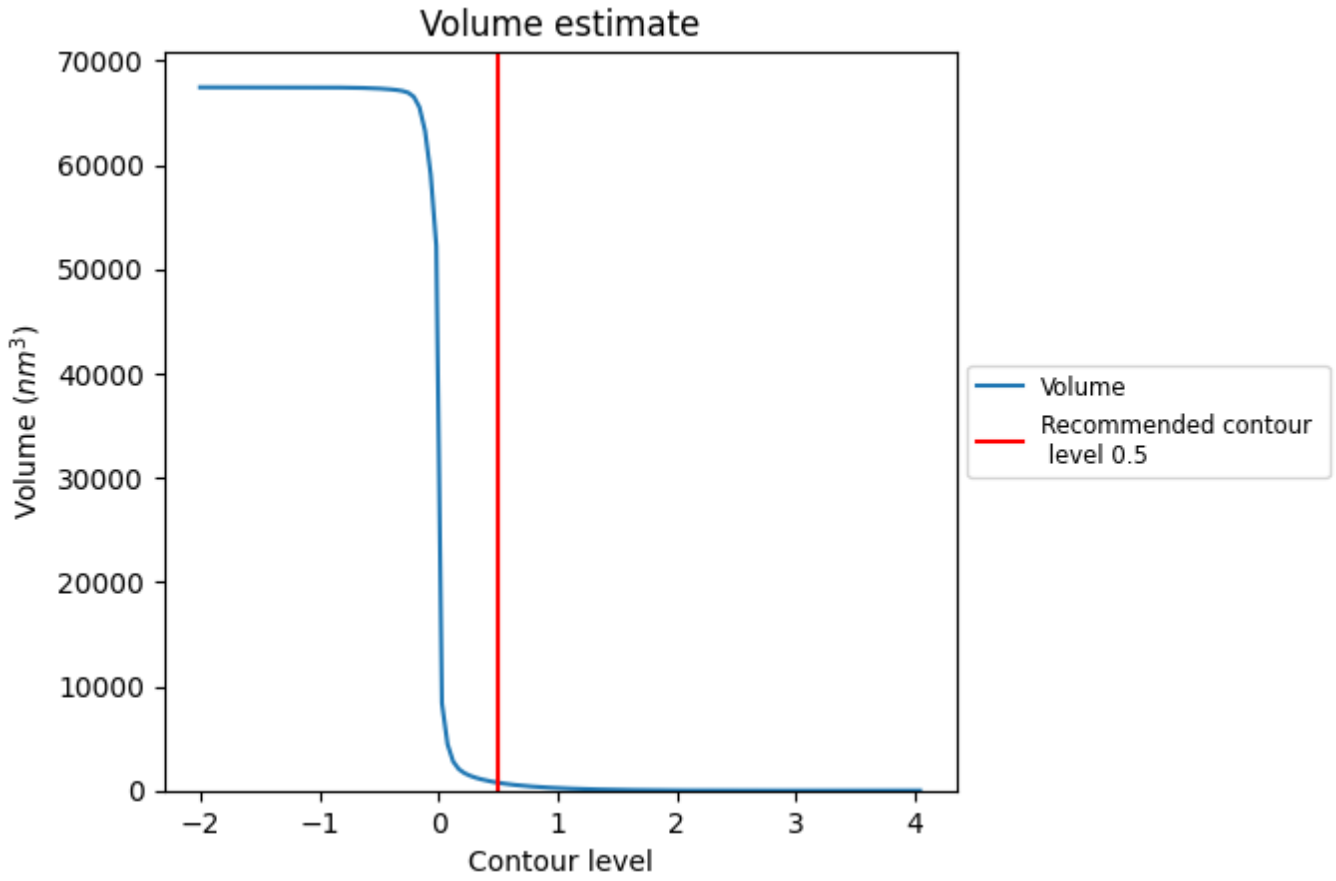
This section contains the results of statistical analysis of the map.

