# Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 10:58 PM EST

| | | |
|---|---|---|
| PDB ID | : | 5T2A |
| EMDB ID | : | EMD-8343 |
| Title | : | CryoEM structure of the Leishmania donovani 80S ribosome at 2.9 Angstrom resolution |
| Authors | : | Zhang, X.; Lai, M.; Zhou, Z.H. |
| Deposited on | : | 2016-08-23 |
| Resolution | : | 2.90 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 (i) 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 (i)) were used in the production of this report:

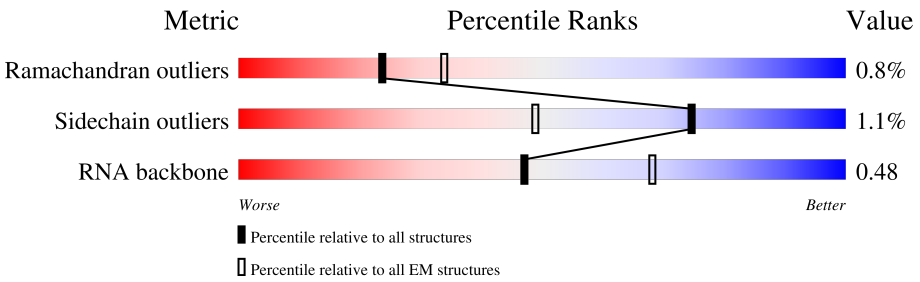
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA)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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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 | A | 1781 | 5% 74% 16% 10% |
| 2 | B | 1465 | 7% 61% 11% 27% |
| 3 | C | 262 | • 52% 9% • 38% |
| 4 | D | 120 | 91% 8% • |
| 5 | E | 213 | 5% 69% 10% 21% |
| 6 | F | 73 | 15% 75% 21% • • |
| 7 | G | 183 | • 89% 11% • |
| 8 | H | 127 | • 62% 11% 27% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | I | 198 | 20% 94% 5% |
| 10 | J | 213 | 29% 97% |
| 11 | K | 188 | 52% 88% 11% |
| 12 | L | 220 | 17% 80% 19% |
| 13 | M | 222 | 17% 96% |
| 14 | N | 175 | 36% 93% |
| 15 | O | 204 | 7% 97% |
| 16 | P | 166 | 7% 92% 7% |
| 17 | Q | 179 | 13% 98% |
| 18 | R | 245 | 24% 79% 20% |
| 19 | S | 159 | 21% 97% |
| 20 | T | 129 | 32% 94% 5% |
| 21 | U | 139 | 9% 99% |
| 22 | V | 145 | 17% 82% 17% |
| 23 | W | 124 | 9% 51% 48% |
| 24 | X | 143 | 15% 82% 16% |
| 25 | Y | 134 | 26% 98% |
| 26 | Z | 145 | 17% 97% |
| 27 | a | 147 | 29% 97% |
| 28 | b | 70 | 26% 96% |
| 29 | c | 260 | 7% 94% |
| 30 | d | 419 | 10% 94% 5% |
| 31 | e | 104 | 15% 84% 5% 10% |
| 32 | f | 183 | 8% 60% 40% |
| 33 | g | 133 | 19% 95% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | h | 168 | 15% 73% 26% |
| 35 | i | 127 | 30% 98% |
| 36 | j | 144 | 13% 90% 8% |
| 37 | k | 105 | 44% 93% 6% |
| 38 | l | 83 | 6% 93% |
| 39 | m | 92 | 14% 98% |
| 40 | n | 83 | 29% 89% 10% |
| 41 | o | 51 | 10% 98% |
| 42 | p | 373 | 23% 96% |
| 43 | q | 128 | 5% 40% 59% |
| 44 | r | 106 | 19% 86% 9% |
| 45 | s | 305 | 28% 87% 13% |
| 46 | t | 195 | 17% 67% 30% |
| 47 | u | 252 | 17% 88% 10% |
| 48 | v | 348 | 21% 66% 34% |
| 49 | w | 190 | 13% 97% |
| 50 | 0 | 264 | 30% 80% 16% |
| 51 | 1 | 273 | 21% 92% 5% |
| 52 | 2 | 2205 | 26% 47% 29% 6% 18% |
| 53 | 3 | 249 | 53% 98% |
| 54 | 4 | 200 | 32% 96% |
| 55 | 5 | 220 | 11% 79% 17% |
| 56 | 6 | 190 | 17% 84% 14% |
| 57 | 7 | 312 | 99% 95% |
| 58 | 8 | 57 | 63% 58% 9% 33% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 59 | AC | 246 | 36% 81% 17% |
| 60 | AD | 153 | 61% 58% 39% |
| 61 | AE | 173 | 8% 78% 19% |
| 62 | AG | 151 | 14% 91% 7% |
| 63 | AH | 144 | 24% 94% 6% |
| 64 | AI | 152 | 80% 74% 20% |
| 65 | AJ | 130 | 10% 93% 5% |
| 66 | AK | 149 | 92% 88% 6% |
| 67 | AL | 143 | 78% 83% 15% |
| 68 | AM | 153 | 95% 89% 7% |
| 69 | AN | 190 | 99% 96% |
| 70 | AO | 179 | 79% 75% 6% 19% |
| 71 | AP | 265 | 19% 85% 15% |
| 72 | AQ | 116 | 81% 86% 12% |
| 73 | AR | 164 | 14% 51% 49% |
| 74 | AS | 143 | 21% 93% 5% |
| 75 | AT | 137 | 42% 90% 8% |
| 76 | AV | 112 | 33% 88% 7% |
| 77 | AW | 86 | 34% 91% 5% 5% |
| 78 | AX | 219 | 86% 86% 5% 7% |
| 79 | AY | 66 | 61% 85% 15% |
| 80 | AZ | 87 | 76% 72% 5% 22% |

# 2 Entry composition (i)

There are 80 unique types of molecules in this entry. The entry contains 200172 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 LSU-alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | A | 1603 | 34365 | 15347 | 6297 | 11118 | 1603 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 761 | U | A | conflict | GB 322500086 |
| A | 1393 | G | A | conflict | GB 322500086 |
| A | ? | - | A | deletion | GB 322500086 |

- Molecule 2 is a RNA chain called LSU-beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | B | 1064 | 22723 | 10152 | 4100 | 7407 | 1064 | 0 | 0 |

- Molecule 3 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 3 | C | 162 | 3449 | 1542 | 615 | 1130 | 162 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | 141 | C | U | conflict | GB 79677111 |
| C | 182 | G | A | conflict | GB 79677111 |
| C | 185 | C | G | conflict | GB 79677111 |
| C | 226 | A | U | conflict | GB 79677111 |
| C | 228 | C | U | conflict | GB 79677111 |
| C | 246 | C | U | conflict | GB 79677111 |

- Molecule 4 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | D | 119 | 2531 | 1132 | 452 | 828 | 119 | 0 | 0 |

- Molecule 5 is a RNA chain called srRNA1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | E | 169 | 3589 | 1604 | 626 | 1190 | 169 | 0 | 0 |

- Molecule 6 is a RNA chain called srRNA3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 6 | F | 71 | 1508 | 676 | 273 | 488 | 71 | 0 | 0 |

- Molecule 7 is a RNA chain called srRNA2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 7 | G | 183 | 3911 | 1744 | 704 | 1280 | 183 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | 169 | U | A | conflict | GB 5019758 |
| G | 171 | U | A | conflict | GB 5019758 |

- Molecule 8 is a RNA chain called srRNA4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 8 | H | 93 | 1996 | 889 | 369 | 645 | 93 | 0 | 0 |

- Molecule 9 is a protein called eL18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | I | 197 | 1539 | 968 | 307 | 258 | 6 | 0 | 0 |

- Molecule 10 is a protein called uL16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | J | 211 | 1704 | 1071 | 338 | 279 | 16 | 0 | 0 |

- Molecule 11 is a protein called uL5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | K | 167 | 1339 | 844 | 249 | 238 | 8 | 0 | 0 |

- Molecule 12 is a protein called eL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | L | 179 | 1435 | 901 | 296 | 230 | 8 | 0 | 0 |

- Molecule 13 is a protein called uL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | M | 221 | 1780 | 1126 | 354 | 293 | 7 | 0 | 0 |

- Molecule 14 is a protein called eL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | N | 168 | 1336 | 832 | 265 | 231 | 8 | 0 | 0 |

- Molecule 15 is a protein called eL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | O | 203 | 1714 | 1080 | 362 | 264 | 8 | 0 | 0 |

- Molecule 16 is a protein called uL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | P | 155 | 1245 | 776 | 246 | 212 | 11 | 0 | 1 |

- Molecule 17 is a protein called eL20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | Q | 178 | 1456 | 927 | 280 | 244 | 5 | 0 | 0 |

- Molecule 18 is a protein called eL19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | R | 196 | 1646 | 1010 | 360 | 271 | 5 | 0 | 0 |

- Molecule 19 is a protein called eL21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | S | 158 | 1261 | 803 | 245 | 208 | 5 | 0 | 0 |

- Molecule 20 is a protein called eL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | T | 123 | 997 | 642 | 179 | 173 | 3 | 0 | 1 |

- Molecule 21 is a protein called uL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | U | 137 | 1035 | 653 | 195 | 181 | 6 | 0 | 0 |

- Molecule 22 is a protein called uL23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | V | 120 | 963 | 611 | 182 | 169 | 1 | 0 | 0 |

- Molecule 23 is a protein called eL24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | W | 65 | 563 | 368 | 110 | 81 | 4 | 0 | 0 |

- Molecule 24 is a protein called uL24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | X | 120 | 965 | 601 | 201 | 159 | 4 | 0 | 0 |

- Molecule 25 is a protein called eL27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | Y | 133 | 1079 | 688 | 215 | 173 | 3 | 0 | 0 |

- Molecule 26 is a protein called uL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | Z | 144 | 1126 | 708 | 226 | 186 | 6 | 0 | 0 |

- Molecule 27 is a protein called eL28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | a | 146 | 1140 | 698 | 243 | 194 | 5 | 0 | 0 |

- Molecule 28 is a protein called eL29.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 28 | b | 69 | 554 | 339 | 127 | 88 | 0 | 0 |

- Molecule 29 is a protein called uL2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | c | 253 | 1921 | 1193 | 392 | 326 | 10 | 0 | 1 |

- Molecule 30 is a protein called uL3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | d | 399 | 3183 | 2003 | 629 | 538 | 13 | 0 | 0 |

- Molecule 31 is a protein called eL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | e | 94 | 720 | 448 | 131 | 136 | 5 | 0 | 0 |

- Molecule 32 is a protein called eL31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 32 | f | 110 | 878 | 561 | 166 | 149 | 2 | 0 | 0 |

- Molecule 33 is a protein called eL32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | g | 129 | 1050 | 664 | 209 | 174 | 3 | 0 | 0 |

- Molecule 34 is a protein called eL34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | h | 124 | 1014 | 624 | 221 | 163 | 6 | 0 | 0 |

- Molecule 35 is a protein called uL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 35 | i | 126 | 1056 | 658 | 218 | 176 | 4 | 0 | 0 |

- Molecule 36 is a protein called eL33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 36 | j | 132 | 1060 | 663 | 221 | 171 | 5 | 0 | 0 |

- Molecule 37 is a protein called eL36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 37 | k | 99 | 787 | 497 | 160 | 128 | 2 | 0 | 0 |

- Molecule 38 is a protein called eL37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 38 | l | 81 | 674 | 410 | 154 | 104 | 6 | 0 | 0 |

- Molecule 39 is a protein called eL43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 39 | m | 91 | 712 | 443 | 146 | 117 | 6 | 0 | 0 |

- Molecule 40 is a protein called eL38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | n | 75 | 605 | 383 | 118 | 101 | 3 | 0 | 0 |

- Molecule 41 is a protein called eL39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | o | 50 | 450 | 291 | 95 | 63 | 1 | 0 | 0 |

- Molecule 42 is a protein called uL4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 42 | p | 365 | 2825 | 1761 | 563 | 486 | 15 | 0 | 1 |

- Molecule 43 is a protein called eL40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 43 | q | 52 | 425 | 266 | 88 | 64 | 7 | 0 | 0 |

- Molecule 44 is a protein called eL42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 44 | r | 96 | 779 | 493 | 157 | 124 | 5 | 0 | 0 |

- Molecule 45 is a protein called uL18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 45 | s | 266 | 2094 | 1334 | 397 | 357 | 6 | 0 | 0 |

- Molecule 46 is a protein called eL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 46 | t | 137 | 1054 | 668 | 197 | 187 | 2 | 0 | 0 |

- Molecule 47 is a protein called uL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 47 | u | 228 | 1857 | 1180 | 358 | 308 | 11 | 0 | 0 |

- Molecule 48 is a protein called eL8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 48 | v | 230 | 1850 | 1160 | 368 | 315 | 7 | 0 | 0 |

- Molecule 49 is a protein called uL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 49 | w | 187 | 1484 | 938 | 273 | 267 | 6 | 0 | 0 |

- Molecule 50 is a protein called eS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 50 | 0 | 221 | 1786 | 1121 | 338 | 316 | 11 | 0 | 0 |

- Molecule 51 is a protein called eS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 51 | 1 | 258 | 2037 | 1291 | 387 | 350 | 9 | 0 | 0 |

- Molecule 52 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 52 | 2 | 1814 | 38724 | 17307 | 6969 | 12635 | 1813 | 0 | 0 |

- Molecule 53 is a protein called eS6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 53 | 3 | 249 | 1994 | 1243 | 409 | 339 | 3 | 0 | 0 |

- Molecule 54 is a protein called eS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 54 | 4 | 200 | 1667 | 1059 | 324 | 276 | 8 | 0 | 0 |

- Molecule 55 is a protein called eS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 55 | 5 | 183 | 1473 | 921 | 308 | 242 | 2 | 0 | 1 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 5 | 220 | ARG | LYS | conflict | UNP E9BH78 |

- Molecule 56 is a protein called uS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 56 | 6 | 164 | 1362 | 862 | 265 | 227 | 8 | 0 | 0 |

- Molecule 57 is a protein called RACK1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 57 | 7 | 308 | 2394 | 1500 | 426 | 456 | 12 | 0 | 0 |

- Molecule 58 is a protein called uS14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 58 | 8 | 38 | 314 | 194 | 63 | 52 | 5 | 0 | 0 |

- Molecule 59 is a protein called uS2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 59 | AC | 203 | 1622 | 1033 | 294 | 283 | 12 | 0 | 0 |

- Molecule 60 is a protein called eS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 60 | AD | 93 | 767 | 491 | 136 | 133 | 7 | 0 | 0 |

- Molecule 61 is a protein called uS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 61 | AE | 140 | 1148 | 725 | 229 | 189 | 5 | 0 | 0 |

- Molecule 62 is a protein called uS15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 62 | AG | 141 | 1157 | 730 | 229 | 190 | 8 | 0 | 0 |

- Molecule 63 is a protein called uS11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 63 | AH | 136 | 1023 | 631 | 200 | 184 | 8 | 0 | 0 |

- Molecule 64 is a protein called uS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 64 | AI | 121 | 984 | 626 | 188 | 166 | 4 | 0 | 0 |

- Molecule 65 is a protein called uS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 65 | AJ | 129 | 1020 | 646 | 188 | 178 | 8 | 0 | 0 |

- Molecule 66 is a protein called uS9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 66 | AK | 140 | 1108 | 710 | 206 | 189 | 3 | 0 | 0 |

- Molecule 67 is a protein called eS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 67 | AL | 121 | 983 | 613 | 192 | 173 | 5 | 0 | 0 |

- Molecule 68 is a protein called uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 68 | AM | 148 | 1186 | 743 | 237 | 202 | 4 | 0 | 0 |

- Molecule 69 is a protein called uS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 69 | AN | 190 | 1493 | 927 | 287 | 271 | 8 | 0 | 0 |

- Molecule 70 is a protein called eS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 70 | AO | 145 | 1150 | 729 | 224 | 193 | 4 | 0 | 0 |

- Molecule 71 is a protein called uS5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 71 | AP | 224 | 1722 | 1096 | 304 | 312 | 10 | 0 | 1 |

- Molecule 72 is a protein called uS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 72 | AQ | 102 | 807 | 504 | 148 | 153 | 2 | 0 | 0 |

- Molecule 73 is a protein called eS21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 73 | AR | 83 | 630 | 388 | 116 | 122 | 4 | 0 | 0 |

- Molecule 74 is a protein called uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 74 | AS | 142 | 1114 | 703 | 222 | 187 | 2 | 0 | 0 |

- Molecule 75 is a protein called eS24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 75 | AT | 126 | 1033 | 661 | 198 | 172 | 2 | 0 | 0 |

- Molecule 76 is a protein called eS26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 76 | AV | 104 | 828 | 515 | 175 | 130 | 8 | 0 | 0 |

- Molecule 77 is a protein called eS27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 77 | AW | 82 | 646 | 396 | 128 | 114 | 8 | 0 | 0 |

- Molecule 78 is a protein called uS3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 78 | AX | 203 | 1595 | 1003 | 295 | 284 | 13 | 0 | 0 |

- Molecule 79 is a protein called eS30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 79 | AY | 56 | 452 | 285 | 94 | 72 | 1 | 0 | 0 |

- Molecule 80 is a protein called eS28.

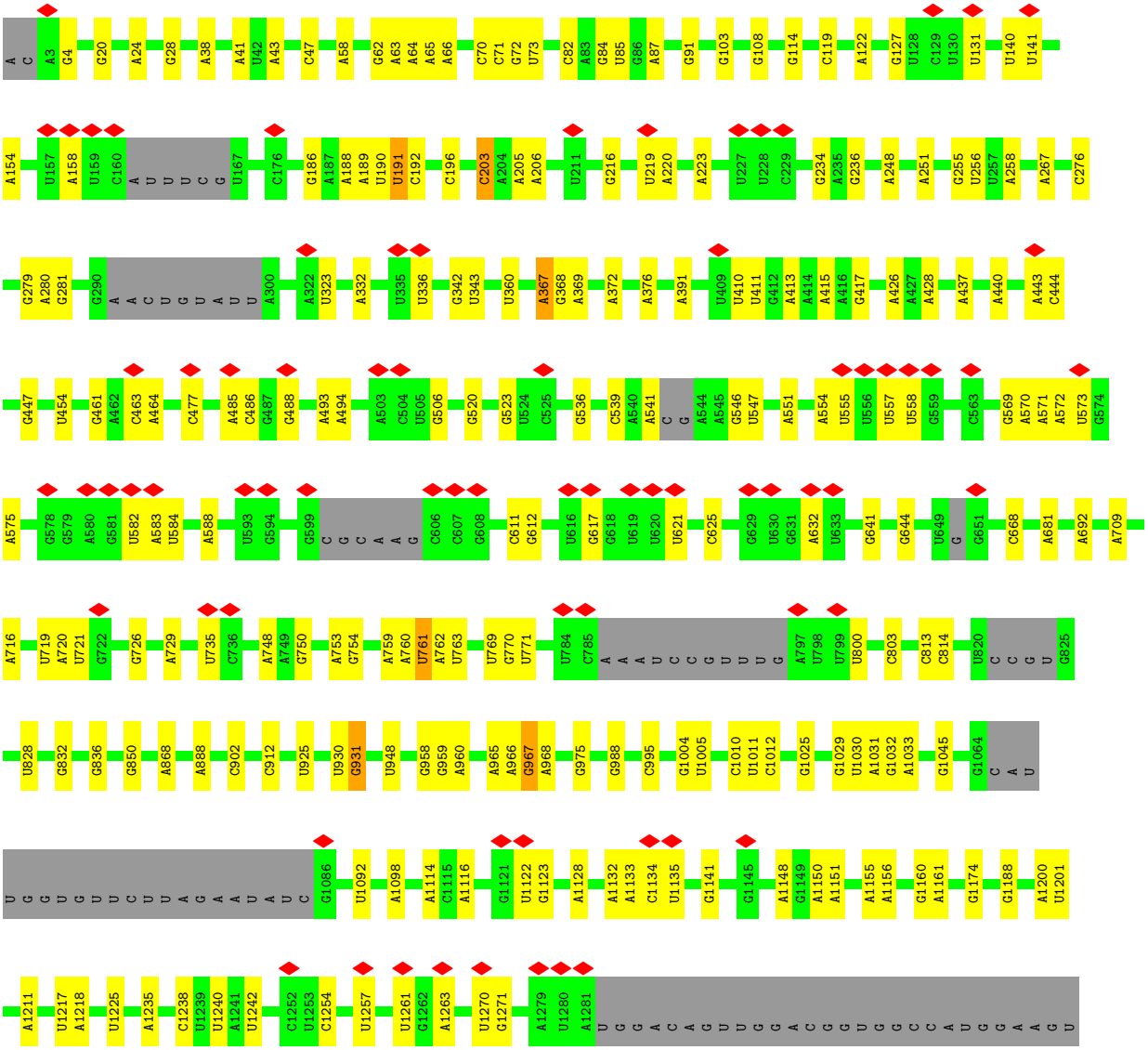
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 80 | AZ | 68 | 526 | 319 | 106 | 97 | 4 | 0 | 0 |

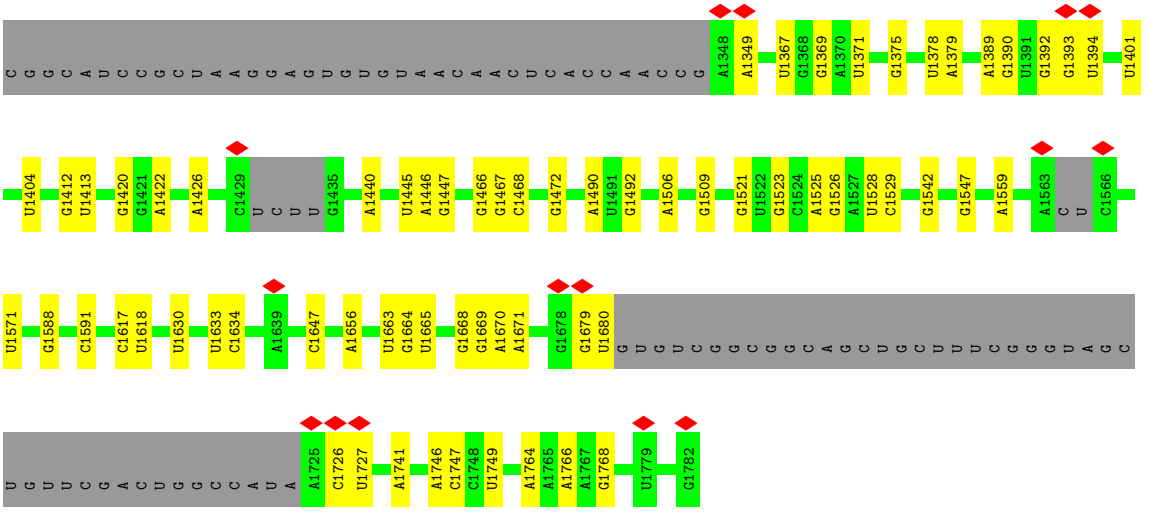
# 3 Residue-property plots (i)