## 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.

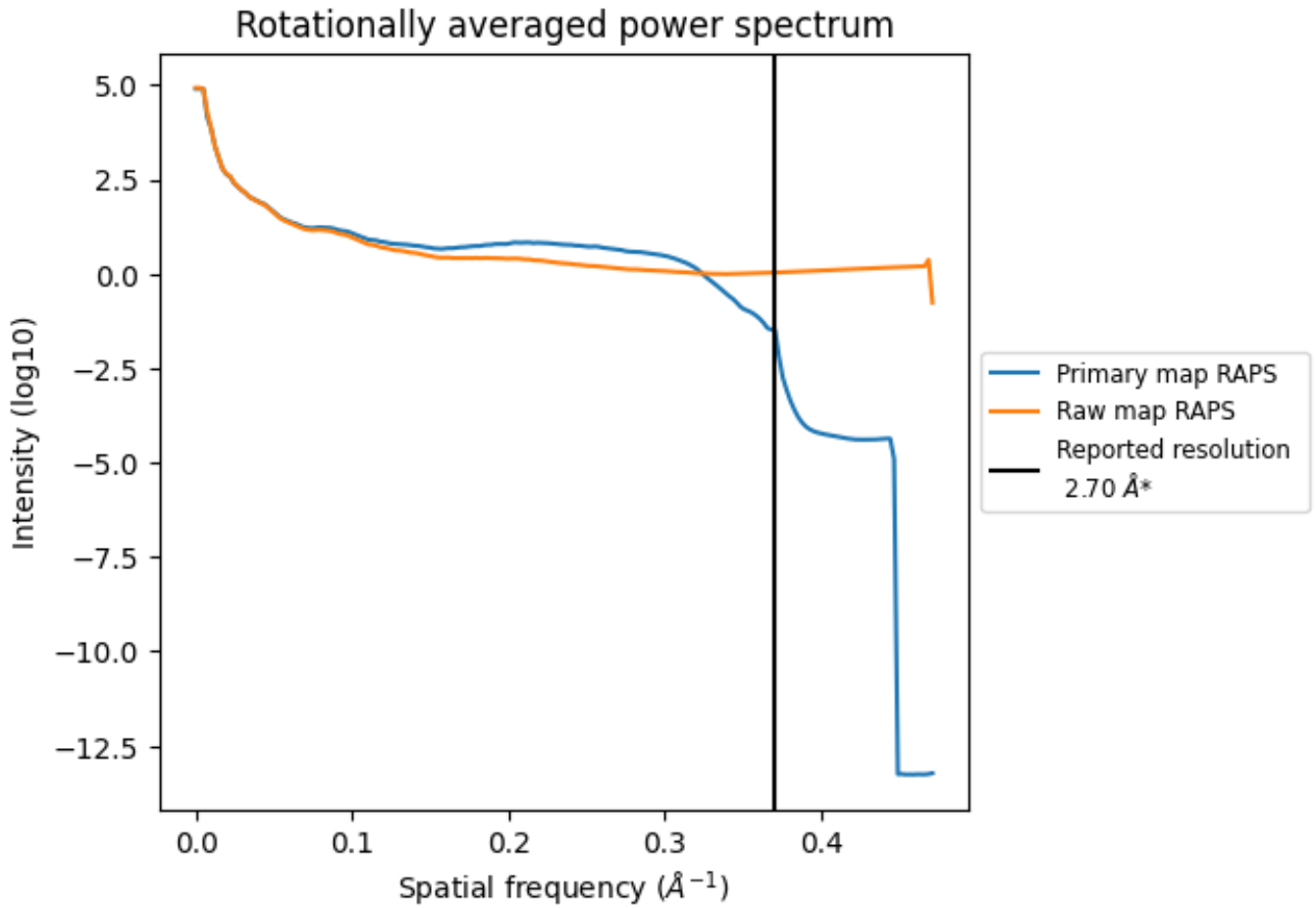
## 7.2 Volume estimate




The volume at the recommended contour level is 752 $nm^3$; this corresponds to an approximate mass of 679 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)

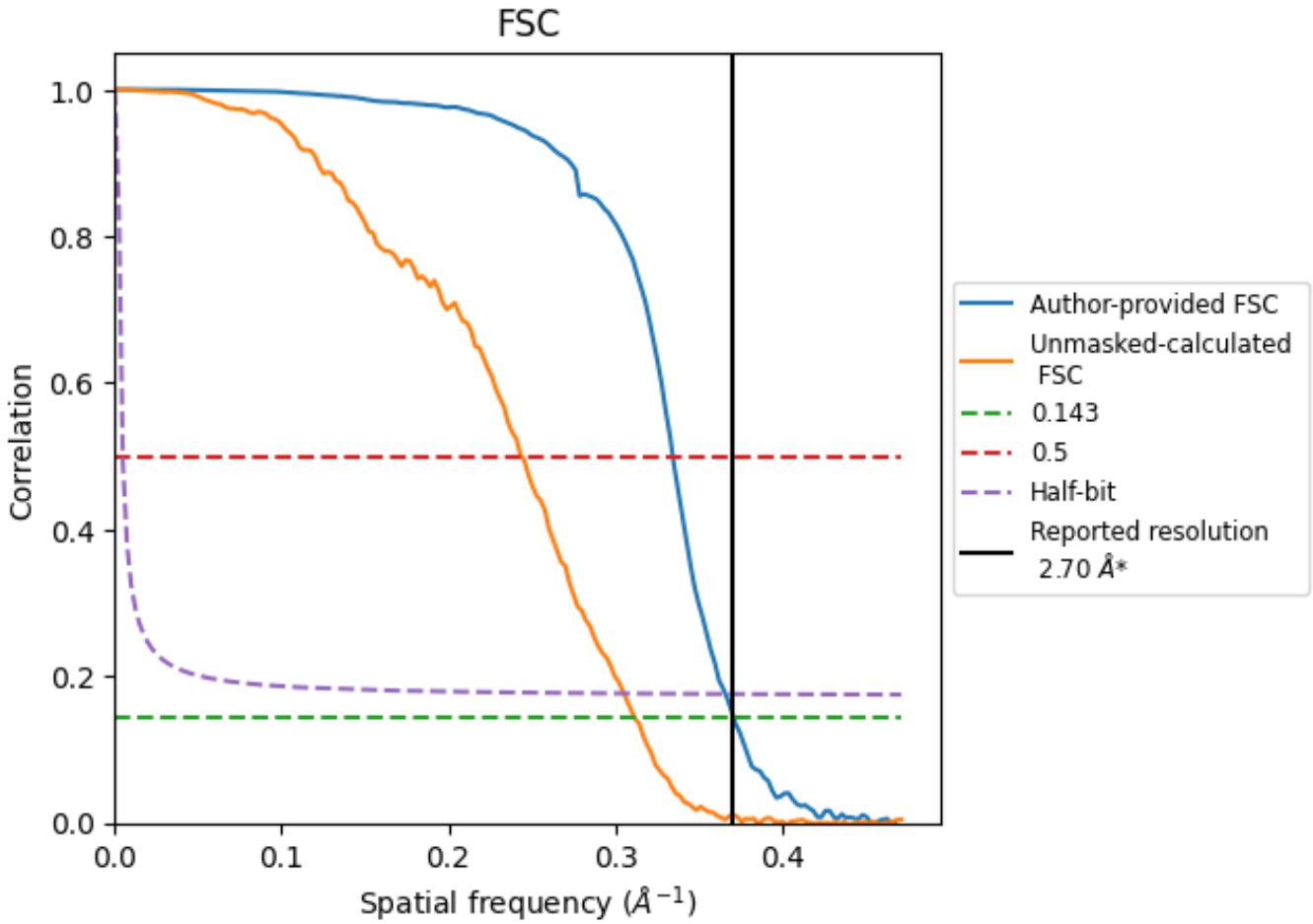



*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

# 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 0.370 Å$^{-1}$

## 8.2 Resolution estimates (i)

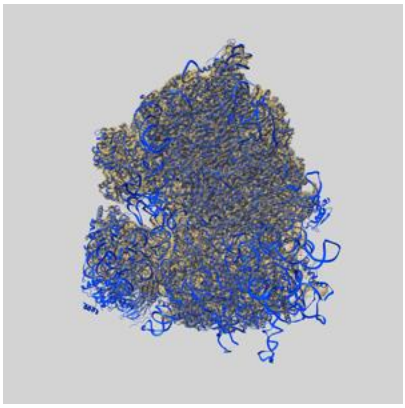
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.70 | - | - |
| Author-provided FSC curve | 2.69 | 2.99 | 2.73 |
| Unmasked-calculated* | 3.21 | 4.10 | 3.27 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.21 differs from the reported value 2.7 by more than 10 %