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: LSU-alpha

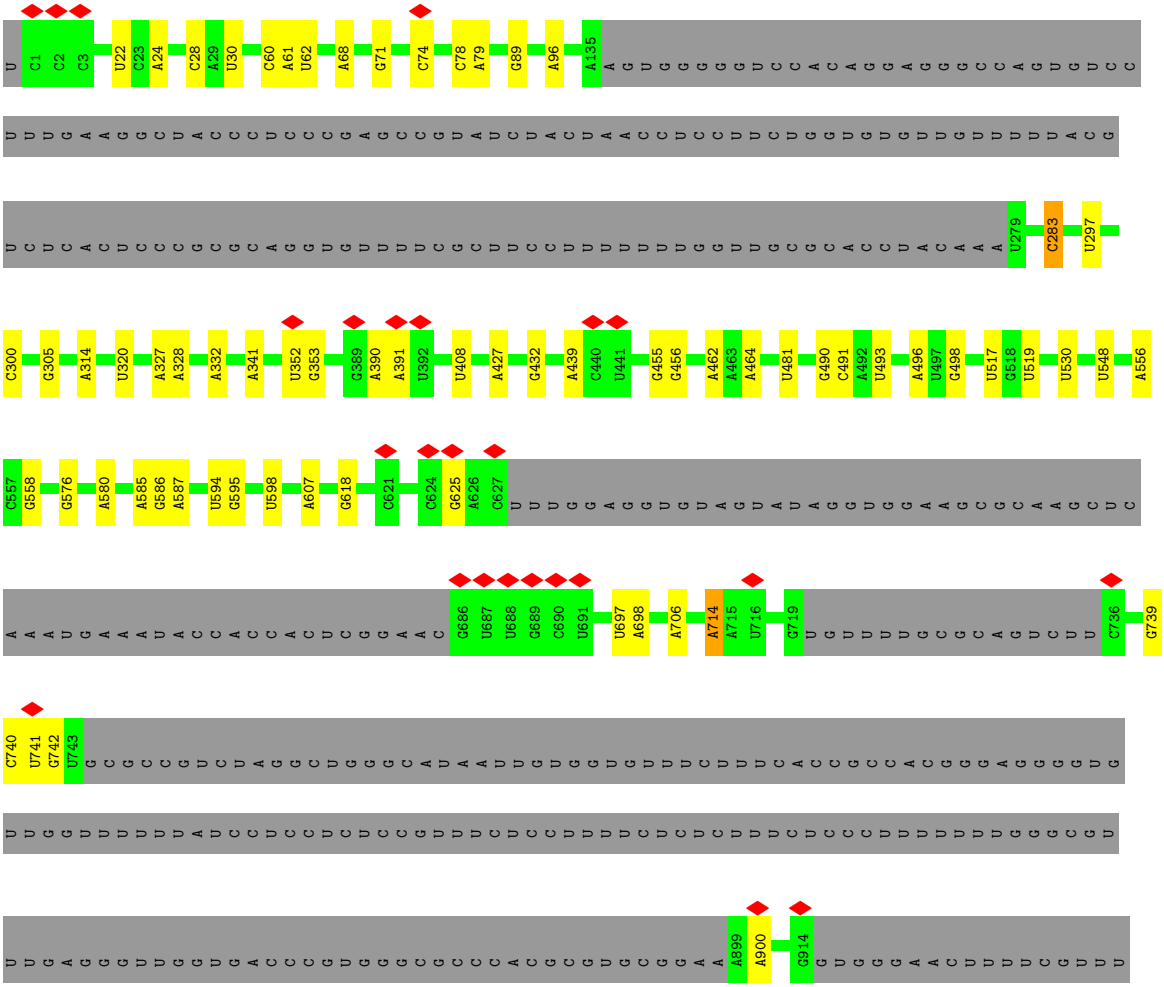
Chain A: 5% 74% 16% 10%

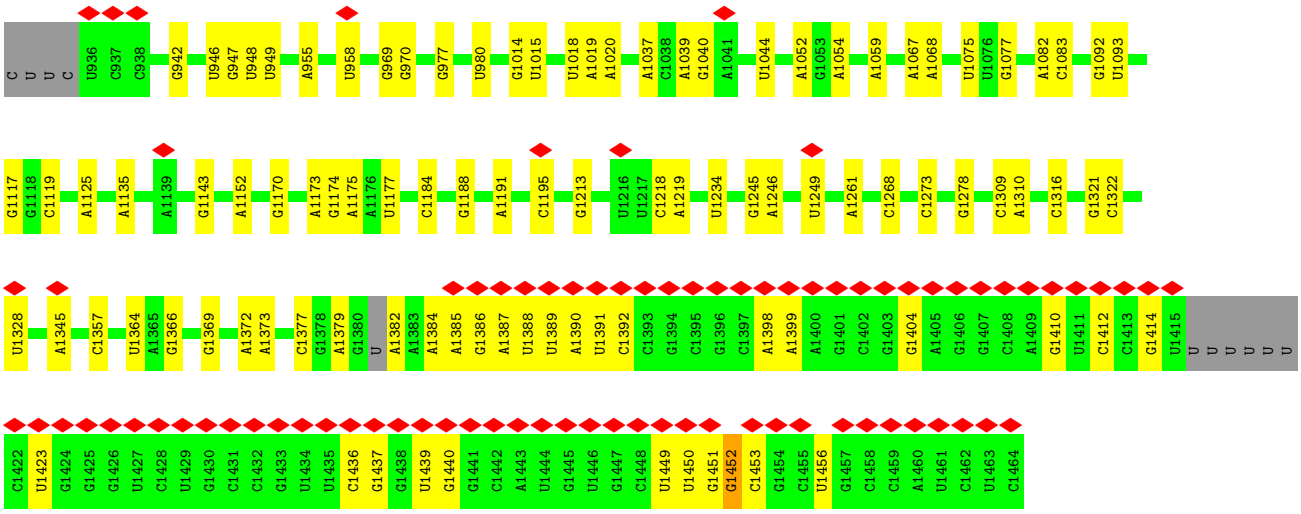




• Molecule 2: LSU-beta

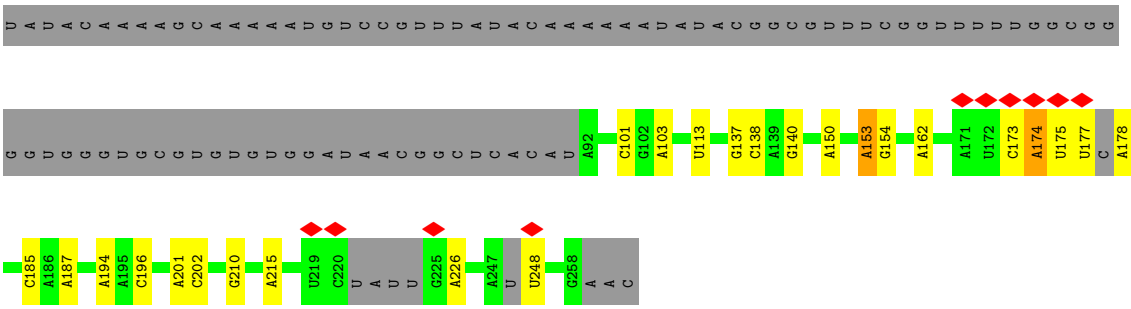
Chain B: 7% 61% 11% 27%





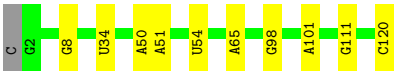
- Molecule 3: 5.8S rRNA

Chain C: 52% 9% 38%



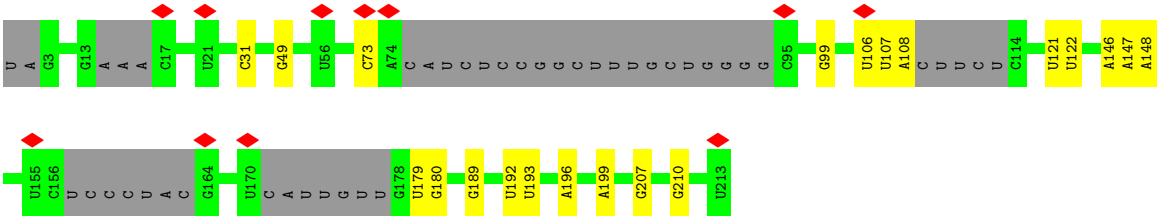
- Molecule 4: 5S rRNA

Chain D: 91% 8%



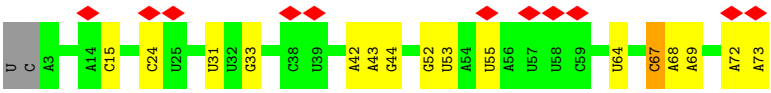
- Molecule 5: srRNA1

Chain E: 5% 69% 10% 21%



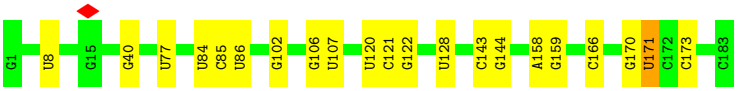
- Molecule 6: srRNA3

Chain F: 15% 75% 21%



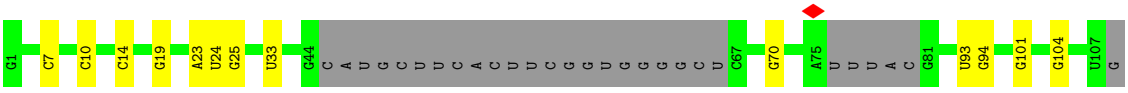

- Molecule 7: srRNA2

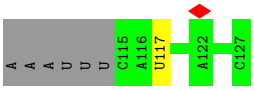
Chain G:




- Molecule 8: srRNA4

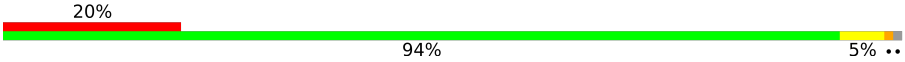
Chain H:

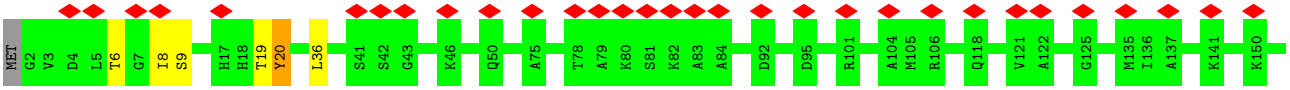


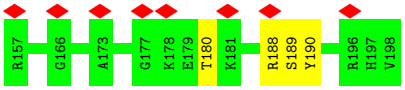




- Molecule 9: eL18

Chain I:

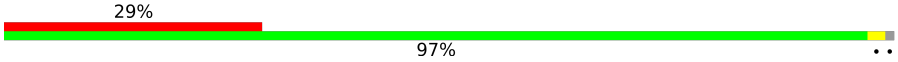


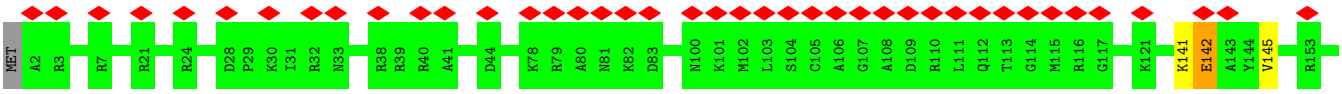



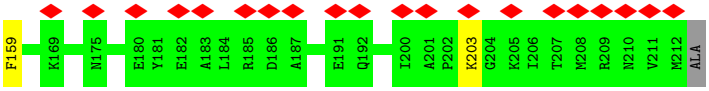




- Molecule 10: uL16

Chain J:

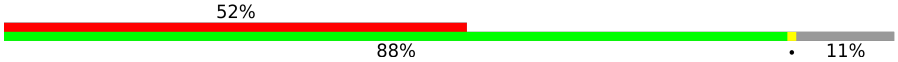


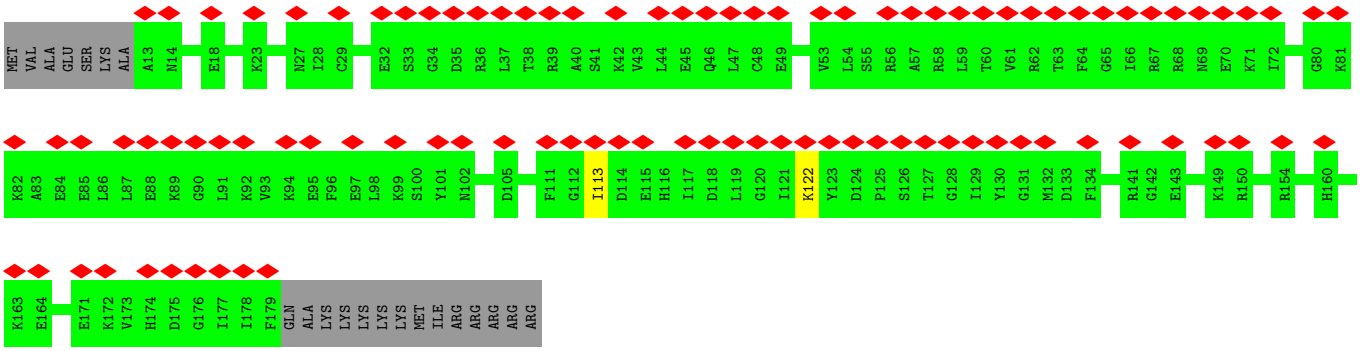




- Molecule 11: uL5

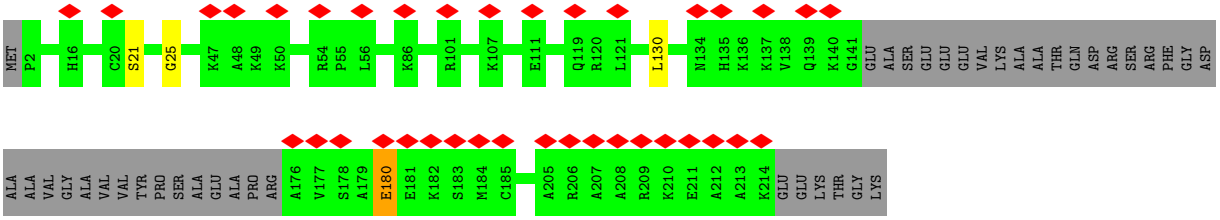
Chain K:





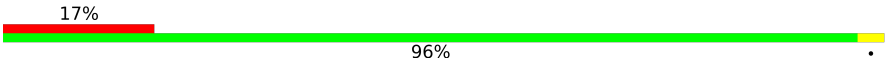

- Molecule 12: eL13

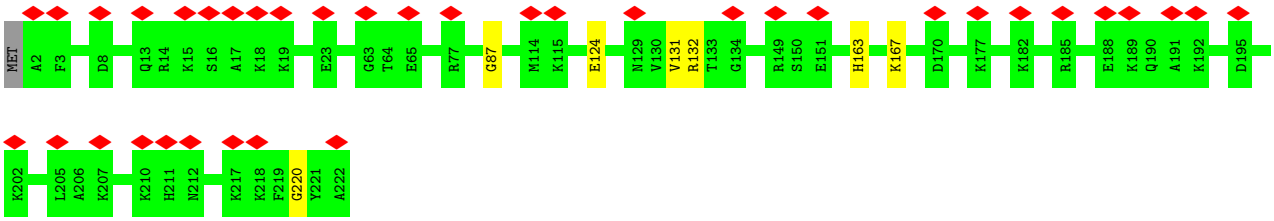
Chain L:




- Molecule 13: uL13

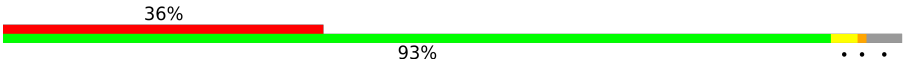
Chain M:

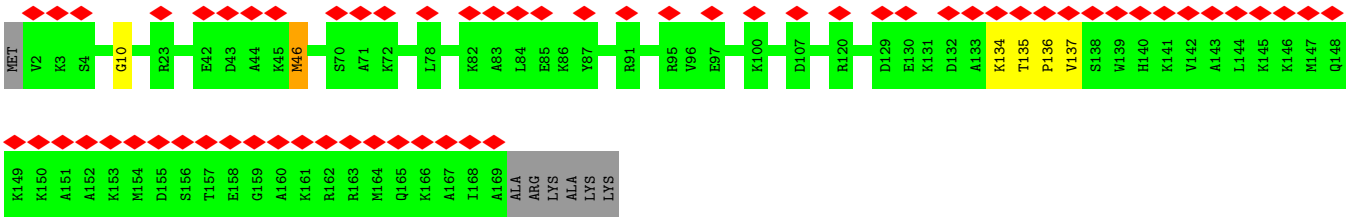



- Molecule 14: eL14

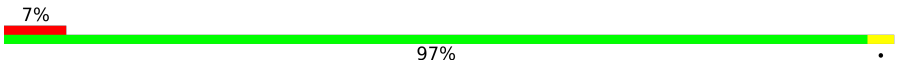
Chain N:

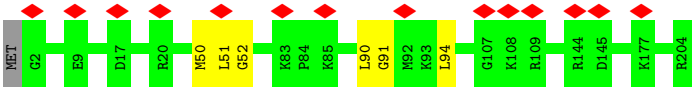



- Molecule 15: eL15

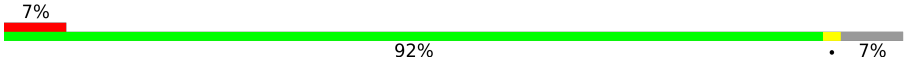
Chain O:

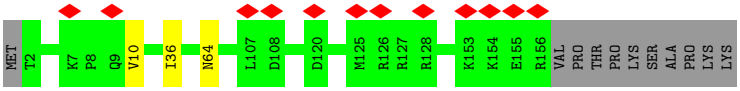





- Molecule 16: uL22

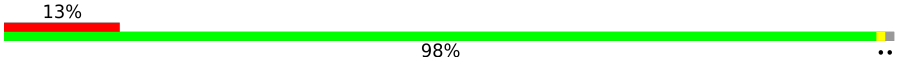
Chain P:

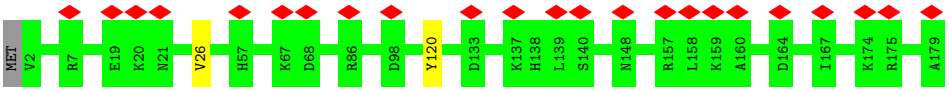



- Molecule 17: eL20

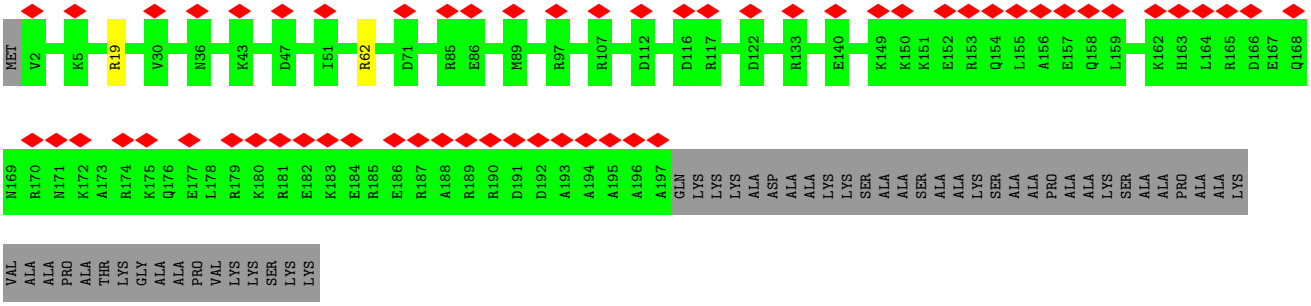
Chain Q:



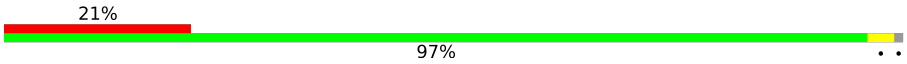

- Molecule 18: eL19

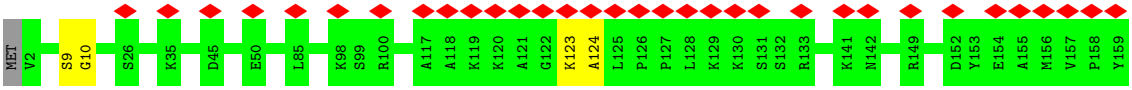
Chain R:




- Molecule 19: eL21

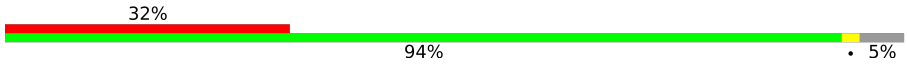
Chain S:

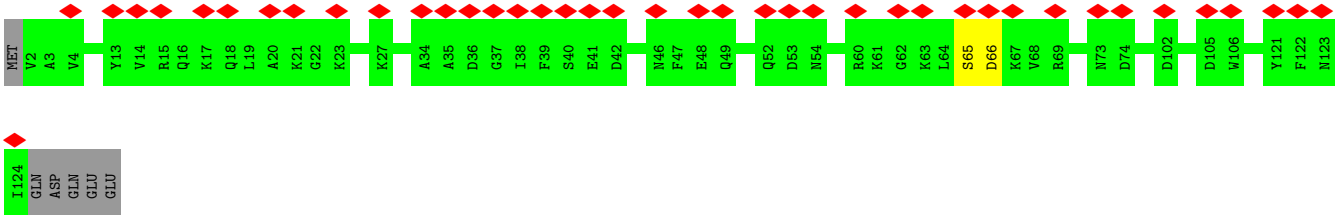



- Molecule 20: eL22

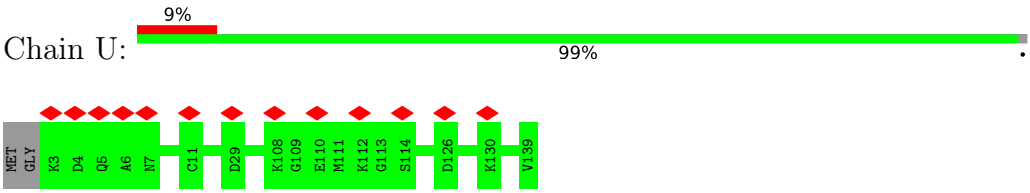
Chain T:



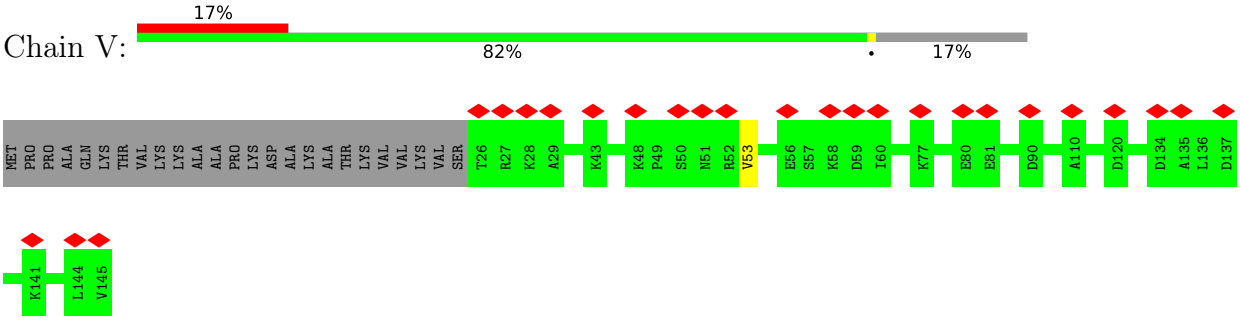
- Molecule 21: uL14

Chain U:



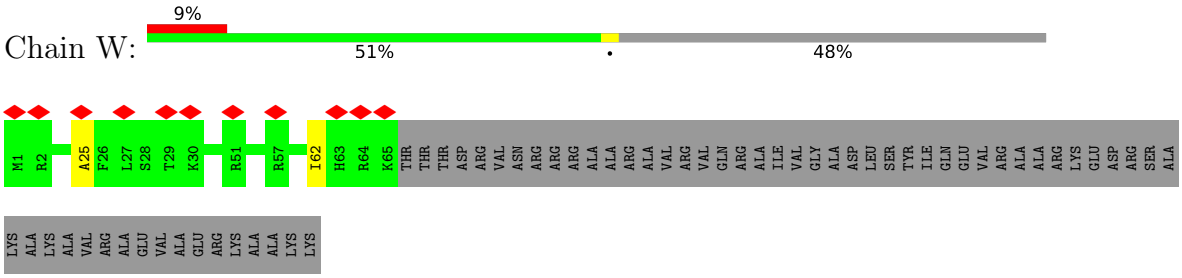

- Molecule 22: uL23

Chain V:



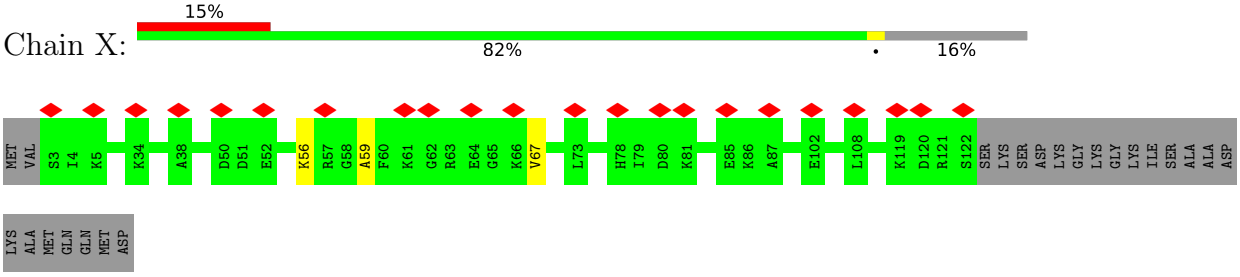

- Molecule 23: eL24

Chain W:



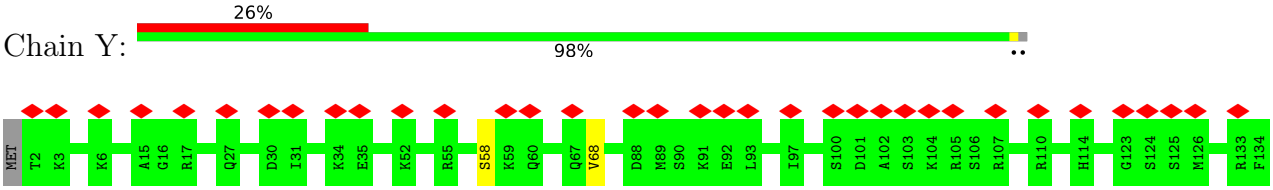

- Molecule 24: uL24

Chain X:



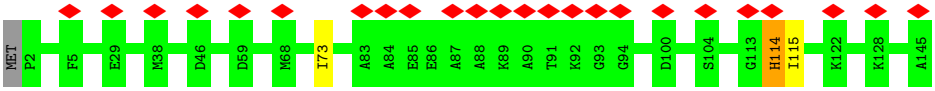

- Molecule 25: eL27

Chain Y:



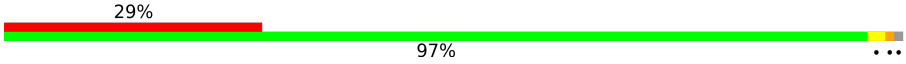

- Molecule 26: uL15

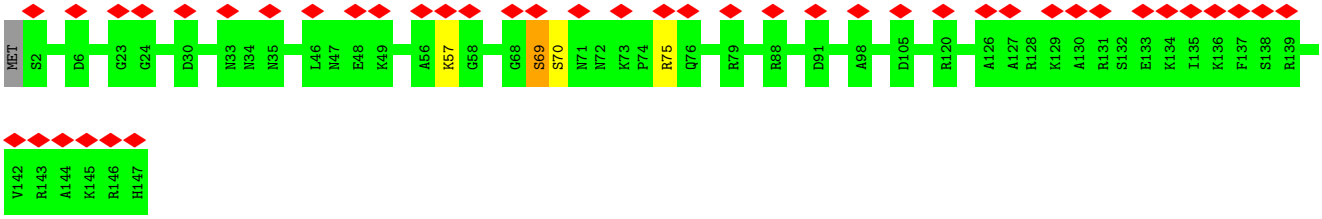
Chain Z:




- Molecule 27: eL28

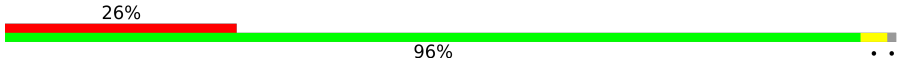
Chain a:

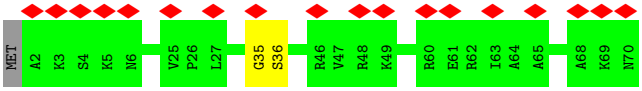



- Molecule 28: eL29

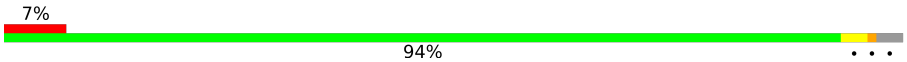
Chain b:

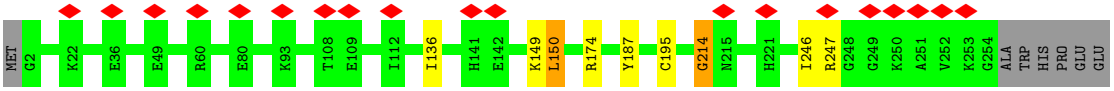



- Molecule 29: uL2

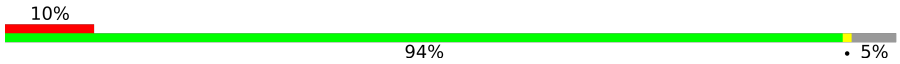
Chain c:

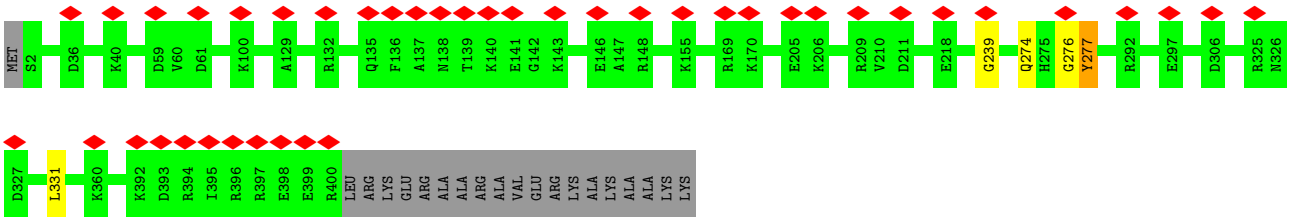



- Molecule 30: uL3

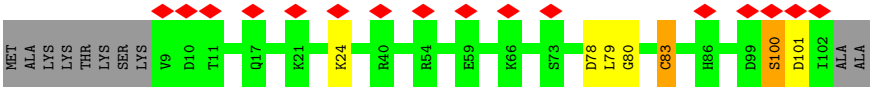
Chain d:



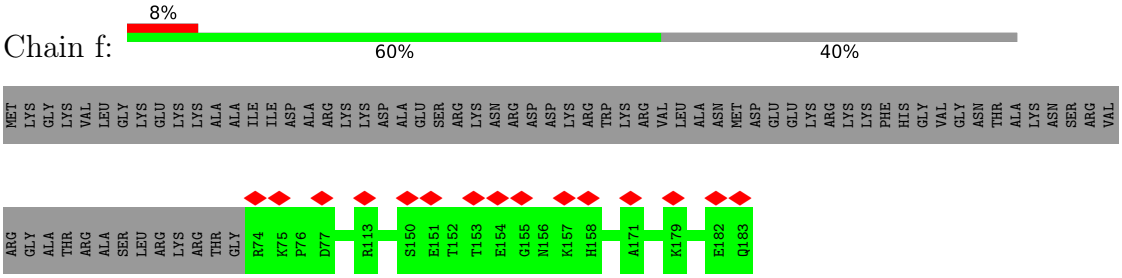

- Molecule 31: eL30

Chain e:



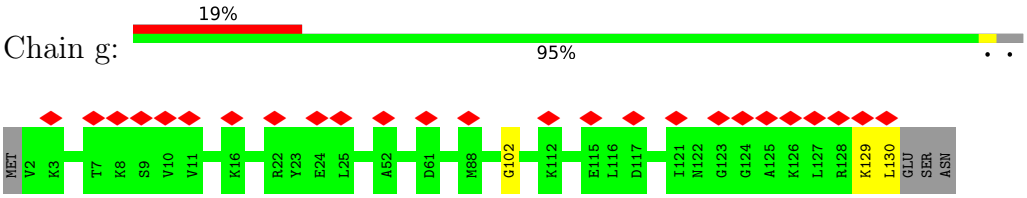

- Molecule 32: eL31

Chain f:



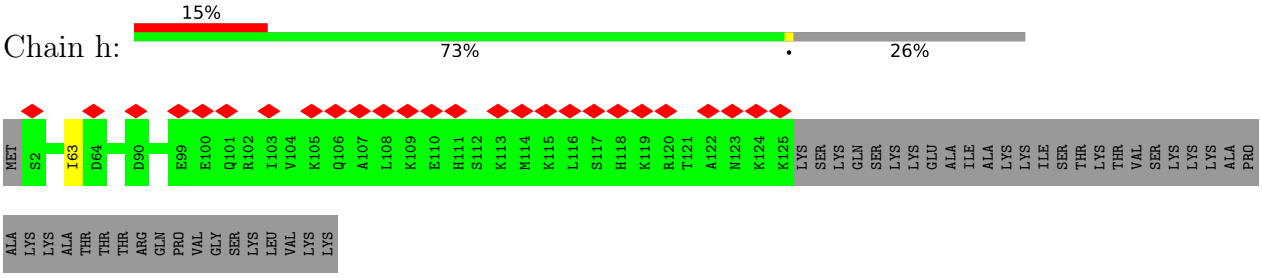

- Molecule 33: eL32

Chain g:



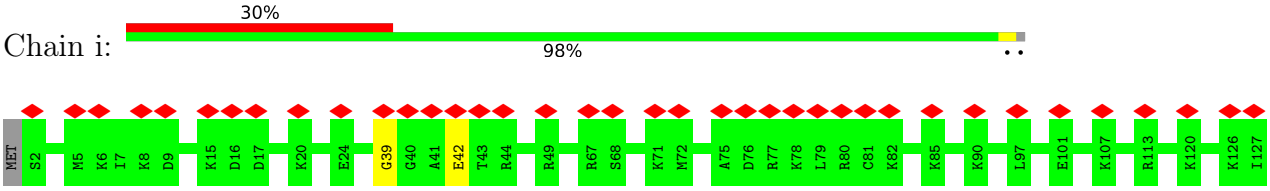

- Molecule 34: eL34

Chain h:



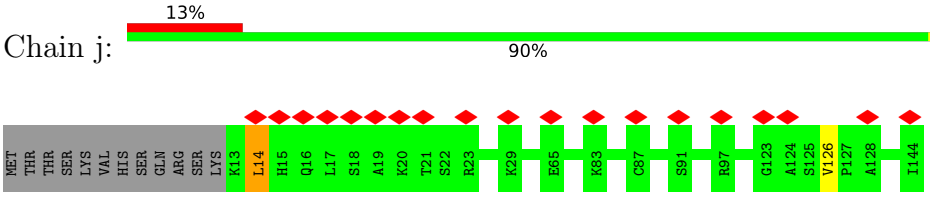

- Molecule 35: uL29

Chain i:



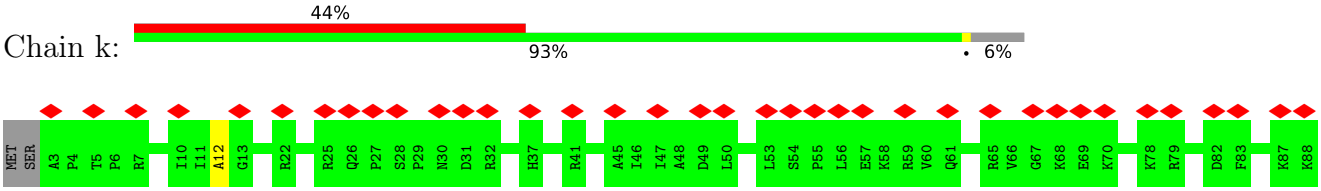

- Molecule 36: eL33

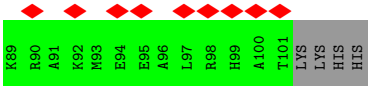
Chain j:




- Molecule 37: eL36

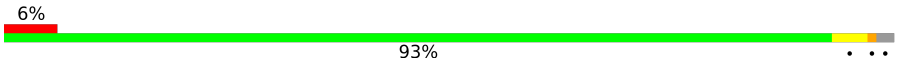
Chain k:

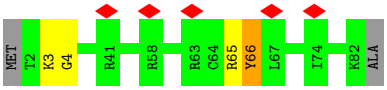





- Molecule 38: eL37

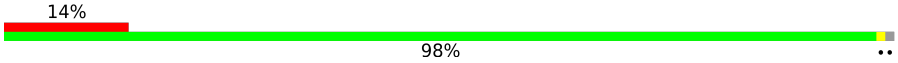
Chain l:

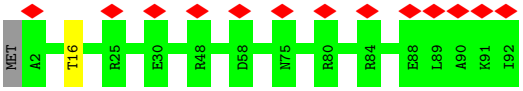



- Molecule 39: eL43

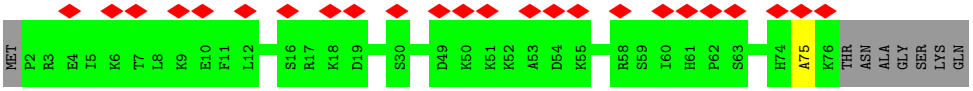
Chain m:



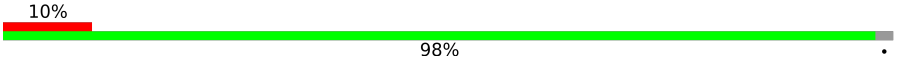

- Molecule 40: eL38

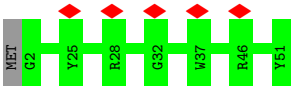
Chain n:




- Molecule 41: eL39

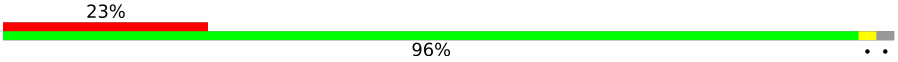
Chain o:

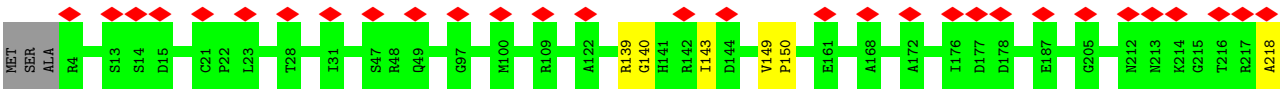


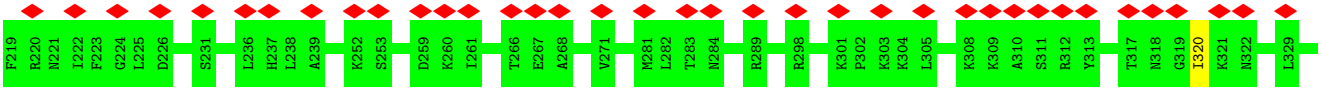



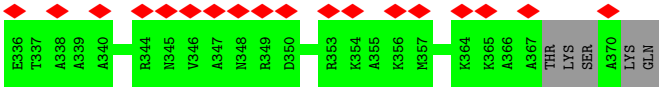

- Molecule 42: uL4

Chain p:



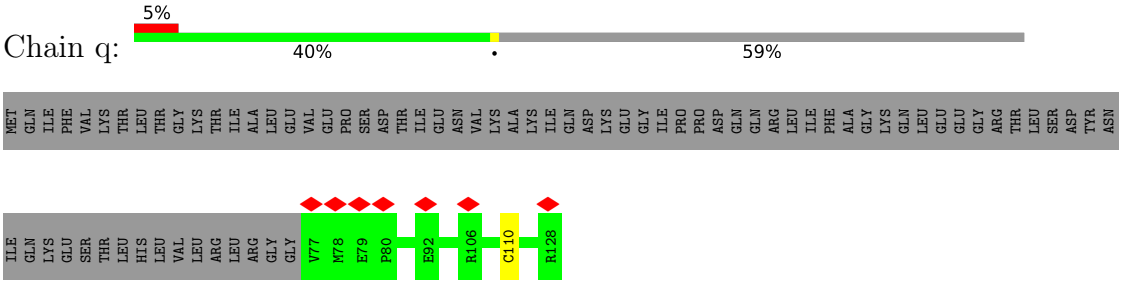



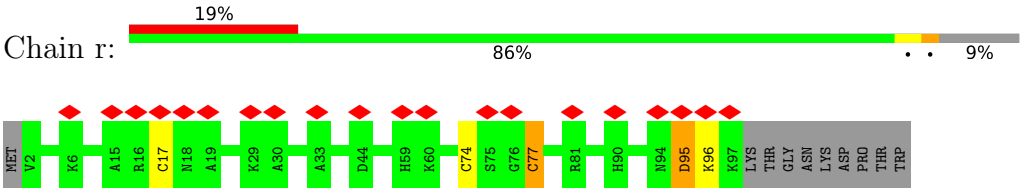

- Molecule 43: eL40

Chain q:



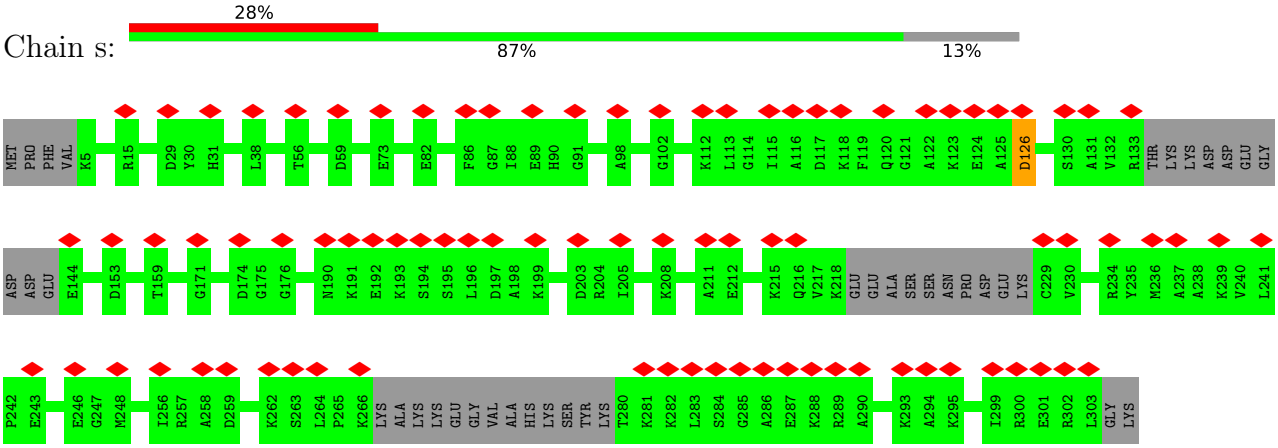

- Molecule 44: eL42

Chain r:



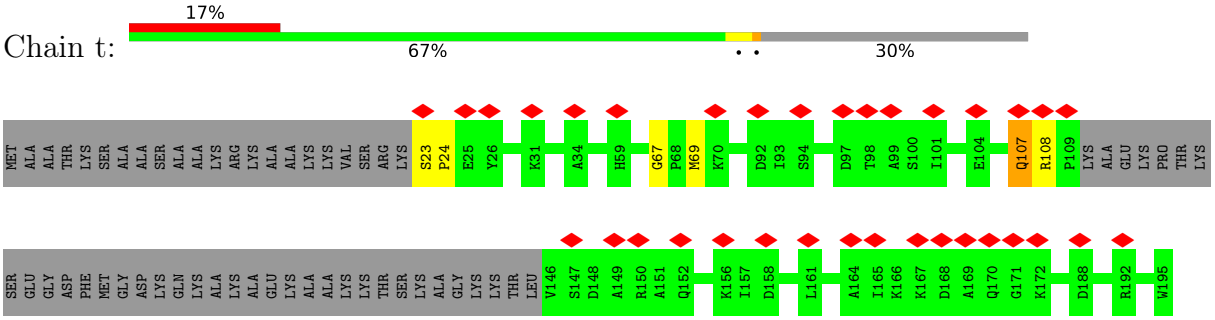

- Molecule 45: uL18

Chain s:



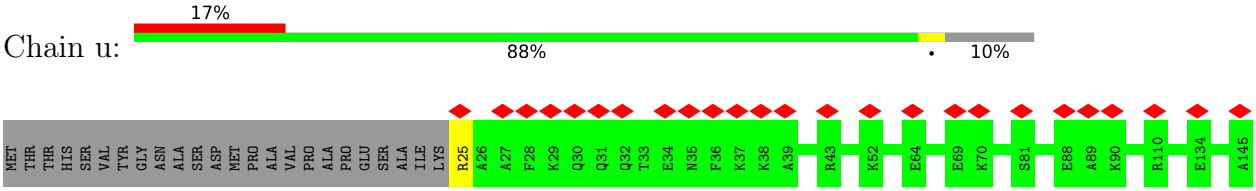

- Molecule 46: eL6

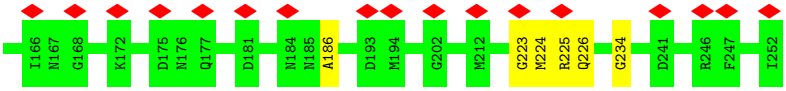
Chain t:



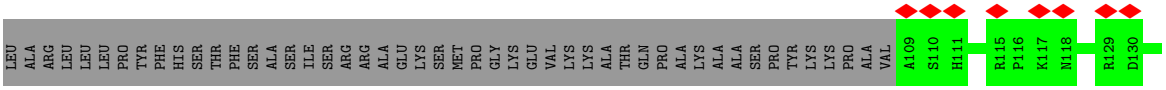

- Molecule 47: uL30

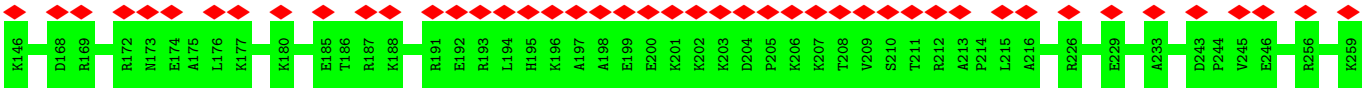
Chain u:

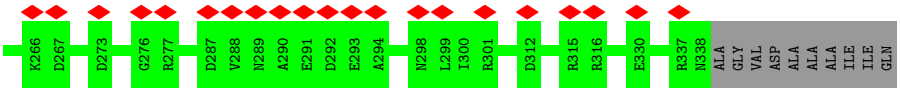




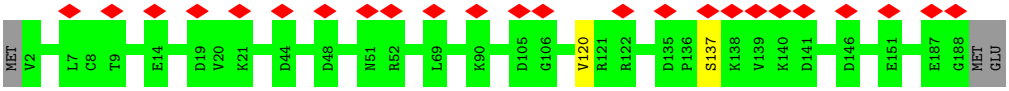

- Molecule 48: eL8



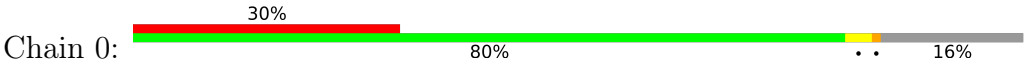



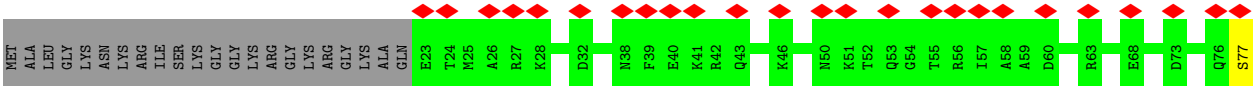



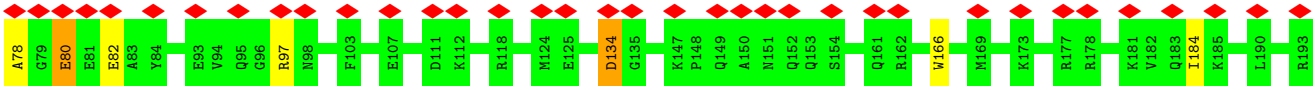

- Molecule 49: uL6

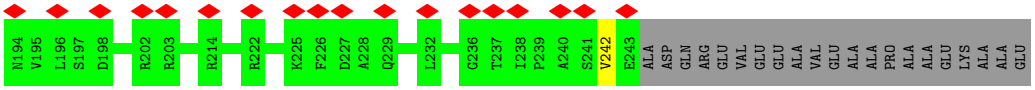



- Molecule 50: eS1

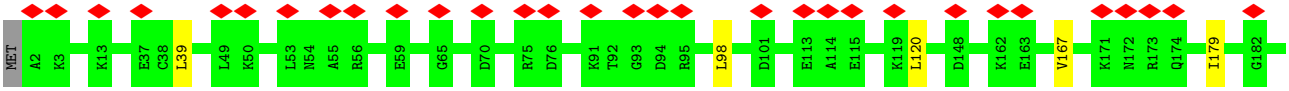


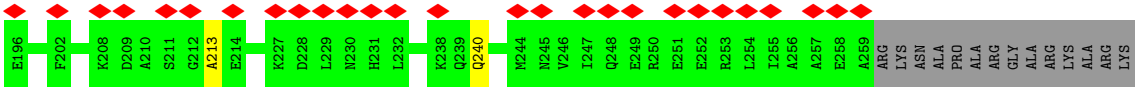



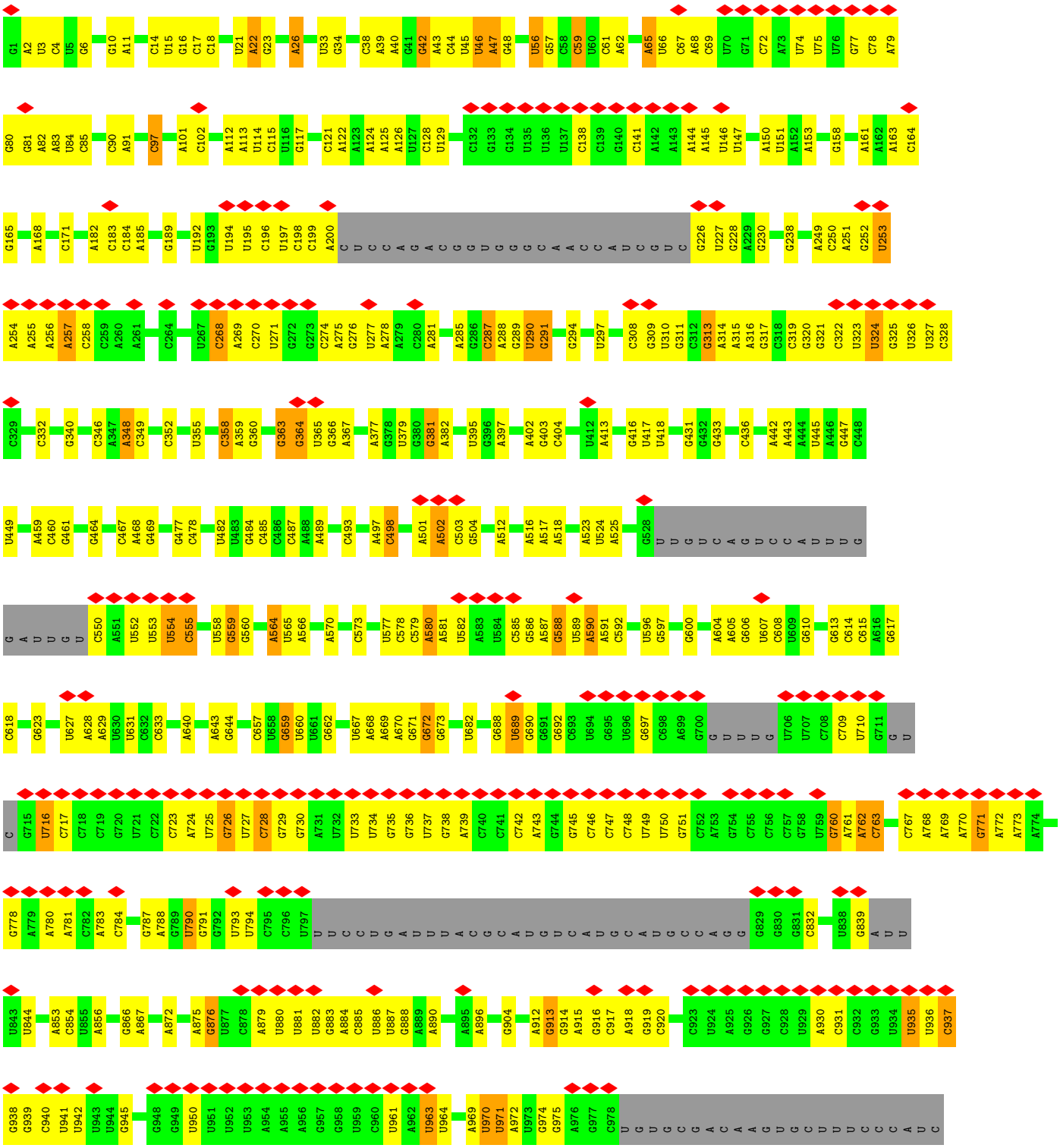

- Molecule 51: eS4

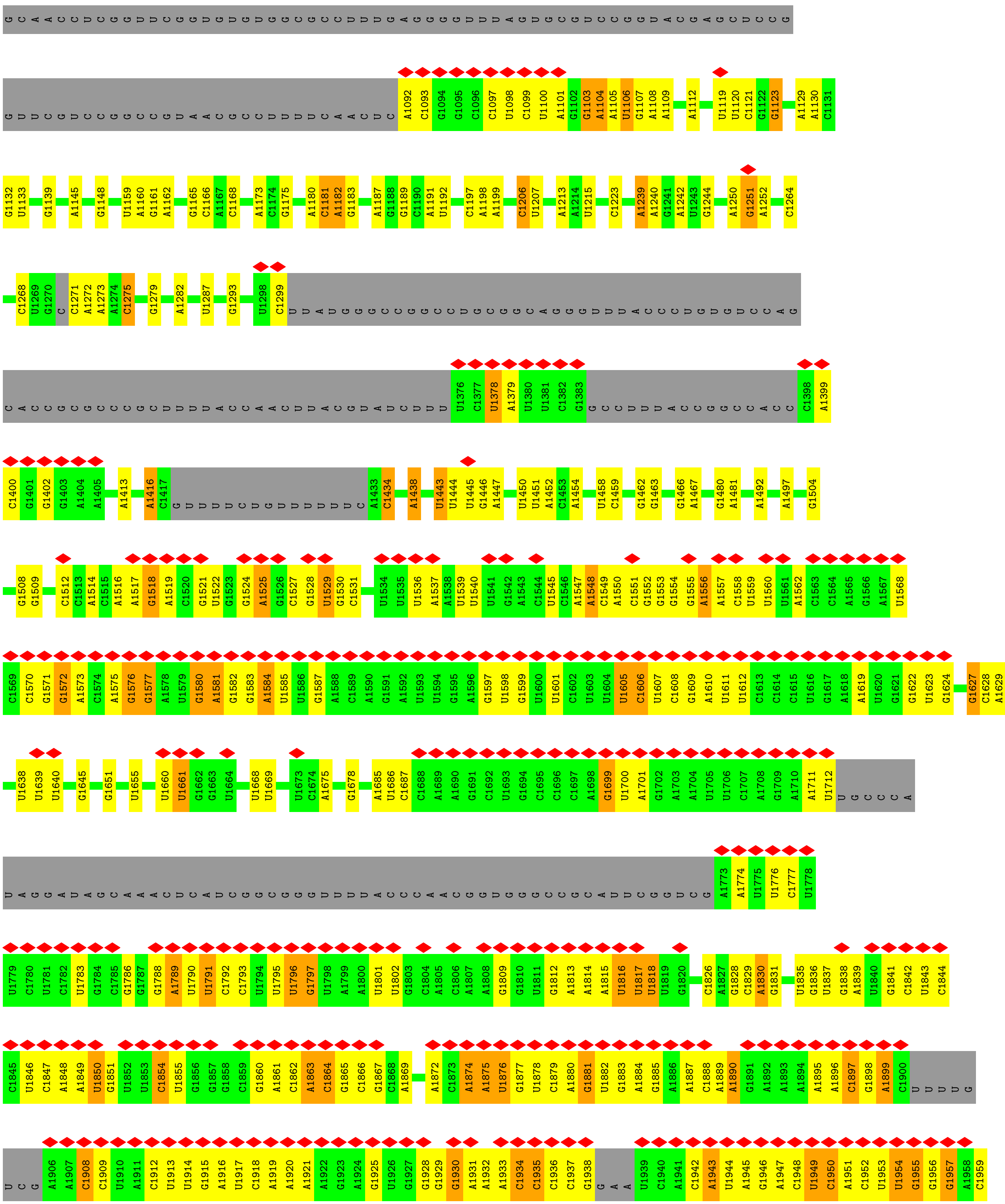


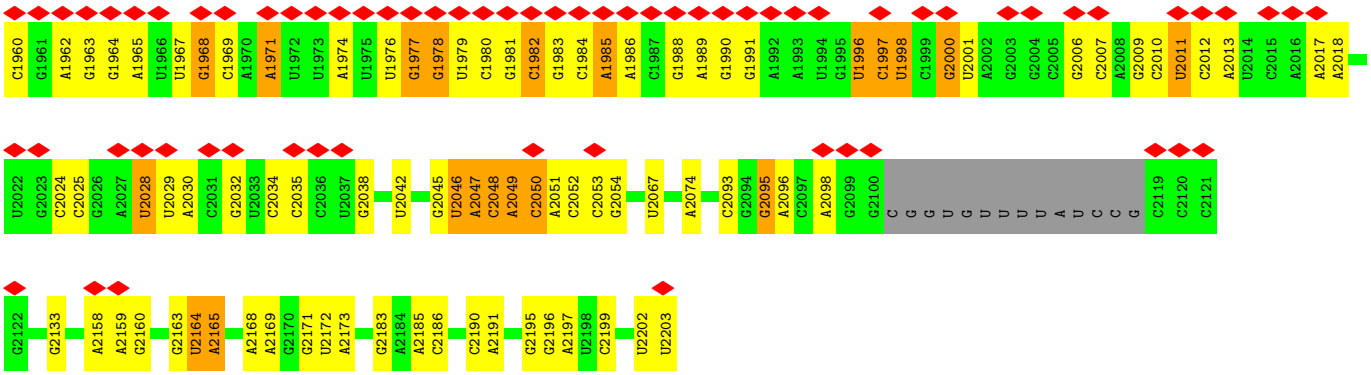



• Molecule 52: 18S rRNA

Chain 2:

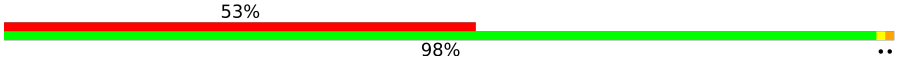


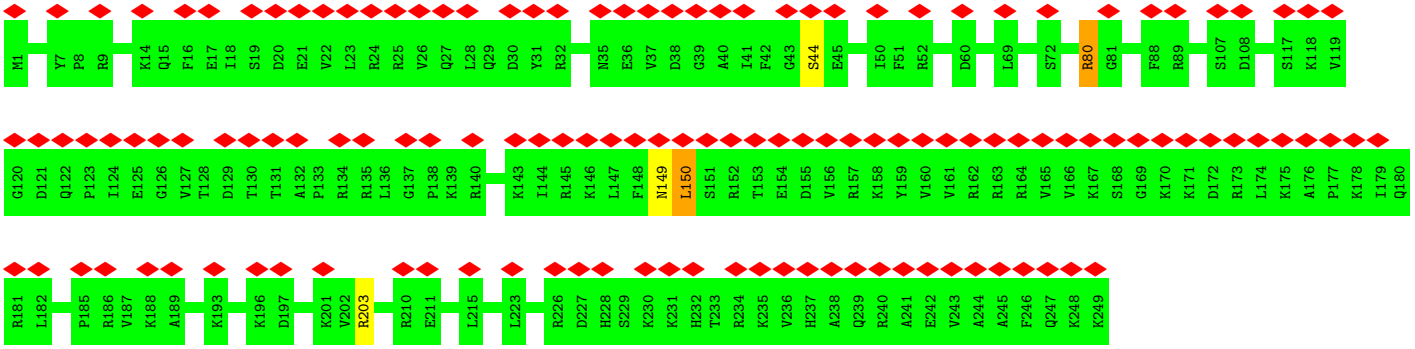

G C A A C C U C G G U U C G G G U G U G U G G C G C C U U U G A G G G G U U U A G U G C G U C C G G U A C G A G C U C C G
G U U C G U C C G G C C G U A A C G C C U U U U C A A C U C A1092 C1093 G1094 G1095 C1096 C1097 U1098 C1099 U1100 A1101 G1102 G1103 A1104 A1105 U1106 G1107 A1108 A1109 A1112 U1119 U1120 C1121 G1122 G1123 A1129 A1130 C1131
G1132 U1133 G1139 A1145 G1148 U1159 A1160 G1161 A1162 G1165 C1166 A1167 C1168 A1173 C1174 G1175 A1180 C1181 A1182 G1183 A1187 G1188 G1189 C1190 A1191 U1192 C1197 A1198 A1199 C1206 U1207 A1213 A1214 U1215 C1223 A1239 A1240 G1241 A1242 U1243 G1244 A1250 G1251 A1252 C1264
C1268 U1269 G1270 C C1271 A1272 A1273 A1274 C1275 G1279 A1282 U1287 G1293 U1298 C1299 U U A U G G G C C G G C C U G C G G C A G G G U U U A C C C U G U G U C C A G
C A C C G C G C C C G C U U U U A C C A A C U U A C G U A U C U U U U1376 C1377 U1378 A1379 U1380 U1381 C1382 G1383 G C C U U U A C C G G C C A C C C1398 A1399
C1400 G1401 G1402 G1403 A1404 A1405 A1413 A1416 C1417 G U U U U C U G U U U U U C A1433 C1434 A1438 U1443 U1444 U1445 G1446 A1447 U1450 U1451 A1452 C1453 A1454 U1458 C1459 G1462 G1463 G1466 A1467 G1480 A1481 A1492 A1497 G1504
G1508 G1509 C1512 C1513 A1514 C1515 A1516 A1517 G1518 A1519 C1520 G1521 U1522 G1523 G1524 A1525 G1526 C1527 G1528 U1529 G1530 C1531 U1534 U1535 U1536 A1537 A1538 U1539 U1540 U1541 G1542 A1543 C1544 U1545 C1546 A1547 A1548 C1549 A1550 C1551 G1552 G1553 G1554 G1555 A1556 A1557 C1558 U1559 U1560 U1561 A1562 C1563 C1564 A1565 G1566 A1567 U1568
C1569 C1570 G1571 G1572 A1573 C1574 A1575 G1576 G1577 A1578 U1579 G1580 A1581 G1582 G1583 A1584 U1585 G1586 G1587 A1588 C1589 A1590 G1591 A1592 U1593 U1594 G1595 A1596 G1597 U1598 G1599 U1600 U1601 C1602 U1603 U1604 U1605 C1606 U1607 C1608 G1609 A1610 U1611 U1612 C1613 C1614 C1615 U1616 G1617 A1618 A1619 U1620 G1621 G1622 U1623 G1624 G1627 C1628 A1629
U1638 U1639 U1640 G1645 G1651 U1655 U1660 U1661 G1662 G1663 U1664 U1668 U1669 U1673 C1674 A1675 G1678 A1685 U1686 C1687 C1688 A1689 A1690 G1691 C1692 U1693 G1694 C1695 C1696 C1697 A1698 G1699 U1700 A1701 G1702 A1703 A1704 U1705 U1706 C1707 A1708 G1709 A1710 A1711 U1712 U G C C C A
U A G G A U A G C A A C U C A U C G G C G G G U U U U A C C C A A C G G U G G G C C G C A U U C G G U C G A1773 A1774 U1775 U1776 C1777 U1778
U1779 C1780 U1781 C1782 U1783 G1784 C1785 G1786 G1787 G1788 A1789 U1790 U1791 C1792 C1793 U1794 U1795 U1796 G1797 U1798 A1799 A1800 U1801 U1802 G1803 C1804 A1805 C1806 A1807 A1808 G1809 G1810 U1811 G1812 A1813 A1814 A1815 U1816 U1817 U1818 U1819 G1820 C1826 A1827 G1828 C1829 A1830 G1831 U1835 G1836 U1837 G1838 A1839 U1840 G1841 C1842 U1843 C1844
C1845 U1846 C1847 A1848 A1849 U1850 G1851 U1852 U1853 C1854 U1855 G1856 G1857 G1858 C1859 G1860 A1861 C1862 A1863 C1864 G1865 C1866 G1867 C1868 A1869 A1872 C1873 A1874 A1875 U1876 G1877 U1878 C1879 A1880 G1881 U1882 G1883 A1884 G1885 A1886 A1887 C1888 A1889 A1890 G1891 A1892 A1893 A1894 A1895 A1896 C1897 G1898 A1899 C1900 U U U U G
U C G A1906 A1907 C1908 C1909 U1910 A1911 C1912 U1913 U1914 G1915 A1916 U1917 C1918 A1919 A1920 A1921 A1922 G1923 A1924 G1925 U1926 G1927 G1928 G1929 G1930 A1931 A1932 A1933 C1934 C1935 C1936 C1937 G1938 G A A U1939 C1940 A1941 C1942 A1943 U1944 A1945 G1946 A1947 C1948 U1949 C1950 A1951 C1952 U1953 U1954 G1955 G1956 G1957 A1958 C1959




- Molecule 53: eS6

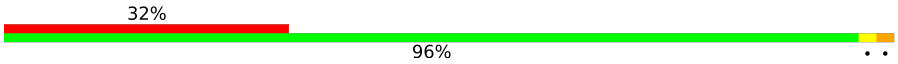
Chain 3:

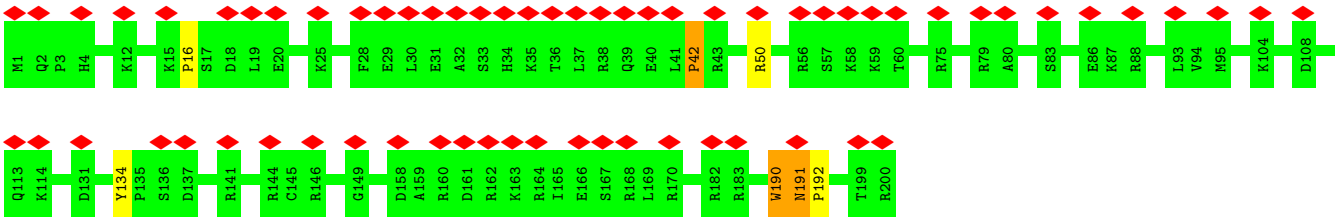



- Molecule 54: eS7

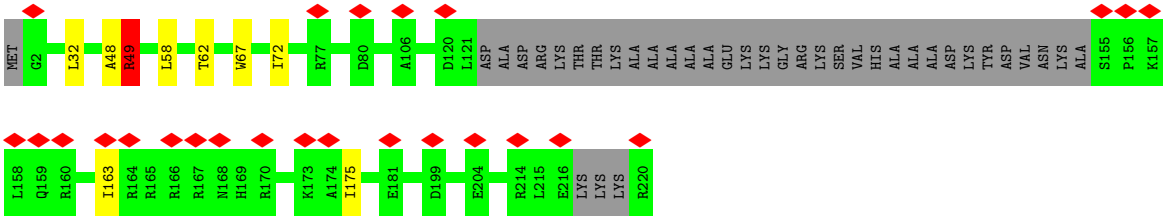
Chain 4:



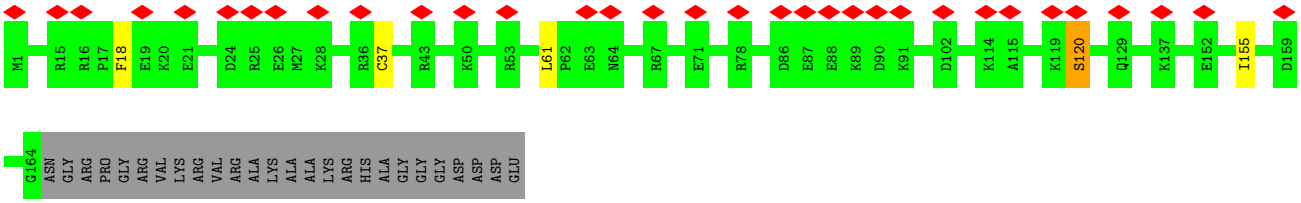

- Molecule 55: eS8

Chain 5:



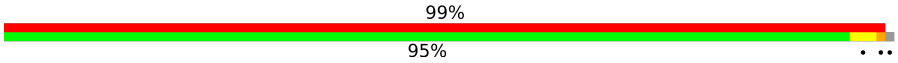

- Molecule 56: uS4

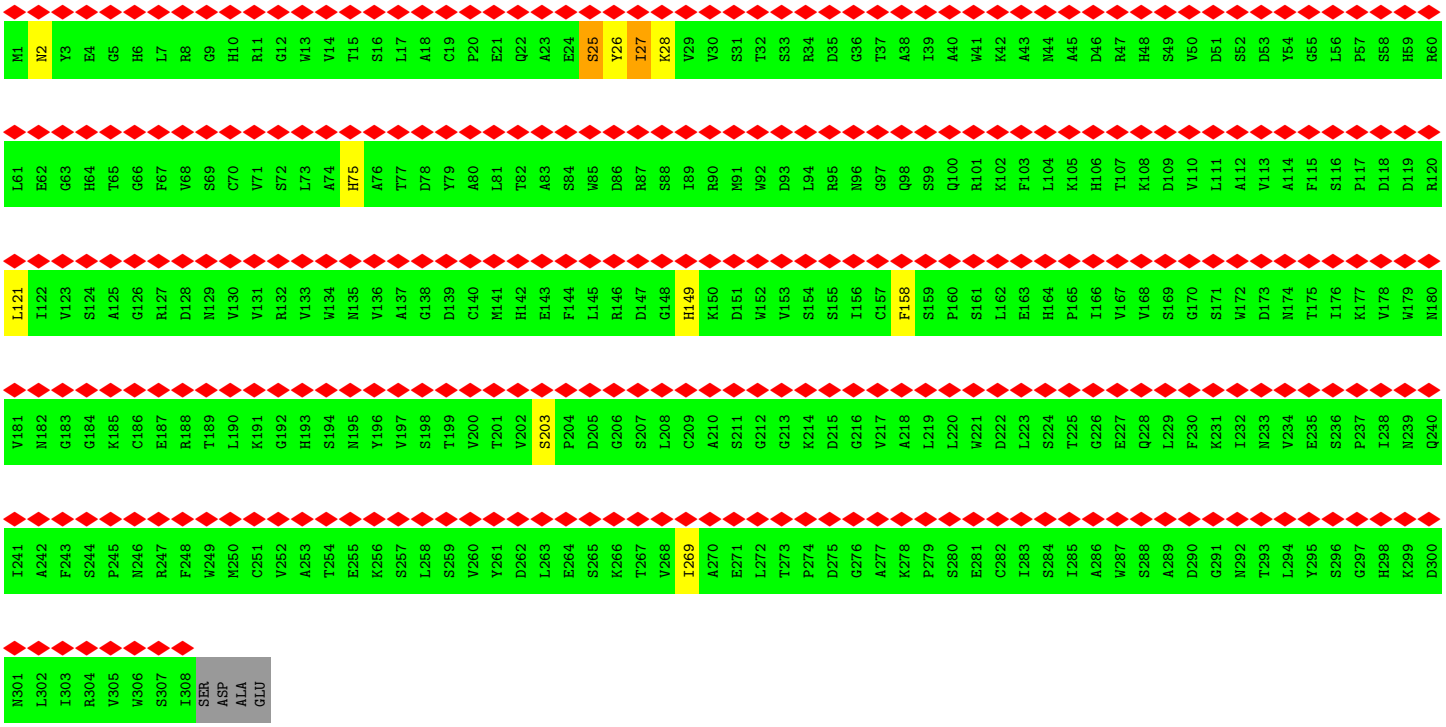
Chain 6:




- Molecule 57: RACK1

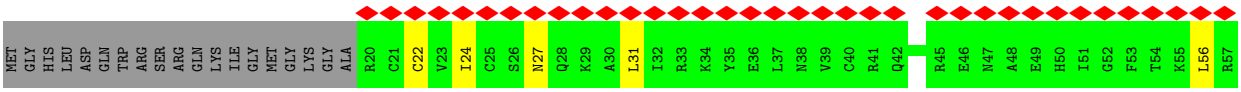
Chain 7:



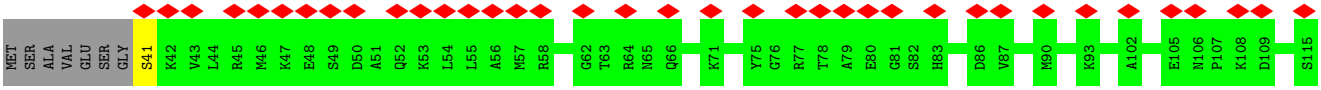

- Molecule 58: uS14

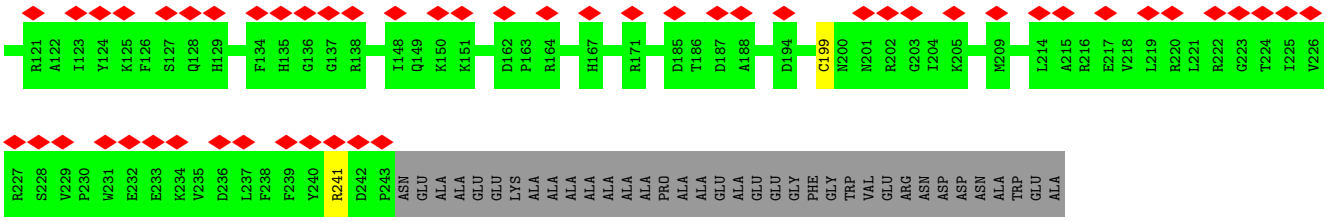
Chain 8:




- Molecule 59: uS2

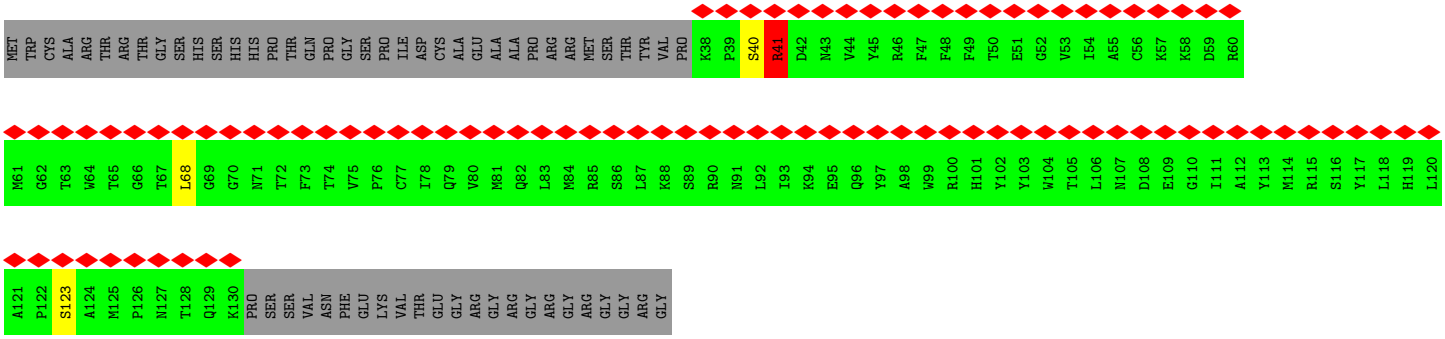
Chain AC:






• Molecule 60: eS10

Chain AD:

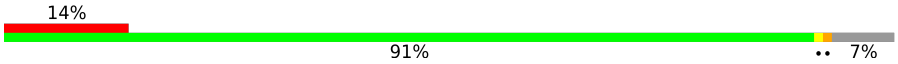


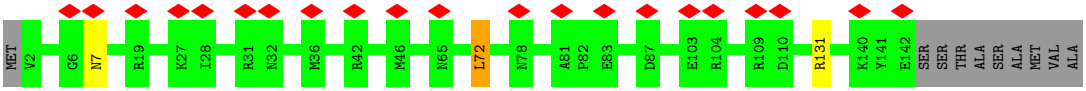

• Molecule 61: uS17

Chain AE:

• Molecule 62: uS15

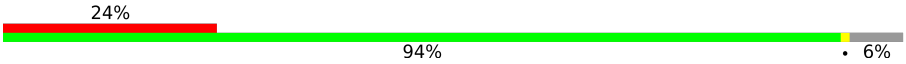
Chain AG:

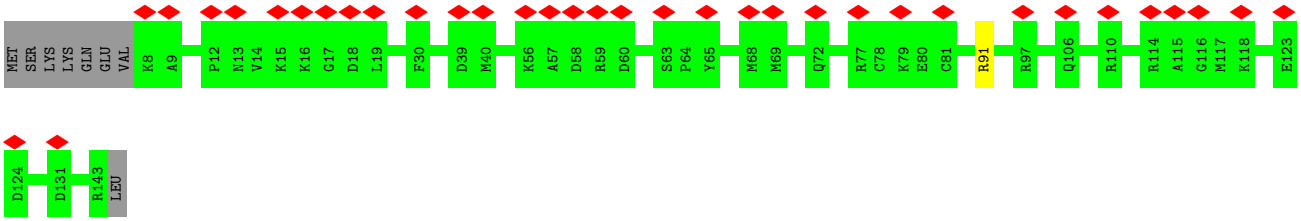



• Molecule 63: uS11

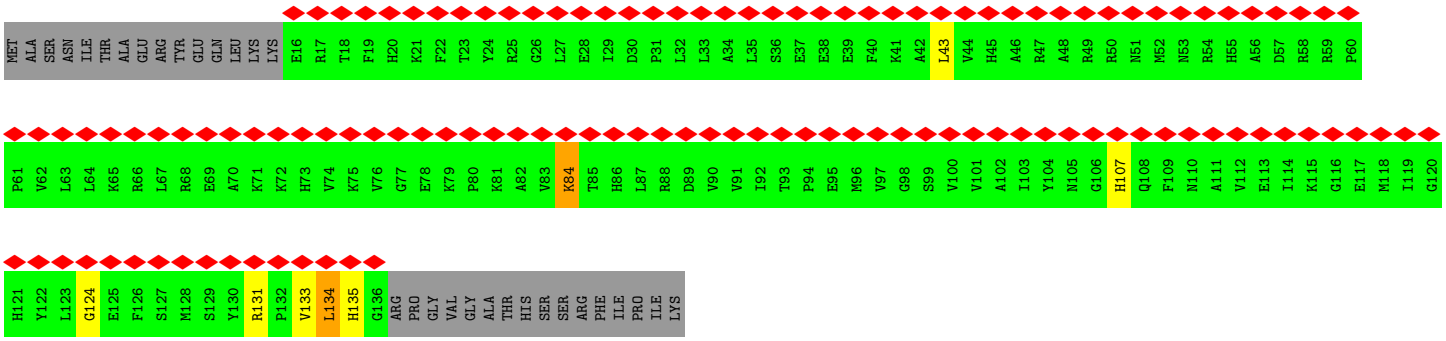
Chain AH:



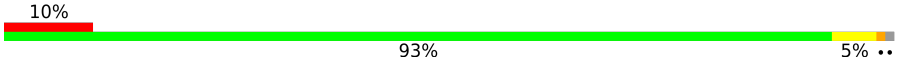
- Molecule 64: uS19

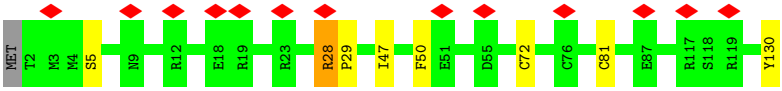
Chain AI:




- Molecule 65: uS8

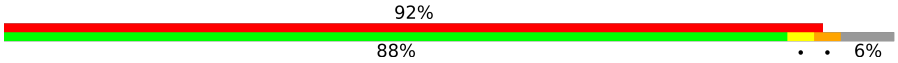
Chain AJ:

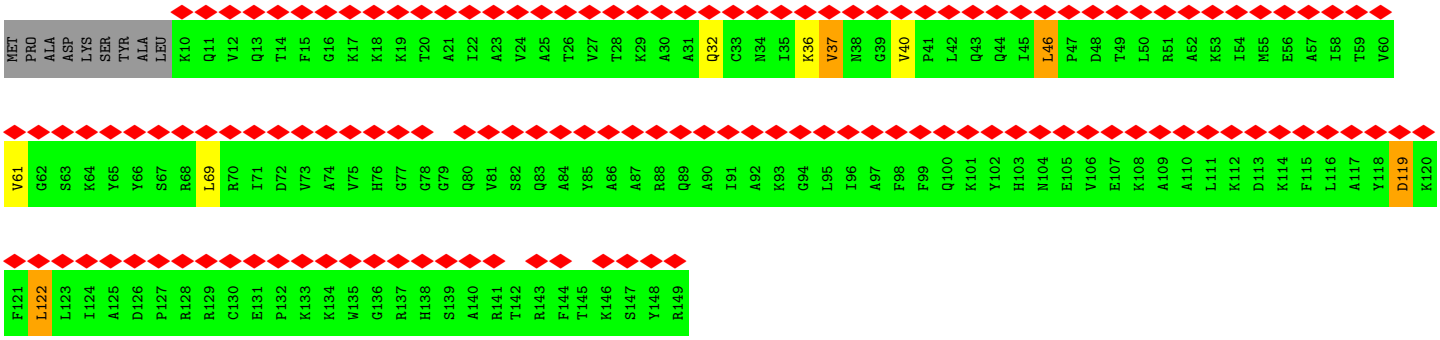



- Molecule 66: uS9

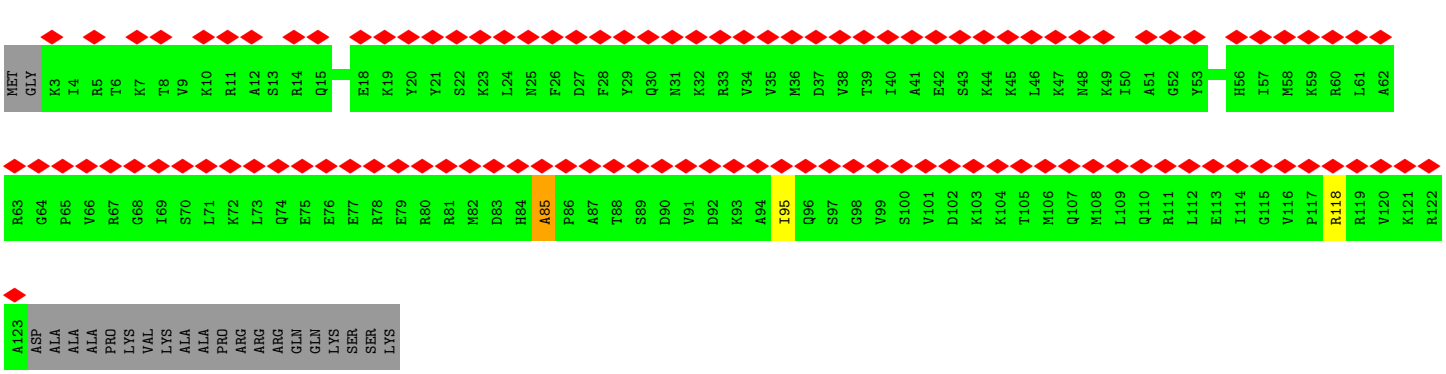
Chain AK:



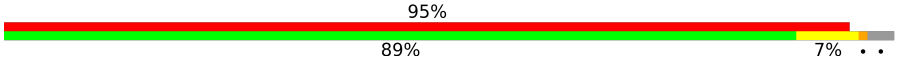

- Molecule 67: eS17

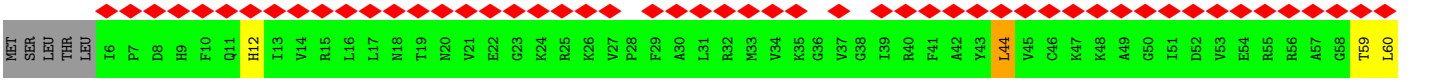
Chain AL:

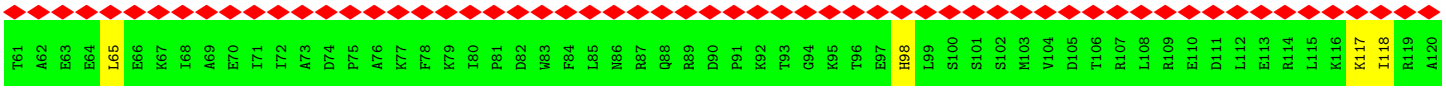


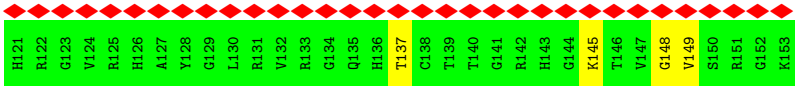
- Molecule 68: uS13

Chain AM:



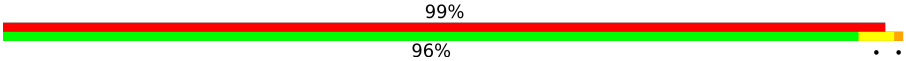



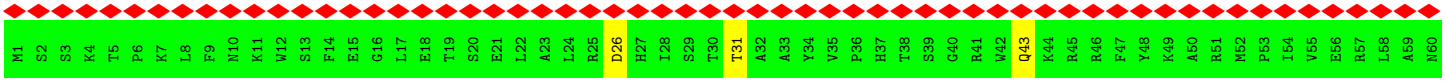



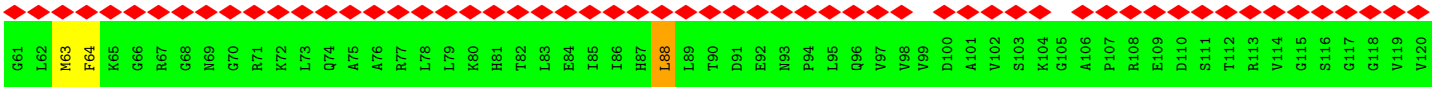



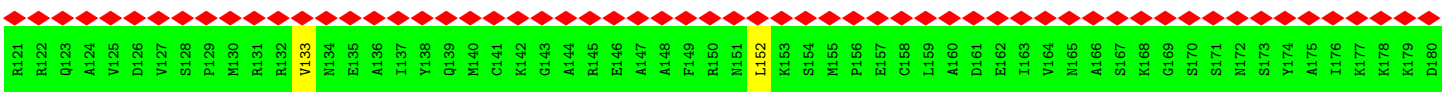

- Molecule 69: uS7

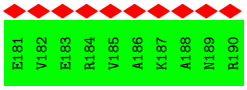
Chain AN:



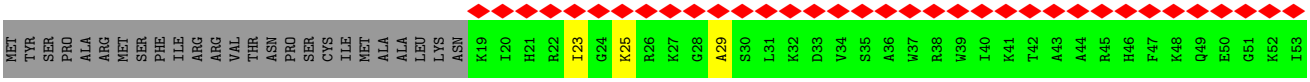



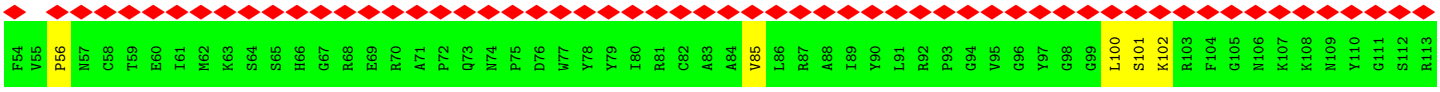



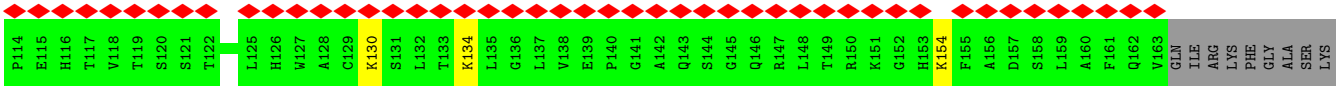




- Molecule 70: eS19

Chain AO:

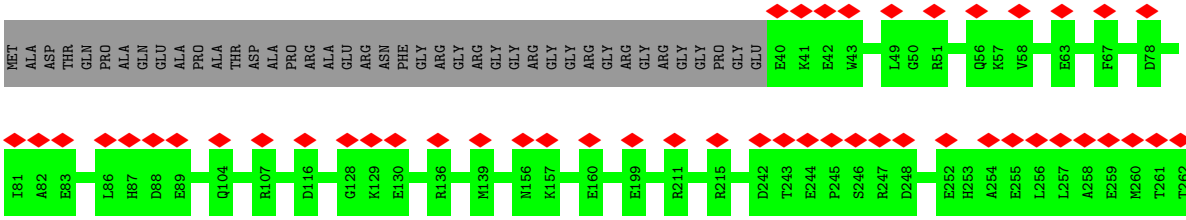



- Molecule 71: uS5

Chain AP:

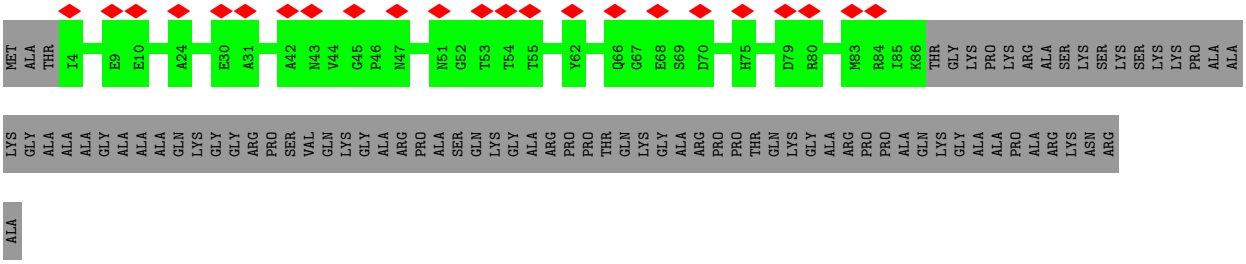



- Molecule 72: uS10

Chain AQ:

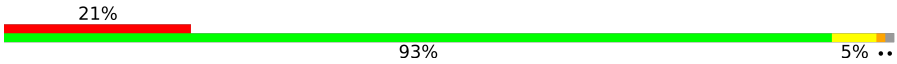
- Molecule 73: eS21

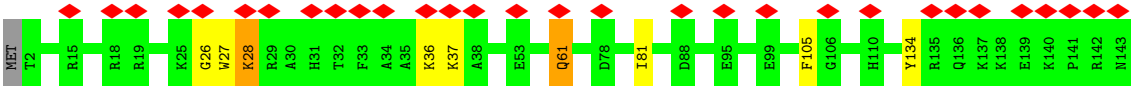
Chain AR:




- Molecule 74: uS12

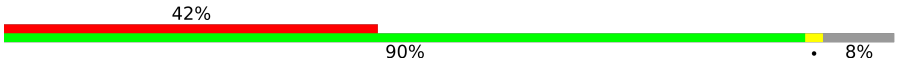
Chain AS:

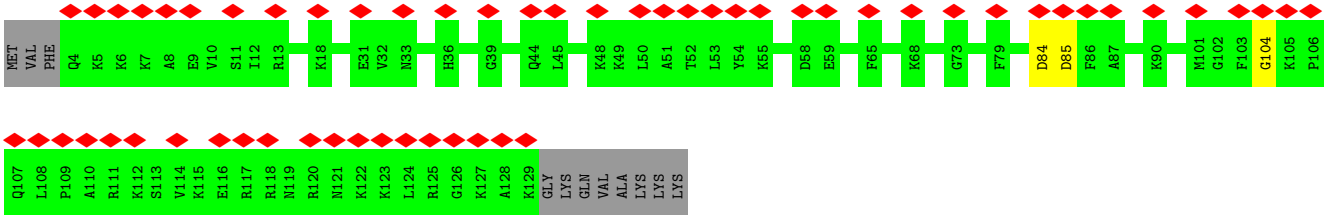



- Molecule 75: eS24

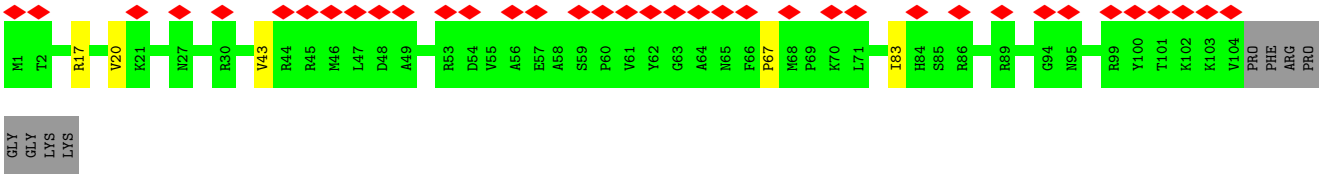
Chain AT:



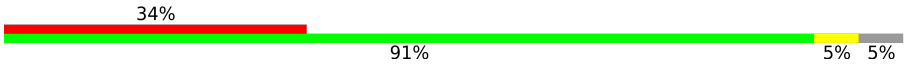

- Molecule 76: eS26

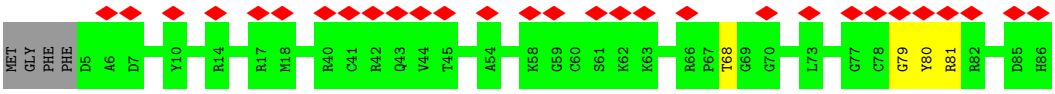
Chain AV:




- Molecule 77: eS27

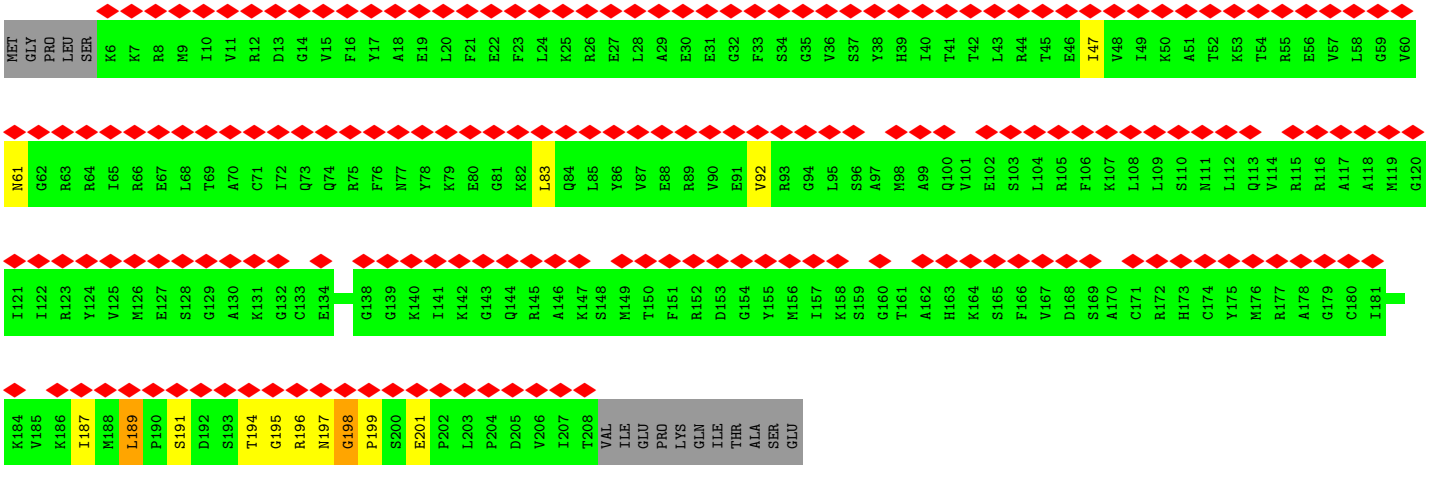
Chain AW:



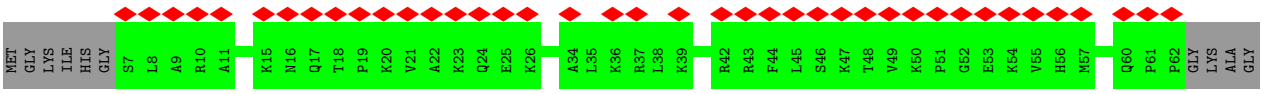

- Molecule 78: uS3

Chain AX:



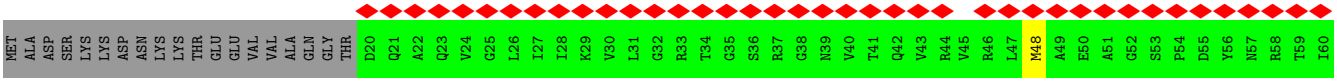

- Molecule 79: eS30

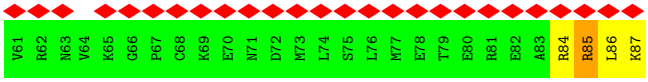
Chain AY:




- Molecule 80: eS28

Chain AZ:




V61
R62
M63
V64
K65
C66
P67
C68
K69
E70
N71
D72
M73
L74
S75
L76
M77
E78
T79
E80
R81
E82
A83
R84
R85
L86
K87

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 213108 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 20 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.039 | Depositor |
| Minimum map value | -0.020 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.01 | Depositor |
| Map size (Å) | 317.31998, 317.31998, 317.31998 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.7932999, 0.7932999, 0.7932999 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 1 | A | 1.03 | 0/38479 | 0.88 | 24/59984 (0.0%) |
| 2 | B | 1.05 | 0/25421 | 0.84 | 8/39614 (0.0%) |
| 3 | C | 0.98 | 1/3855 (0.0%) | 0.89 | 2/6002 (0.0%) |
| 4 | D | 0.93 | 0/2829 | 0.79 | 0/4405 |
| 5 | E | 1.01 | 0/4004 | 0.83 | 1/6223 (0.0%) |
| 6 | F | 0.84 | 0/1686 | 0.86 | 1/2623 (0.0%) |
| 7 | G | 1.11 | 0/4373 | 0.88 | 8/6817 (0.1%) |
| 8 | H | 1.15 | 0/2230 | 0.88 | 2/3470 (0.1%) |
| 9 | I | 0.60 | 1/1564 (0.1%) | 0.75 | 2/2092 (0.1%) |
| 10 | J | 0.53 | 0/1737 | 0.62 | 0/2324 |
| 11 | K | 0.42 | 0/1362 | 0.56 | 0/1821 |
| 12 | L | 0.52 | 0/1463 | 0.60 | 2/1952 (0.1%) |
| 13 | M | 0.59 | 0/1815 | 0.67 | 3/2436 (0.1%) |
| 14 | N | 0.51 | 0/1355 | 0.66 | 3/1814 (0.2%) |
| 15 | O | 0.65 | 2/1754 (0.1%) | 0.71 | 5/2342 (0.2%) |
| 16 | P | 0.61 | 0/1269 | 0.62 | 0/1700 |
| 17 | Q | 0.61 | 0/1490 | 0.60 | 0/2007 |
| 18 | R | 0.50 | 0/1665 | 0.54 | 0/2206 |
| 19 | S | 0.58 | 0/1290 | 0.71 | 2/1734 (0.1%) |
| 20 | T | 0.52 | 0/1013 | 0.61 | 1/1350 (0.1%) |
| 21 | U | 0.64 | 0/1052 | 0.64 | 0/1417 |
| 22 | V | 0.50 | 0/978 | 0.58 | 0/1318 |
| 23 | W | 0.65 | 0/584 | 0.53 | 0/785 |
| 24 | X | 0.54 | 0/980 | 0.67 | 0/1308 |
| 25 | Y | 0.56 | 0/1100 | 0.57 | 0/1470 |
| 26 | Z | 0.57 | 0/1153 | 0.72 | 2/1541 (0.1%) |
| 27 | a | 0.47 | 0/1157 | 0.65 | 2/1548 (0.1%) |
| 28 | b | 0.41 | 0/565 | 0.62 | 1/754 (0.1%) |
| 29 | c | 0.69 | 2/1961 (0.1%) |
| 30 | d | 0.64 | 0/3250 | 0.69 | 4/4368 (0.1%) |
| 31 | e | 0.57 | 0/730 | 0.77 | 3/988 (0.3%) |
| 32 | f | 0.55 | 0/893 | 0.61 | 0/1196 |
| 33 | g | 0.57 | 0/1071 | 0.71 | 1/1432 (0.1%) |
| 34 | h | 0.57 | 0/1030 | 0.62 | 0/1369 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 35 | i | 0.45 | 0/1067 | 0.59 | 1/1416 (0.1%) |
| 36 | j | 0.63 | 0/1082 | 0.68 | 1/1454 (0.1%) |
| 37 | k | 0.42 | 0/802 | 0.50 | 0/1073 |
| 38 | l | 0.64 | 1/688 (0.1%) | 0.87 | 2/918 (0.2%) |
| 39 | m | 0.63 | 0/724 | 0.66 | 0/964 |
| 40 | n | 0.54 | 0/614 | 0.58 | 1/818 (0.1%) |
| 41 | o | 0.58 | 0/463 | 0.65 | 0/617 |
| 42 | p | 0.53 | 0/2874 | 0.67 | 3/3865 (0.1%) |
| 43 | q | 0.61 | 0/431 | 0.66 | 1/572 (0.2%) |
| 44 | r | 0.59 | 1/792 (0.1%) | 0.69 | 2/1046 (0.2%) |
| 45 | s | 0.49 | 0/2129 | 0.58 | 1/2846 (0.0%) |
| 46 | t | 0.57 | 0/1074 | 0.78 | 5/1454 (0.3%) |
| 47 | u | 0.57 | 0/1891 | 0.61 | 2/2531 (0.1%) |
| 48 | v | 0.48 | 0/1878 | 0.57 | 0/2524 |
| 49 | w | 0.56 | 0/1504 | 0.64 | 0/2024 |
| 50 | 0 | 0.70 | 0/1811 | 0.76 | 4/2438 (0.2%) |
| 51 | 1 | 0.80 | 0/2076 | 0.78 | 1/2799 (0.0%) |
| 52 | 2 | 1.66 | 86/43318 (0.2%) | 1.27 | 315/67487 (0.5%) |
| 53 | 3 | 0.66 | 1/2019 (0.0%) | 0.77 | 3/2694 (0.1%) |
| 54 | 4 | 0.76 | 0/1697 | 0.88 | 4/2276 (0.2%) |
| 55 | 5 | 0.89 | 2/1494 (0.1%) | 1.01 | 7/2000 (0.3%) |
| 56 | 6 | 0.75 | 1/1389 (0.1%) | 0.73 | 1/1866 (0.1%) |
| 57 | 7 | 0.46 | 1/2454 (0.0%) | 0.75 | 6/3337 (0.2%) |
| 58 | 8 | 0.73 | 0/317 | 1.00 | 3/421 (0.7%) |
| 59 | AC | 0.68 | 0/1656 | 0.69 | 0/2238 |
| 60 | AD | 0.47 | 0/788 | 0.91 | 3/1064 (0.3%) |
| 61 | AE | 0.98 | 0/1171 | 0.75 | 1/1570 (0.1%) |
| 62 | AG | 0.83 | 0/1180 | 0.80 | 1/1581 (0.1%) |
| 63 | AH | 0.78 | 0/1038 | 0.80 | 1/1392 (0.1%) |
| 64 | AI | 1.11 | 1/1006 (0.1%) | 0.94 | 8/1351 (0.6%) |
| 65 | AJ | 0.94 | 2/1037 (0.2%) | 0.89 | 1/1391 (0.1%) |
| 66 | AK | 0.54 | 0/1128 | 0.82 | 3/1515 (0.2%) |
| 67 | AL | 0.52 | 0/993 | 0.69 | 0/1322 |
| 68 | AM | 0.50 | 0/1206 | 0.88 | 2/1615 (0.1%) |
| 69 | AN | 0.48 | 0/1516 | 0.75 | 2/2034 (0.1%) |
| 70 | AO | 0.51 | 0/1180 | 0.78 | 1/1585 (0.1%) |
| 71 | AP | 0.80 | 0/1758 | 0.76 | 0/2380 |
| 72 | AQ | 0.51 | 0/817 | 0.75 | 0/1107 |
| 73 | AR | 0.67 | 0/639 | 0.72 | 0/866 |
| 74 | AS | 0.81 | 0/1134 | 0.89 | 3/1517 (0.2%) |
| 75 | AT | 0.68 | 0/1054 | 0.70 | 0/1405 |
| 76 | AV | 0.69 | 0/845 | 0.76 | 0/1130 |
| 77 | AW | 1.25 | 2/658 (0.3%) | 0.80 | 1/883 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 78 | AX | 0.56 | 0/1616 | 0.83 | 6/2159 (0.3%) |
| 79 | AY | 0.54 | 0/460 | 0.73 | 0/611 |
| 80 | AZ | 0.60 | 1/528 (0.2%) | 0.83 | 1/705 (0.1%) |
| All | All | 1.06 | 105/215154 (0.0%) | 0.92 | 475/315901 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 9 | I | 0 | 1 |
| 13 | M | 0 | 2 |
| 16 | P | 0 | 2 |
| 20 | T | 0 | 1 |
| 23 | W | 0 | 1 |
| 24 | X | 0 | 1 |
| 28 | b | 0 | 1 |
| 29 | c | 0 | 1 |
| 31 | e | 0 | 1 |
| 37 | k | 0 | 1 |
| 38 | l | 0 | 3 |
| 39 | m | 0 | 1 |
| 47 | u | 0 | 1 |
| 50 | 0 | 0 | 1 |
| 53 | 3 | 0 | 1 |
| 54 | 4 | 0 | 1 |
| 55 | 5 | 0 | 2 |
| 57 | 7 | 0 | 1 |
| 58 | 8 | 0 | 1 |
| 59 | AC | 0 | 3 |
| 61 | AE | 0 | 1 |
| 62 | AG | 0 | 3 |
| 64 | AI | 0 | 3 |
| 66 | AK | 0 | 1 |
| 67 | AL | 0 | 1 |
| 68 | AM | 0 | 7 |
| 69 | AN | 0 | 4 |
| 70 | AO | 0 | 6 |
| 72 | AQ | 0 | 1 |
| 75 | AT | 0 | 2 |
| 77 | AW | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 78 | AX | 0 | 1 |
| All | All | 0 | 58 |

All (105) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 52 | 2 | 1864 | C | N3-C4 | 80.83 | 1.90 | 1.33 |
| 52 | 2 | 1864 | C | C2-N3 | 72.70 | 1.94 | 1.35 |
| 52 | 2 | 1864 | C | N1-C6 | 69.47 | 1.78 | 1.37 |
| 52 | 2 | 1864 | C | N1-C2 | 48.39 | 1.88 | 1.40 |
| 52 | 2 | 1864 | C | C4-C5 | 48.22 | 1.81 | 1.43 |
| 52 | 2 | 1864 | C | C5-C6 | 44.65 | 1.70 | 1.34 |
| 52 | 2 | 1954 | U | O3'-P | 38.92 | 2.07 | 1.61 |
| 64 | AI | 135 | HIS | CB-CG | 30.36 | 2.04 | 1.50 |
| 77 | AW | 80 | TYR | C-N | -20.26 | 0.87 | 1.34 |
| 52 | 2 | 1954 | U | C3'-O3' | 19.37 | 1.69 | 1.42 |
| 77 | AW | 79 | GLY | C-N | 15.09 | 1.68 | 1.34 |
| 29 | c | 246 | ILE | C-N | -14.26 | 1.01 | 1.34 |
| 15 | O | 51 | LEU | C-N | 9.04 | 1.49 | 1.33 |
| 52 | 2 | 1956 | G | N7-C5 | -9.04 | 1.33 | 1.39 |
| 15 | O | 50 | MET | C-N | -8.01 | 1.15 | 1.34 |
| 9 | I | 20 | TYR | C-N | 7.84 | 1.52 | 1.34 |
| 52 | 2 | 969 | A | N9-C4 | -7.78 | 1.33 | 1.37 |
| 29 | c | 247 | ARG | C-N | 7.74 | 1.47 | 1.33 |
| 80 | AZ | 85 | ARG | C-N | 7.69 | 1.51 | 1.34 |
| 52 | 2 | 1899 | A | C1'-N9 | -7.08 | 1.36 | 1.46 |
| 52 | 2 | 1956 | G | N9-C8 | -7.07 | 1.32 | 1.37 |
| 52 | 2 | 913 | G | N9-C4 | -6.80 | 1.32 | 1.38 |
| 52 | 2 | 1645 | G | N3-C4 | -6.62 | 1.30 | 1.35 |
| 38 | l | 66 | TYR | C-N | -6.58 | 1.19 | 1.34 |
| 55 | 5 | 49 | ARG | C-N | -6.48 | 1.21 | 1.33 |
| 52 | 2 | 1525 | A | N7-C5 | -6.41 | 1.35 | 1.39 |
| 52 | 2 | 1977 | G | C1'-N9 | -6.39 | 1.38 | 1.46 |
| 52 | 2 | 640 | A | N9-C4 | -6.38 | 1.34 | 1.37 |
| 52 | 2 | 590 | A | N9-C4 | -6.33 | 1.34 | 1.37 |
| 52 | 2 | 1971 | A | C1'-N9 | -6.31 | 1.38 | 1.46 |
| 52 | 2 | 969 | A | N3-C4 | -6.29 | 1.31 | 1.34 |
| 52 | 2 | 1934 | C | C1'-N1 | 6.27 | 1.58 | 1.48 |
| 52 | 2 | 97 | C | N1-C6 | -6.25 | 1.33 | 1.37 |
| 52 | 2 | 2168 | A | N9-C4 | -6.19 | 1.34 | 1.37 |
| 3 | C | 153 | A | N9-C4 | -6.11 | 1.34 | 1.37 |
| 52 | 2 | 153 | A | N9-C4 | -6.07 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 52 | 2 | 1678 | G | N3-C4 | -6.01 | 1.31 | 1.35 |
| 52 | 2 | 1480 | G | C5-C4 | -5.99 | 1.34 | 1.38 |
| 44 | r | 77 | CYS | CB-SG | -5.97 | 1.72 | 1.81 |
| 52 | 2 | 315 | A | N9-C4 | -5.93 | 1.34 | 1.37 |
| 52 | 2 | 1864 | C | P-O5' | 5.92 | 1.65 | 1.59 |
| 52 | 2 | 1459 | C | N3-C4 | -5.90 | 1.29 | 1.33 |
| 52 | 2 | 1935 | C | C1'-N1 | 5.88 | 1.57 | 1.48 |
| 52 | 2 | 381 | G | C5-C4 | -5.87 | 1.34 | 1.38 |
| 52 | 2 | 1459 | C | N1-C6 | -5.81 | 1.33 | 1.37 |
| 52 | 2 | 726 | G | C1'-N9 | -5.80 | 1.38 | 1.46 |
| 65 | AJ | 72 | CYS | CB-SG | -5.80 | 1.72 | 1.81 |
| 52 | 2 | 1438 | A | N3-C4 | -5.74 | 1.31 | 1.34 |
| 52 | 2 | 771 | G | N9-C4 | -5.72 | 1.33 | 1.38 |
| 52 | 2 | 2049 | A | N9-C4 | -5.71 | 1.34 | 1.37 |
| 52 | 2 | 1645 | G | N9-C4 | -5.71 | 1.33 | 1.38 |
| 56 | 6 | 37 | CYS | CB-SG | -5.67 | 1.72 | 1.81 |
| 52 | 2 | 1864 | C | C5'-C4' | 5.64 | 1.58 | 1.51 |
| 52 | 2 | 2173 | A | N9-C4 | -5.62 | 1.34 | 1.37 |
| 52 | 2 | 1955 | G | N7-C5 | -5.60 | 1.35 | 1.39 |
| 52 | 2 | 1413 | A | N9-C4 | -5.58 | 1.34 | 1.37 |
| 52 | 2 | 1182 | A | N9-C4 | -5.58 | 1.34 | 1.37 |
| 52 | 2 | 969 | A | N7-C5 | -5.57 | 1.35 | 1.39 |
| 52 | 2 | 1223 | C | N1-C6 | -5.56 | 1.33 | 1.37 |
| 52 | 2 | 348 | A | N9-C4 | -5.54 | 1.34 | 1.37 |
| 52 | 2 | 124 | A | N9-C4 | -5.54 | 1.34 | 1.37 |
| 52 | 2 | 1239 | A | N3-C4 | -5.53 | 1.31 | 1.34 |
| 52 | 2 | 1282 | A | N9-C4 | -5.52 | 1.34 | 1.37 |
| 52 | 2 | 1872 | A | N9-C4 | -5.49 | 1.34 | 1.37 |
| 52 | 2 | 1132 | G | N3-C4 | -5.42 | 1.31 | 1.35 |
| 52 | 2 | 1438 | A | C6-N1 | -5.42 | 1.31 | 1.35 |
| 52 | 2 | 22 | A | N9-C4 | -5.41 | 1.34 | 1.37 |
| 52 | 2 | 1678 | G | N9-C4 | -5.41 | 1.33 | 1.38 |
| 52 | 2 | 597 | G | N9-C4 | -5.41 | 1.33 | 1.38 |
| 52 | 2 | 670 | A | N9-C4 | -5.40 | 1.34 | 1.37 |
| 52 | 2 | 489 | A | N9-C4 | -5.39 | 1.34 | 1.37 |
| 52 | 2 | 1112 | A | N9-C4 | -5.38 | 1.34 | 1.37 |
| 52 | 2 | 1651 | G | C5-C4 | -5.37 | 1.34 | 1.38 |
| 52 | 2 | 1458 | U | N1-C2 | -5.37 | 1.33 | 1.38 |
| 52 | 2 | 969 | A | C5-C6 | -5.36 | 1.36 | 1.41 |
| 52 | 2 | 517 | A | N9-C4 | -5.35 | 1.34 | 1.37 |
| 52 | 2 | 377 | A | N9-C4 | -5.34 | 1.34 | 1.37 |
| 57 | 7 | 203 | SER | C-N | -5.32 | 1.24 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 52 | 2 | 682 | U | N1-C2 | -5.29 | 1.33 | 1.38 |
| 65 | AJ | 81 | CYS | CB-SG | -5.26 | 1.73 | 1.81 |
| 52 | 2 | 2190 | C | N1-C6 | -5.25 | 1.34 | 1.37 |
| 52 | 2 | 359 | A | N3-C4 | -5.24 | 1.31 | 1.34 |
| 52 | 2 | 1275 | C | N1-C6 | -5.24 | 1.34 | 1.37 |
| 52 | 2 | 436 | C | N3-C4 | -5.24 | 1.30 | 1.33 |
| 52 | 2 | 379 | U | C2-N3 | -5.21 | 1.34 | 1.37 |
| 52 | 2 | 771 | G | N3-C4 | -5.16 | 1.31 | 1.35 |
| 52 | 2 | 1215 | U | N1-C2 | -5.14 | 1.33 | 1.38 |
| 52 | 2 | 1497 | A | N9-C4 | -5.12 | 1.34 | 1.37 |
| 52 | 2 | 26 | A | C5-C4 | -5.12 | 1.35 | 1.38 |
| 52 | 2 | 16 | G | C5-C4 | -5.09 | 1.34 | 1.38 |
| 52 | 2 | 40 | A | C5-C4 | -5.06 | 1.35 | 1.38 |
| 52 | 2 | 2191 | A | N9-C4 | -5.06 | 1.34 | 1.37 |
| 52 | 2 | 121 | C | N1-C6 | -5.06 | 1.34 | 1.37 |
| 52 | 2 | 358 | C | N1-C6 | -5.05 | 1.34 | 1.37 |
| 52 | 2 | 2190 | C | C4-C5 | -5.05 | 1.39 | 1.43 |
| 52 | 2 | 1123 | G | N9-C8 | -5.04 | 1.34 | 1.37 |
| 53 | 3 | 80 | ARG | CB-CG | -5.04 | 1.39 | 1.52 |
| 55 | 5 | 48 | ALA | C-N | -5.04 | 1.22 | 1.34 |
| 52 | 2 | 1264 | C | N1-C6 | -5.02 | 1.34 | 1.37 |
| 52 | 2 | 1965 | A | N9-C4 | -5.02 | 1.34 | 1.37 |
| 52 | 2 | 670 | A | N3-C4 | -5.02 | 1.31 | 1.34 |
| 52 | 2 | 1481 | A | N9-C4 | -5.02 | 1.34 | 1.37 |
| 52 | 2 | 16 | G | N3-C4 | -5.01 | 1.31 | 1.35 |
| 52 | 2 | 397 | A | N3-C4 | -5.01 | 1.31 | 1.34 |
| 52 | 2 | 1108 | A | N9-C4 | -5.01 | 1.34 | 1.37 |