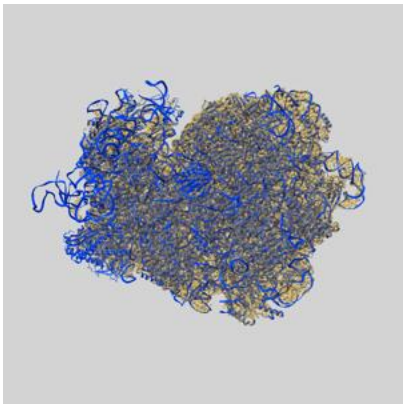
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24307 and PDB model 7R81. Per-residue inclusion information can be found in section 3 on page 20.

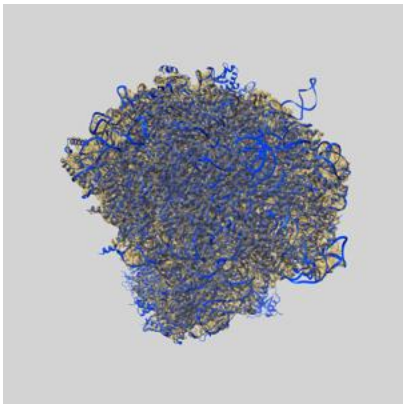
## 9.1 Map-model overlay



X



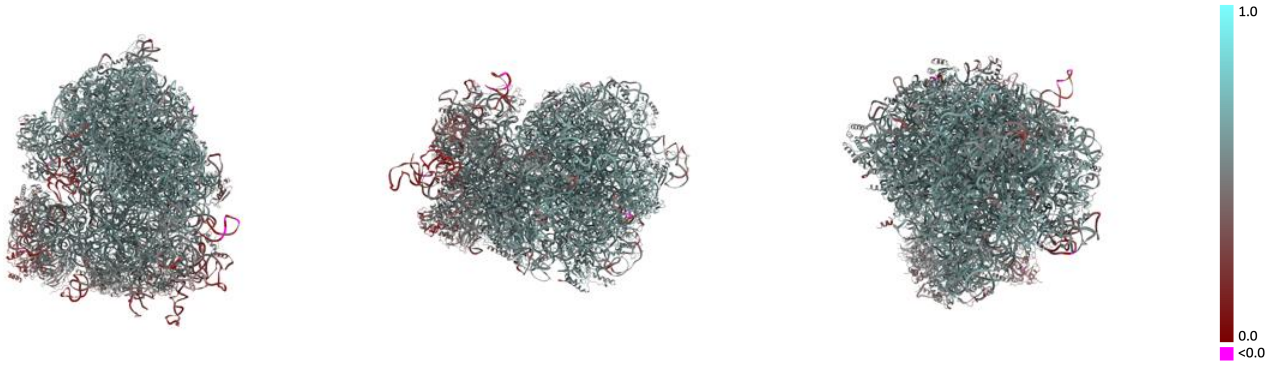
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

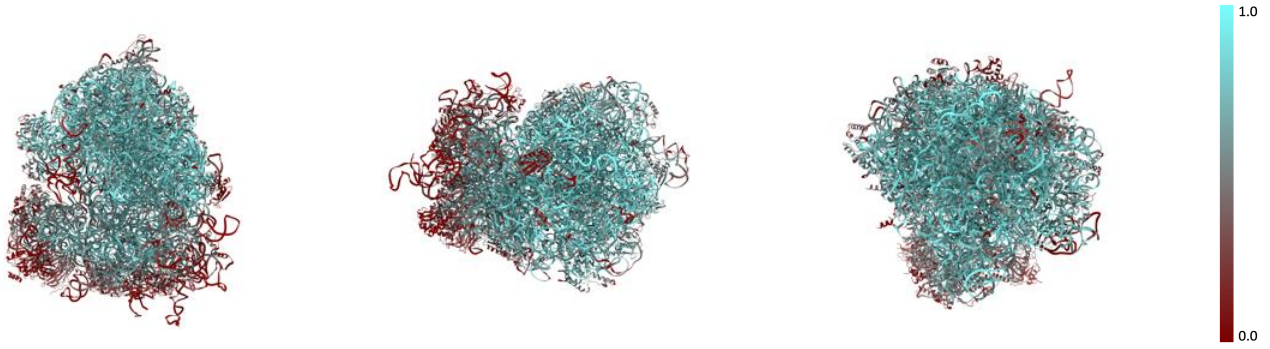
## 9.2 Q-score mapped to coordinate model (i)




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.

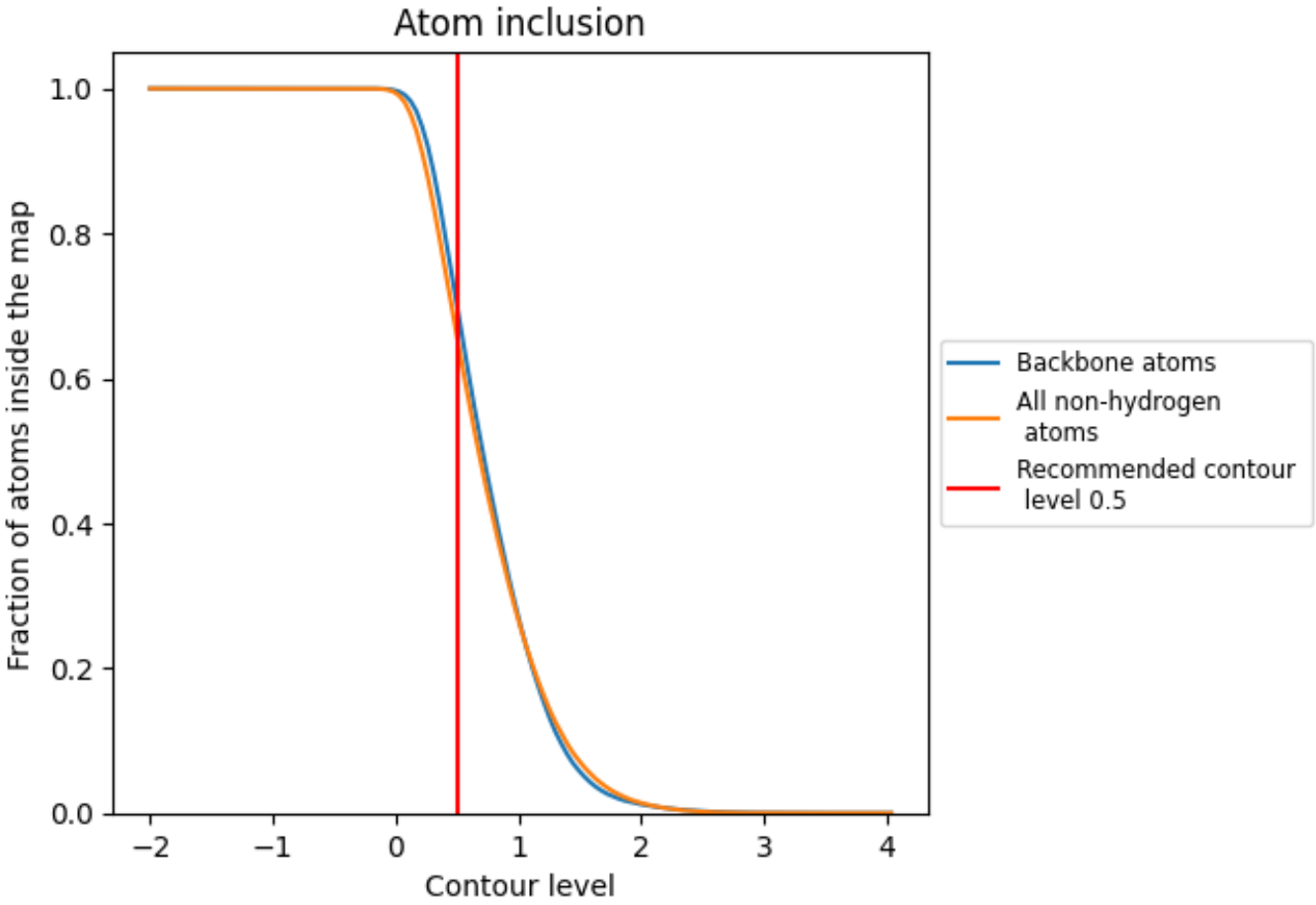
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.5).