All (475) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 52 | 2 | 971 | U | O5'-P-OP2 | -31.09 | 73.39 | 110.70 |
| 52 | 2 | 1954 | U | P-O3'-C3' | 28.04 | 153.35 | 119.70 |
| 52 | 2 | 1818 | U | O5'-P-OP2 | -26.60 | 78.78 | 110.70 |
| 52 | 2 | 1818 | U | O5'-P-OP1 | -22.31 | 83.92 | 110.70 |
| 52 | 2 | 971 | U | O5'-P-OP1 | -21.05 | 85.44 | 110.70 |
| 55 | 5 | 49 | ARG | O-C-N | -20.08 | 89.07 | 123.20 |
| 52 | 2 | 1577 | G | N7-C8-N9 | 16.50 | 121.35 | 113.10 |
| 52 | 2 | 1818 | U | OP1-P-OP2 | 16.10 | 143.75 | 119.60 |
| 52 | 2 | 1577 | G | C8-N9-C4 | -15.47 | 100.21 | 106.40 |
| 52 | 2 | 1577 | G | C4-N9-C1' | 13.33 | 143.83 | 126.50 |
| 52 | 2 | 1955 | G | O5'-P-OP2 | -13.07 | 93.94 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 46 | t | 108 | ARG | C-N-CD | -13.04 | 91.91 | 120.60 |
| 52 | 2 | 970 | U | OP2-P-O3' | -12.83 | 76.97 | 105.20 |
| 52 | 2 | 1817 | U | OP2-P-O3' | -12.81 | 77.02 | 105.20 |
| 52 | 2 | 971 | U | OP1-P-OP2 | 12.71 | 138.67 | 119.60 |
| 52 | 2 | 1875 | A | C8-N9-C4 | -12.64 | 100.74 | 105.80 |
| 64 | AI | 131 | ARG | N-CA-C | -12.64 | 76.87 | 111.00 |
| 54 | 4 | 191 | ASN | C-N-CD | -12.33 | 93.47 | 120.60 |
| 38 | l | 66 | TYR | O-C-N | -12.25 | 103.11 | 122.70 |
| 52 | 2 | 1817 | U | OP1-P-O3' | -11.89 | 79.05 | 105.20 |
| 52 | 2 | 970 | U | OP1-P-O3' | -11.84 | 79.16 | 105.20 |
| 30 | d | 239 | GLY | C-N-CA | -11.63 | 92.62 | 121.70 |
| 52 | 2 | 550 | C | N1-C2-O2 | 11.61 | 125.86 | 118.90 |
| 52 | 2 | 771 | G | N3-C4-N9 | -11.47 | 119.12 | 126.00 |
| 60 | AD | 40 | SER | N-CA-C | -11.42 | 80.16 | 111.00 |
| 52 | 2 | 1605 | U | OP1-P-O3' | -11.31 | 80.31 | 105.20 |
| 52 | 2 | 1796 | U | OP1-P-O3' | -11.21 | 80.53 | 105.20 |
| 52 | 2 | 2028 | U | OP1-P-O3' | -11.15 | 80.67 | 105.20 |
| 52 | 2 | 1955 | G | N7-C8-N9 | 11.05 | 118.63 | 113.10 |
| 52 | 2 | 1788 | G | OP1-P-O3' | -10.98 | 81.05 | 105.20 |
| 52 | 2 | 2028 | U | OP2-P-O3' | -10.80 | 81.43 | 105.20 |
| 52 | 2 | 56 | U | C2-N1-C1' | 10.64 | 130.47 | 117.70 |
| 31 | e | 83 | CYS | N-CA-C | -10.32 | 83.13 | 111.00 |
| 52 | 2 | 1796 | U | OP2-P-O3' | -10.32 | 82.49 | 105.20 |
| 52 | 2 | 1875 | A | N7-C8-N9 | 10.32 | 118.96 | 113.80 |
| 52 | 2 | 1605 | U | OP2-P-O3' | -10.27 | 82.61 | 105.20 |
| 52 | 2 | 1955 | G | C8-N9-C4 | -10.11 | 102.35 | 106.40 |
| 52 | 2 | 1864 | C | C4-C5-C6 | 10.06 | 122.43 | 117.40 |
| 38 | l | 65 | ARG | C-N-CA | -9.98 | 96.75 | 121.70 |
| 52 | 2 | 1577 | G | C5-N7-C8 | -9.96 | 99.32 | 104.30 |
| 52 | 2 | 2050 | C | N1-C2-O2 | 9.90 | 124.84 | 118.90 |
| 52 | 2 | 1955 | G | OP1-P-OP2 | -9.79 | 104.91 | 119.60 |
| 64 | AI | 135 | HIS | CA-CB-CG | 9.53 | 129.79 | 113.60 |
| 52 | 2 | 1955 | G | O5'-P-OP1 | -9.50 | 97.15 | 105.70 |
| 52 | 2 | 1577 | G | C6-C5-N7 | -9.36 | 124.78 | 130.40 |
| 52 | 2 | 1956 | G | C4-N9-C1' | 9.17 | 138.42 | 126.50 |
| 52 | 2 | 550 | C | N3-C2-O2 | -9.14 | 115.50 | 121.90 |
| 26 | Z | 114 | HIS | O-C-N | -9.00 | 108.30 | 122.70 |
| 52 | 2 | 1788 | G | OP2-P-O3' | -8.95 | 85.51 | 105.20 |
| 60 | AD | 68 | LEU | N-CA-C | 8.95 | 135.16 | 111.00 |
| 63 | AH | 91 | ARG | NE-CZ-NH1 | -8.91 | 115.85 | 120.30 |
| 52 | 2 | 1956 | G | C4-C5-C6 | 8.88 | 124.13 | 118.80 |
| 52 | 2 | 364 | G | O4'-C1'-N9 | 8.87 | 115.29 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 66 | AK | 122 | LEU | C-N-CA | -8.86 | 99.54 | 121.70 |
| 15 | O | 51 | LEU | N-CA-C | -8.86 | 87.08 | 111.00 |
| 52 | 2 | 1863 | A | P-O3'-C3' | 8.81 | 130.27 | 119.70 |
| 52 | 2 | 56 | U | C6-N1-C1' | -8.79 | 108.89 | 121.20 |
| 52 | 2 | 1960 | C | O5'-P-OP1 | -8.78 | 97.80 | 105.70 |
| 29 | c | 214 | GLY | N-CA-C | 8.74 | 134.94 | 113.10 |
| 52 | 2 | 1864 | C | O4'-C1'-N1 | 8.72 | 115.18 | 108.20 |
| 52 | 2 | 1843 | U | N3-C2-O2 | -8.70 | 116.11 | 122.20 |
| 52 | 2 | 1955 | G | C6-C5-N7 | -8.67 | 125.20 | 130.40 |
| 52 | 2 | 1206 | C | C2-N1-C1' | 8.64 | 128.31 | 118.80 |
| 52 | 2 | 1954 | U | OP2-P-O3' | 8.63 | 124.19 | 105.20 |
| 52 | 2 | 2029 | U | N3-C2-O2 | -8.59 | 116.19 | 122.20 |
| 52 | 2 | 1864 | C | N3-C4-C5 | -8.59 | 118.46 | 121.90 |
| 52 | 2 | 1577 | G | C8-N9-C1' | -8.55 | 115.89 | 127.00 |
| 52 | 2 | 2050 | C | C2-N1-C1' | 8.54 | 128.19 | 118.80 |
| 52 | 2 | 550 | C | C2-N1-C1' | 8.53 | 128.19 | 118.80 |
| 52 | 2 | 1816 | U | C2-N1-C1' | 8.49 | 127.89 | 117.70 |
| 52 | 2 | 913 | G | N3-C4-C5 | 8.46 | 132.83 | 128.60 |
| 52 | 2 | 1843 | U | N1-C2-O2 | 8.42 | 128.69 | 122.80 |
| 52 | 2 | 1645 | G | C2-N3-C4 | -8.33 | 107.74 | 111.90 |
| 45 | s | 126 | ASP | N-CA-C | -8.31 | 88.55 | 111.00 |
| 52 | 2 | 364 | G | O5'-P-OP1 | -8.31 | 98.22 | 105.70 |
| 52 | 2 | 2029 | U | N1-C2-O2 | 8.31 | 128.62 | 122.80 |
| 52 | 2 | 771 | G | N3-C2-N2 | -8.29 | 114.10 | 119.90 |
| 52 | 2 | 1678 | G | N3-C4-N9 | -8.27 | 121.04 | 126.00 |
| 52 | 2 | 913 | G | N3-C4-N9 | -8.23 | 121.06 | 126.00 |
| 52 | 2 | 1956 | G | C6-C5-N7 | -8.13 | 125.52 | 130.40 |
| 70 | AO | 100 | LEU | CA-CB-CG | 8.11 | 133.96 | 115.30 |
| 52 | 2 | 1864 | C | N1-C2-N3 | -8.08 | 113.54 | 119.20 |
| 52 | 2 | 56 | U | C5-C6-N1 | 8.06 | 126.73 | 122.70 |
| 52 | 2 | 771 | G | N3-C4-C5 | 8.03 | 132.62 | 128.60 |
| 74 | AS | 28 | LYS | N-CA-C | -7.99 | 89.42 | 111.00 |
| 52 | 2 | 1875 | A | C5'-C4'-O4' | -7.99 | 99.51 | 109.10 |
| 52 | 2 | 1997 | C | C2-N1-C1' | 7.97 | 127.57 | 118.80 |
| 46 | t | 67 | GLY | N-CA-C | -7.94 | 93.24 | 113.10 |
| 52 | 2 | 1956 | G | C8-N9-C1' | -7.94 | 116.67 | 127.00 |
| 52 | 2 | 969 | A | C2-N3-C4 | -7.94 | 106.63 | 110.60 |
| 52 | 2 | 2029 | U | C2-N1-C1' | 7.89 | 127.17 | 117.70 |
| 52 | 2 | 1997 | C | N1-C2-O2 | 7.86 | 123.61 | 118.90 |
| 53 | 3 | 150 | LEU | N-CA-C | 7.83 | 132.15 | 111.00 |
| 52 | 2 | 1967 | U | N1-C2-O2 | 7.79 | 128.25 | 122.80 |
| 52 | 2 | 1930 | G | C4-C5-N7 | 7.78 | 113.91 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 761 | U | C2-N1-C1' | 7.68 | 126.91 | 117.70 |
| 51 | 1 | 120 | LEU | CA-CB-CG | 7.67 | 132.93 | 115.30 |
| 52 | 2 | 1789 | A | OP1-P-OP2 | 7.63 | 131.05 | 119.60 |
| 44 | r | 17 | CYS | CA-CB-SG | 7.62 | 127.72 | 114.00 |
| 52 | 2 | 1525 | A | C4-C5-C6 | 7.62 | 120.81 | 117.00 |
| 52 | 2 | 1955 | G | C4-N9-C1' | 7.61 | 136.39 | 126.50 |
| 52 | 2 | 46 | U | C2-N1-C1' | 7.60 | 126.82 | 117.70 |
| 52 | 2 | 1443 | U | N3-C2-O2 | -7.57 | 116.90 | 122.20 |
| 52 | 2 | 760 | G | C5-C6-N1 | 7.57 | 115.28 | 111.50 |
| 7 | G | 85 | C | N3-C2-O2 | -7.55 | 116.61 | 121.90 |
| 52 | 2 | 1997 | C | O5'-P-OP1 | -7.54 | 98.92 | 105.70 |
| 7 | G | 85 | C | N1-C2-O2 | 7.47 | 123.38 | 118.90 |
| 77 | AW | 79 | GLY | O-C-N | -7.46 | 110.77 | 122.70 |
| 52 | 2 | 1955 | G | N3-C4-C5 | -7.44 | 124.88 | 128.60 |
| 52 | 2 | 1518 | G | O4'-C1'-N9 | 7.44 | 114.15 | 108.20 |
| 52 | 2 | 1577 | G | N1-C6-O6 | 7.42 | 124.36 | 119.90 |
| 33 | g | 102 | GLY | N-CA-C | 7.38 | 131.55 | 113.10 |
| 1 | A | 461 | G | N3-C4-N9 | -7.37 | 121.58 | 126.00 |
| 52 | 2 | 1678 | G | N3-C2-N2 | -7.36 | 114.75 | 119.90 |
| 52 | 2 | 2050 | C | N3-C2-O2 | -7.35 | 116.75 | 121.90 |
| 57 | 7 | 27 | ILE | N-CA-C | 7.35 | 130.85 | 111.00 |
| 52 | 2 | 2046 | U | C5-C6-N1 | 7.35 | 126.37 | 122.70 |
| 15 | O | 51 | LEU | O-C-N | 7.32 | 135.65 | 123.20 |
| 52 | 2 | 502 | A | N1-C2-N3 | 7.30 | 132.95 | 129.30 |
| 52 | 2 | 904 | G | C6-C5-N7 | -7.28 | 126.03 | 130.40 |
| 52 | 2 | 1950 | C | C5-C6-N1 | 7.26 | 124.63 | 121.00 |
| 52 | 2 | 771 | G | C4-N9-C1' | -7.25 | 117.08 | 126.50 |
| 69 | AN | 88 | LEU | CA-CB-CG | 7.24 | 131.94 | 115.30 |
| 64 | AI | 133 | VAL | N-CA-C | 7.23 | 130.53 | 111.00 |
| 13 | M | 220 | GLY | N-CA-C | 7.23 | 131.18 | 113.10 |
| 19 | S | 123 | LYS | N-CA-C | -7.23 | 91.48 | 111.00 |
| 55 | 5 | 49 | ARG | CA-C-N | 7.22 | 130.65 | 116.20 |
| 52 | 2 | 1956 | G | N3-C4-C5 | -7.19 | 125.00 | 128.60 |
| 55 | 5 | 67 | TRP | CA-CB-CG | 7.19 | 127.36 | 113.70 |
| 52 | 2 | 1797 | G | OP1-P-OP2 | 7.18 | 130.37 | 119.60 |
| 52 | 2 | 771 | G | N9-C4-C5 | 7.17 | 108.27 | 105.40 |
| 52 | 2 | 1606 | C | OP1-P-OP2 | 7.15 | 130.32 | 119.60 |
| 52 | 2 | 771 | G | C8-N9-C1' | 7.13 | 136.28 | 127.00 |
| 7 | G | 85 | C | C2-N1-C1' | 7.12 | 126.63 | 118.80 |
| 52 | 2 | 38 | C | C5-C6-N1 | -7.12 | 117.44 | 121.00 |
| 52 | 2 | 1850 | U | N3-C2-O2 | -7.10 | 117.23 | 122.20 |
| 52 | 2 | 1955 | G | N3-C4-N9 | 7.10 | 130.26 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 52 | 2 | 1874 | A | O4'-C1'-N9 | 7.08 | 113.86 | 108.20 |
| 52 | 2 | 1956 | G | N3-C4-N9 | 7.08 | 130.25 | 126.00 |
| 52 | 2 | 1930 | G | C5-C6-O6 | -7.07 | 124.36 | 128.60 |
| 52 | 2 | 2050 | C | C6-N1-C1' | -7.04 | 112.35 | 120.80 |
| 52 | 2 | 59 | C | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 52 | 2 | 1968 | G | O4'-C1'-N9 | 6.96 | 113.77 | 108.20 |
| 52 | 2 | 1967 | U | N3-C2-O2 | -6.96 | 117.33 | 122.20 |
| 62 | AG | 72 | LEU | CA-CB-CG | 6.95 | 131.29 | 115.30 |
| 1 | A | 461 | G | N3-C4-C5 | 6.95 | 132.07 | 128.60 |
| 52 | 2 | 1930 | G | N1-C6-O6 | 6.91 | 124.04 | 119.90 |
| 52 | 2 | 1206 | C | N3-C2-O2 | -6.88 | 117.08 | 121.90 |
| 19 | S | 10 | GLY | C-N-CA | -6.85 | 104.57 | 121.70 |
| 52 | 2 | 728 | C | C2-N1-C1' | 6.85 | 126.33 | 118.80 |
| 52 | 2 | 1529 | U | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 52 | 2 | 1206 | C | N1-C2-O2 | 6.83 | 123.00 | 118.90 |
| 42 | p | 140 | GLY | C-N-CA | -6.80 | 104.70 | 121.70 |
| 31 | e | 100 | SER | N-CA-C | -6.80 | 92.65 | 111.00 |
| 52 | 2 | 763 | C | N3-C2-O2 | -6.79 | 117.15 | 121.90 |
| 52 | 2 | 1239 | A | C2-N3-C4 | -6.72 | 107.24 | 110.60 |
| 52 | 2 | 1860 | G | N3-C4-N9 | -6.71 | 121.97 | 126.00 |
| 52 | 2 | 324 | U | N1-C2-O2 | 6.71 | 127.50 | 122.80 |
| 2 | B | 980 | U | N3-C2-O2 | -6.69 | 117.51 | 122.20 |
| 58 | 8 | 31 | LEU | CA-CB-CG | 6.69 | 130.69 | 115.30 |
| 52 | 2 | 2164 | U | P-O3'-C3' | 6.68 | 127.72 | 119.70 |
| 52 | 2 | 1955 | G | O4'-C1'-N9 | 6.66 | 113.53 | 108.20 |
| 30 | d | 276 | GLY | N-CA-C | 6.66 | 129.75 | 113.10 |
| 58 | 8 | 24 | ILE | CG1-CB-CG2 | -6.66 | 96.76 | 111.40 |
| 9 | I | 36 | LEU | CA-CB-CG | 6.62 | 130.51 | 115.30 |
| 52 | 2 | 1864 | C | C6-N1-C2 | 6.61 | 122.94 | 120.30 |
| 52 | 2 | 1816 | U | C6-N1-C1' | -6.60 | 111.96 | 121.20 |
| 52 | 2 | 2029 | U | OP1-P-OP2 | 6.60 | 129.50 | 119.60 |
| 1 | A | 814 | C | N3-C2-O2 | -6.57 | 117.30 | 121.90 |
| 78 | AX | 198 | GLY | C-N-CD | -6.57 | 106.14 | 120.60 |
| 50 | 0 | 134 | ASP | N-CA-C | -6.56 | 93.28 | 111.00 |
| 52 | 2 | 1577 | G | N3-C4-C5 | -6.55 | 125.32 | 128.60 |
| 52 | 2 | 1930 | G | C6-C5-N7 | -6.55 | 126.47 | 130.40 |
| 52 | 2 | 1954 | U | O3'-P-O5' | 6.53 | 116.40 | 104.00 |
| 52 | 2 | 559 | G | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |
| 52 | 2 | 1791 | U | P-O3'-C3' | 6.51 | 127.51 | 119.70 |
| 52 | 2 | 42 | G | P-O3'-C3' | 6.51 | 127.51 | 119.70 |
| 1 | A | 186 | G | N3-C4-C5 | 6.50 | 131.85 | 128.60 |
| 52 | 2 | 1997 | C | C6-N1-C1' | -6.50 | 113.00 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 52 | 2 | 1434 | C | C2-N1-C1' | 6.49 | 125.94 | 118.80 |
| 52 | 2 | 1872 | A | C2-N3-C4 | -6.49 | 107.36 | 110.60 |
| 52 | 2 | 1985 | A | N1-C6-N6 | -6.47 | 114.72 | 118.60 |
| 52 | 2 | 1930 | G | N9-C4-C5 | -6.46 | 102.82 | 105.40 |
| 7 | G | 85 | C | C6-N1-C2 | -6.45 | 117.72 | 120.30 |
| 2 | B | 1453 | C | C5-C6-N1 | 6.42 | 124.21 | 121.00 |
| 52 | 2 | 904 | G | C4-N9-C1' | 6.41 | 134.83 | 126.50 |
| 1 | A | 186 | G | N3-C4-N9 | -6.38 | 122.17 | 126.00 |
| 52 | 2 | 1978 | G | C8-N9-C1' | 6.36 | 135.27 | 127.00 |
| 43 | q | 110 | CYS | CA-CB-SG | 6.34 | 125.41 | 114.00 |
| 78 | AX | 199 | PRO | N-CA-C | 6.33 | 128.54 | 112.10 |
| 30 | d | 277 | TYR | CA-CB-CG | 6.32 | 125.41 | 113.40 |
| 52 | 2 | 1964 | G | C2-N3-C4 | -6.32 | 108.74 | 111.90 |
| 1 | A | 761 | U | N1-C2-O2 | 6.30 | 127.21 | 122.80 |
| 52 | 2 | 1183 | G | N3-C4-N9 | -6.29 | 122.23 | 126.00 |
| 52 | 2 | 1525 | A | C6-C5-N7 | -6.28 | 127.91 | 132.30 |