## 9.4 Atom inclusion (i)




At the recommended contour level, 70% of all backbone atoms, 66% 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 (0.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6573 | 0.5390 |
| A1 | 0.8444 | 0.5780 |
| A2 | 0.6061 | 0.4900 |
| B1 | 0.8618 | 0.5770 |
| B2 | 0.3199 | 0.4800 |
| C1 | 0.8173 | 0.5650 |
| C2 | 0.3499 | 0.4980 |
| D1 | 0.8181 | 0.6080 |
| D2 | 0.4523 | 0.5170 |
| E1 | 0.7685 | 0.5980 |
| E2 | 0.2685 | 0.4600 |
| F1 | 0.7326 | 0.5830 |
| F2 | 0.2656 | 0.4850 |
| G1 | 0.5689 | 0.5380 |
| G2 | 0.3556 | 0.4860 |
| H1 | 0.5222 | 0.5380 |
| H2 | 0.1851 | 0.4520 |
| I1 | 0.7180 | 0.5720 |
| I2 | 0.1581 | 0.4150 |
| J1 | 0.6047 | 0.5430 |
| J2 | 0.5018 | 0.5280 |
| K1 | 0.6205 | 0.5620 |
| K2 | 0.3243 | 0.4670 |
| L1 | 0.6653 | 0.5600 |
| L2 | 0.1858 | 0.4420 |
| M1 | 0.5000 | 0.5250 |
| M2 | 0.5717 | 0.5500 |
| N1 | 0.6800 | 0.5600 |
| N2 | 0.0000 | 0.2160 |
| O1 | 0.6277 | 0.5590 |
| O2 | 0.4374 | 0.5140 |
| P1 | 0.8444 | 0.6110 |
| P2 | 0.5248 | 0.5260 |
| Q1 | 0.7696 | 0.5930 |
| Q2 | 0.2301 | 0.4520 |


*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| R1 | 0.7761 | 0.5900 |
| R2 | 0.3776 | 0.5090 |
| S1 | 0.7747 | 0.6000 |
| S2 | 0.2370 | 0.4420 |
| T1 | 0.6460 | 0.5410 |
| T2 | 0.3039 | 0.4770 |
| U1 | 0.7469 | 0.5910 |
| U2 | 0.3049 | 0.4810 |
| V1 | 0.7030 | 0.5780 |
| V2 | 0.2725 | 0.4500 |
| W1 | 0.0474 | 0.4640 |
| W2 | 0.3498 | 0.4830 |
| X1 | 0.7325 | 0.5950 |
| X2 | 0.4931 | 0.5250 |
| Y1 | 0.7510 | 0.5960 |
| Y2 | 0.5897 | 0.5640 |
| Z1 | 0.6677 | 0.5750 |
| Z2 | 0.2027 | 0.4480 |
| a1 | 0.7000 | 0.5720 |
| a2 | 0.1775 | 0.4400 |
| b1 | 0.6474 | 0.5570 |
| b2 | 0.5816 | 0.5280 |
| c1 | 0.7843 | 0.6000 |
| c2 | 0.2429 | 0.4600 |
| d1 | 0.7018 | 0.5730 |
| d2 | 0.3227 | 0.5020 |
| e1 | 0.6771 | 0.5710 |
| e2 | 0.4590 | 0.5160 |
| f1 | 0.7567 | 0.5890 |
| f2 | 0.3254 | 0.4860 |
| g1 | 0.7792 | 0.5980 |
| g2 | 0.0000 | 0.2560 |
| h1 | 0.7956 | 0.6070 |
| h2 | 0.0814 | 0.4240 |
| i1 | 0.7652 | 0.5960 |
| j1 | 0.6322 | 0.5570 |
| k1 | 0.6763 | 0.5650 |
| l1 | 0.8256 | 0.6030 |
| m1 | 0.3962 | 0.5020 |
| n1 | 0.7029 | 0.5700 |
| o1 | 0.7513 | 0.5940 |
| p1 | 0.6822 | 0.5940 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| q1 | 0.7182 | 0.5780 |
| r1 | 0.7628 | 0.5870 |
| s1 | 0.5925 | 0.5610 |
| t1 | 0.4300 | 0.4890 |
| u1 | 0.5321 | 0.5080 |
| v1 | 0.2000 | 0.5090 |
| w1 | 0.4794 | 0.4360 |