| 52 | 2 | 290 | U | N3-C2-O2 | -6.27 | 117.81 | 122.20 |
| 52 | 2 | 1908 | C | C2-N1-C1' | 6.26 | 125.69 | 118.80 |
| 52 | 2 | 38 | C | C4-C5-C6 | 6.26 | 120.53 | 117.40 |
| 52 | 2 | 963 | U | OP1-P-O3' | 6.26 | 118.98 | 105.20 |
| 52 | 2 | 1239 | A | N1-C2-N3 | 6.26 | 132.43 | 129.30 |
| 52 | 2 | 56 | U | C4-C5-C6 | -6.25 | 115.95 | 119.70 |
| 52 | 2 | 56 | U | O5'-P-OP2 | 6.25 | 118.20 | 110.70 |
| 52 | 2 | 1949 | U | P-O3'-C3' | 6.25 | 127.20 | 119.70 |
| 52 | 2 | 1416 | A | O5'-P-OP1 | -6.24 | 100.08 | 105.70 |
| 52 | 2 | 1860 | G | N3-C4-C5 | 6.23 | 131.71 | 128.60 |
| 52 | 2 | 1181 | C | C2-N1-C1' | 6.22 | 125.64 | 118.80 |
| 52 | 2 | 1104 | A | N7-C8-N9 | 6.21 | 116.91 | 113.80 |
| 52 | 2 | 716 | U | C2'-C3'-O3' | 6.16 | 123.56 | 113.70 |
| 52 | 2 | 1876 | U | P-O5'-C5' | 6.16 | 130.75 | 120.90 |
| 52 | 2 | 1869 | A | C5-C6-N1 | 6.16 | 120.78 | 117.70 |
| 54 | 4 | 190 | TRP | N-CA-C | 6.15 | 127.61 | 111.00 |
| 52 | 2 | 1850 | U | N1-C2-O2 | 6.15 | 127.10 | 122.80 |
| 52 | 2 | 762 | A | OP1-P-OP2 | -6.14 | 110.38 | 119.60 |
| 52 | 2 | 1881 | G | N3-C4-N9 | 6.14 | 129.68 | 126.00 |
| 52 | 2 | 493 | C | C6-N1-C2 | 6.13 | 122.75 | 120.30 |
| 52 | 2 | 1678 | G | N9-C4-C5 | 6.13 | 107.85 | 105.40 |
| 52 | 2 | 1106 | U | C3'-C2'-C1' | 6.13 | 106.40 | 101.50 |
| 80 | AZ | 85 | ARG | C-N-CA | 6.12 | 137.01 | 121.70 |
| 52 | 2 | 1400 | C | C5-C6-N1 | -6.12 | 117.94 | 121.00 |
| 52 | 2 | 1967 | U | C2-N1-C1' | 6.12 | 125.04 | 117.70 |
| 31 | e | 80 | GLY | C-N-CA | -6.11 | 106.42 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 0 | 78 | ALA | N-CA-C | 6.10 | 127.48 | 111.00 |
| 52 | 2 | 1843 | U | C2-N1-C1' | 6.10 | 125.02 | 117.70 |
| 26 | Z | 114 | HIS | CA-C-N | 6.10 | 130.62 | 117.20 |
| 52 | 2 | 10 | G | C4-N9-C1' | 6.09 | 134.42 | 126.50 |
| 52 | 2 | 1864 | C | C5'-C4'-O4' | 6.08 | 116.40 | 109.10 |
| 52 | 2 | 2030 | A | N1-C2-N3 | 6.08 | 132.34 | 129.30 |
| 52 | 2 | 1548 | A | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 30 | d | 331 | LEU | CA-CB-CG | 6.07 | 129.27 | 115.30 |
| 1 | A | 367 | A | C2-N3-C4 | -6.07 | 107.57 | 110.60 |
| 52 | 2 | 550 | C | C6-N1-C1' | -6.06 | 113.53 | 120.80 |
| 52 | 2 | 10 | G | C8-N9-C1' | -6.06 | 119.13 | 127.00 |
| 52 | 2 | 1955 | G | C5-C6-O6 | -6.04 | 124.98 | 128.60 |
| 2 | B | 1452 | G | C4-N9-C1' | 6.02 | 134.33 | 126.50 |
| 52 | 2 | 153 | A | O5'-P-OP1 | -6.02 | 100.28 | 105.70 |
| 52 | 2 | 416 | G | C8-N9-C1' | -6.02 | 119.17 | 127.00 |
| 15 | O | 91 | GLY | C-N-CA | -6.02 | 106.65 | 121.70 |
| 60 | AD | 41 | ARG | C-N-CA | -6.02 | 106.66 | 121.70 |
| 52 | 2 | 1527 | C | C6-N1-C2 | -6.01 | 117.90 | 120.30 |
| 64 | AI | 134 | LEU | N-CA-C | 6.00 | 127.20 | 111.00 |
| 52 | 2 | 363 | G | OP1-P-O3' | 6.00 | 118.40 | 105.20 |
| 52 | 2 | 38 | C | N1-C2-O2 | -5.99 | 115.30 | 118.90 |
| 52 | 2 | 1576 | G | P-O3'-C3' | 5.97 | 126.86 | 119.70 |
| 54 | 4 | 50 | ARG | NE-CZ-NH1 | -5.96 | 117.32 | 120.30 |
| 47 | u | 223 | GLY | N-CA-C | 5.95 | 127.96 | 113.10 |
| 9 | I | 20 | TYR | O-C-N | 5.94 | 132.21 | 122.70 |
| 52 | 2 | 1525 | A | C8-N9-C4 | -5.94 | 103.42 | 105.80 |
| 52 | 2 | 1206 | C | C6-N1-C1' | -5.93 | 113.68 | 120.80 |
| 52 | 2 | 2011 | U | P-O3'-C3' | 5.93 | 126.81 | 119.70 |
| 52 | 2 | 1955 | G | C5-N7-C8 | -5.92 | 101.34 | 104.30 |
| 52 | 2 | 319 | C | N3-C2-O2 | 5.92 | 126.04 | 121.90 |
| 53 | 3 | 80 | ARG | CG-CD-NE | -5.91 | 99.38 | 111.80 |
| 52 | 2 | 1570 | C | C6-N1-C2 | 5.89 | 122.66 | 120.30 |
| 7 | G | 166 | C | C2-N1-C1' | 5.89 | 125.28 | 118.80 |
| 61 | AE | 55 | LEU | CA-CB-CG | -5.88 | 101.77 | 115.30 |
| 52 | 2 | 969 | A | C5-N7-C8 | -5.88 | 100.96 | 103.90 |
| 78 | AX | 189 | LEU | N-CA-C | -5.87 | 95.15 | 111.00 |
| 15 | O | 94 | LEU | CA-CB-CG | 5.87 | 128.79 | 115.30 |
| 8 | H | 7 | C | C2-N1-C1' | 5.86 | 125.25 | 118.80 |
| 52 | 2 | 1627 | G | P-O3'-C3' | 5.86 | 126.74 | 119.70 |
| 1 | A | 761 | U | N3-C2-O2 | -5.85 | 118.10 | 122.20 |
| 46 | t | 107 | GLN | N-CA-C | 5.85 | 126.80 | 111.00 |
| 52 | 2 | 1239 | A | O4'-C1'-N9 | 5.84 | 112.88 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 52 | 2 | 1875 | A | N9-C4-C5 | 5.84 | 108.14 | 105.80 |
| 52 | 2 | 1577 | G | C5-C6-O6 | -5.84 | 125.10 | 128.60 |
| 40 | n | 75 | ALA | N-CA-C | -5.82 | 95.30 | 111.00 |
| 52 | 2 | 1796 | U | C5-C6-N1 | 5.82 | 125.61 | 122.70 |
| 52 | 2 | 1930 | G | O4'-C1'-N9 | -5.79 | 103.57 | 108.20 |
| 52 | 2 | 771 | G | C6-C5-N7 | 5.79 | 133.87 | 130.40 |
| 7 | G | 171 | U | C2-N1-C1' | 5.79 | 124.64 | 117.70 |
| 1 | A | 360 | U | C2-N1-C1' | 5.78 | 124.64 | 117.70 |
| 74 | AS | 61 | GLN | C-N-CD | 5.78 | 140.54 | 128.40 |
| 12 | L | 25 | GLY | N-CA-C | 5.78 | 127.54 | 113.10 |
| 52 | 2 | 1104 | A | C8-N9-C4 | -5.77 | 103.49 | 105.80 |
| 57 | 7 | 25 | SER | N-CA-C | 5.77 | 126.57 | 111.00 |
| 74 | AS | 26 | GLY | N-CA-C | -5.76 | 98.70 | 113.10 |
| 52 | 2 | 253 | U | OP1-P-O3' | 5.76 | 117.86 | 105.20 |
| 52 | 2 | 1378 | U | P-O3'-C3' | 5.76 | 126.61 | 119.70 |
| 52 | 2 | 1525 | A | N7-C8-N9 | 5.76 | 116.68 | 113.80 |
| 52 | 2 | 1584 | A | N9-C1'-C2' | -5.76 | 105.67 | 112.00 |
| 52 | 2 | 1996 | U | C5-C6-N1 | -5.75 | 119.82 | 122.70 |
| 52 | 2 | 257 | A | OP1-P-O3' | 5.75 | 117.85 | 105.20 |
| 52 | 2 | 1955 | G | N1-C6-O6 | 5.75 | 123.35 | 119.90 |
| 52 | 2 | 1645 | G | N1-C2-N3 | 5.75 | 127.35 | 123.90 |
| 52 | 2 | 1577 | G | C4-C5-C6 | 5.74 | 122.24 | 118.80 |
| 52 | 2 | 790 | U | P-O3'-C3' | 5.73 | 126.57 | 119.70 |
| 52 | 2 | 1206 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 52 | 2 | 659 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 52 | 2 | 672 | G | N3-C4-C5 | 5.71 | 131.46 | 128.60 |
| 55 | 5 | 58 | LEU | CA-CB-CG | 5.71 | 128.44 | 115.30 |
| 52 | 2 | 689 | U | N1-C2-O2 | 5.70 | 126.79 | 122.80 |
| 57 | 7 | 27 | ILE | C-N-CA | 5.70 | 135.96 | 121.70 |
| 52 | 2 | 1982 | C | C5-C6-N1 | 5.70 | 123.85 | 121.00 |
| 52 | 2 | 597 | G | N3-C4-C5 | 5.69 | 131.45 | 128.60 |
| 52 | 2 | 1400 | C | OP1-P-OP2 | -5.69 | 111.07 | 119.60 |
| 44 | r | 74 | CYS | CA-CB-SG | 5.68 | 124.23 | 114.00 |
| 52 | 2 | 771 | G | C4-C5-N7 | -5.68 | 108.53 | 110.80 |
| 65 | AJ | 28 | ARG | C-N-CD | 5.68 | 140.33 | 128.40 |
| 1 | A | 461 | G | C2-N3-C4 | -5.68 | 109.06 | 111.90 |
| 52 | 2 | 1434 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 1 | A | 447 | G | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 52 | 2 | 1148 | G | O4'-C1'-N9 | 5.64 | 112.72 | 108.20 |
| 52 | 2 | 1964 | G | N1-C2-N3 | 5.64 | 127.29 | 123.90 |
| 52 | 2 | 46 | U | C6-N1-C1' | -5.64 | 113.30 | 121.20 |
| 53 | 3 | 203 | ARG | NE-CZ-NH1 | -5.63 | 117.48 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 191 | U | O4'-C1'-N1 | 5.63 | 112.71 | 108.20 |
| 52 | 2 | 416 | G | C4-N9-C1' | 5.62 | 133.81 | 126.50 |
| 52 | 2 | 689 | U | C2-N1-C1' | 5.62 | 124.45 | 117.70 |
| 52 | 2 | 1685 | A | C2-N3-C4 | 5.62 | 113.41 | 110.60 |
| 56 | 6 | 61 | LEU | CA-CB-CG | 5.62 | 128.23 | 115.30 |
| 52 | 2 | 1983 | G | N3-C4-C5 | 5.62 | 131.41 | 128.60 |
| 12 | L | 130 | LEU | C-N-CA | -5.61 | 107.67 | 121.70 |
| 52 | 2 | 1943 | A | C8-N9-C4 | -5.61 | 103.56 | 105.80 |
| 52 | 2 | 1998 | U | C2-N1-C1' | -5.61 | 110.97 | 117.70 |
| 52 | 2 | 1580 | G | C4-N9-C1' | -5.60 | 119.22 | 126.50 |
| 52 | 2 | 1791 | U | OP2-P-O3' | 5.59 | 117.50 | 105.20 |
| 52 | 2 | 1556 | A | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 52 | 2 | 313 | G | C4-N9-C1' | 5.58 | 133.75 | 126.50 |
| 52 | 2 | 2029 | U | C6-N1-C1' | -5.57 | 113.40 | 121.20 |
| 57 | 7 | 121 | LEU | CA-CB-CG | 5.57 | 128.11 | 115.30 |
| 52 | 2 | 913 | G | C2-N3-C4 | -5.57 | 109.12 | 111.90 |
| 52 | 2 | 1982 | C | C2-N1-C1' | 5.56 | 124.92 | 118.80 |
| 52 | 2 | 555 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 52 | 2 | 1645 | G | N3-C4-N9 | -5.55 | 122.67 | 126.00 |
| 52 | 2 | 692 | G | N3-C4-C5 | 5.54 | 131.37 | 128.60 |
| 47 | u | 234 | GLY | N-CA-C | -5.54 | 99.25 | 113.10 |
| 57 | 7 | 158 | PHE | N-CA-C | -5.53 | 96.07 | 111.00 |
| 36 | j | 14 | LEU | CA-CB-CG | 5.52 | 128.00 | 115.30 |
| 42 | p | 150 | PRO | N-CA-C | -5.52 | 97.74 | 112.10 |
| 50 | 0 | 166 | TRP | CA-CB-CG | 5.52 | 124.19 | 113.70 |
| 1 | A | 367 | A | N1-C2-N3 | 5.52 | 132.06 | 129.30 |
| 52 | 2 | 618 | C | O5'-P-OP1 | -5.52 | 100.73 | 105.70 |
| 52 | 2 | 1996 | U | C6-N1-C2 | 5.52 | 124.31 | 121.00 |
| 52 | 2 | 1645 | G | N3-C4-C5 | 5.52 | 131.36 | 128.60 |
| 52 | 2 | 2048 | C | C2-N1-C1' | 5.51 | 124.87 | 118.80 |
| 52 | 2 | 47 | A | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 68 | AM | 44 | LEU | CA-CB-CG | 5.51 | 127.97 | 115.30 |
| 52 | 2 | 1525 | A | N1-C6-N6 | 5.50 | 121.90 | 118.60 |
| 52 | 2 | 1876 | U | C6-N1-C2 | -5.50 | 117.70 | 121.00 |
| 52 | 2 | 316 | A | O5'-P-OP2 | -5.50 | 100.75 | 105.70 |
| 14 | N | 46 | MET | N-CA-C | -5.49 | 96.18 | 111.00 |
| 52 | 2 | 1572 | G | O4'-C1'-N9 | -5.48 | 103.81 | 108.20 |
| 2 | B | 958 | U | N1-C2-O2 | 5.47 | 126.63 | 122.80 |
| 52 | 2 | 573 | C | C6-N1-C2 | -5.46 | 118.11 | 120.30 |
| 78 | AX | 83 | LEU | CB-CG-CD2 | -5.46 | 101.73 | 111.00 |
| 52 | 2 | 1897 | C | P-O3'-C3' | 5.44 | 126.23 | 119.70 |
| 64 | AI | 131 | ARG | C-N-CD | 5.44 | 139.82 | 128.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 52 | 2 | 1955 | G | C4-C5-C6 | 5.43 | 122.06 | 118.80 |
| 14 | N | 10 | GLY | C-N-CA | -5.43 | 108.13 | 121.70 |
| 27 | a | 70 | SER | N-CA-C | -5.43 | 96.34 | 111.00 |
| 52 | 2 | 728 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 52 | 2 | 2165 | A | O5'-P-OP1 | -5.42 | 100.82 | 105.70 |
| 52 | 2 | 1577 | G | C4-C5-N7 | 5.42 | 112.97 | 110.80 |
| 52 | 2 | 667 | U | OP2-P-O3' | 5.41 | 117.10 | 105.20 |
| 27 | a | 69 | SER | N-CA-C | 5.41 | 125.61 | 111.00 |
| 66 | AK | 46 | LEU | C-N-CD | 5.41 | 139.76 | 128.40 |
| 1 | A | 203 | C | N3-C2-O2 | -5.40 | 118.12 | 121.90 |
| 52 | 2 | 1103 | G | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 52 | 2 | 38 | C | C2-N3-C4 | -5.39 | 117.20 | 119.90 |
| 6 | F | 67 | C | N1-C2-O2 | 5.39 | 122.14 | 118.90 |
| 58 | 8 | 56 | LEU | CA-CB-CG | -5.39 | 102.90 | 115.30 |
| 68 | AM | 149 | VAL | CA-CB-CG2 | 5.39 | 118.99 | 110.90 |
| 52 | 2 | 1104 | A | P-O3'-C3' | 5.39 | 126.16 | 119.70 |
| 52 | 2 | 771 | G | N1-C2-N2 | 5.38 | 121.04 | 116.20 |
| 13 | M | 124 | GLU | C-N-CA | -5.37 | 111.02 | 122.30 |
| 52 | 2 | 1864 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 64 | AI | 84 | LYS | C-N-CA | 5.37 | 135.12 | 121.70 |
| 1 | A | 761 | U | C6-N1-C1' | -5.36 | 113.69 | 121.20 |
| 52 | 2 | 1863 | A | N1-C6-N6 | -5.36 | 115.38 | 118.60 |
| 52 | 2 | 1576 | G | N3-C4-C5 | -5.36 | 125.92 | 128.60 |
| 52 | 2 | 1881 | G | C6-C5-N7 | -5.36 | 127.19 | 130.40 |
| 52 | 2 | 2000 | G | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 52 | 2 | 1950 | C | C4-C5-C6 | -5.35 | 114.73 | 117.40 |
| 52 | 2 | 1576 | G | C4-C5-C6 | 5.34 | 122.01 | 118.80 |
| 64 | AI | 84 | LYS | N-CA-C | 5.34 | 125.41 | 111.00 |
| 52 | 2 | 596 | U | N1-C2-O2 | -5.33 | 119.07 | 122.80 |
| 52 | 2 | 46 | U | N1-C2-O2 | 5.33 | 126.53 | 122.80 |
| 5 | E | 73 | C | C2-N1-C1' | 5.32 | 124.66 | 118.80 |
| 2 | B | 283 | C | N3-C2-O2 | -5.32 | 118.17 | 121.90 |
| 52 | 2 | 1606 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 52 | 2 | 896 | A | O4'-C1'-N9 | 5.31 | 112.45 | 108.20 |
| 52 | 2 | 876 | G | C4-N9-C1' | 5.30 | 133.39 | 126.50 |
| 78 | AX | 61 | ASN | N-CA-C | -5.30 | 96.69 | 111.00 |
| 52 | 2 | 268 | C | OP1-P-O3' | 5.30 | 116.86 | 105.20 |
| 1 | A | 203 | C | C6-N1-C2 | -5.29 | 118.18 | 120.30 |
| 1 | A | 814 | C | C2-N1-C1' | 5.29 | 124.62 | 118.80 |
| 52 | 2 | 937 | C | P-O3'-C3' | 5.29 | 126.05 | 119.70 |
| 52 | 2 | 2046 | U | C6-N1-C2 | -5.29 | 117.83 | 121.00 |
| 52 | 2 | 1580 | G | OP1-P-O3' | 5.29 | 116.83 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 46 | t | 67 | GLY | C-N-CD | 5.28 | 139.49 | 128.40 |
| 2 | B | 320 | U | C2-N1-C1' | 5.28 | 124.03 | 117.70 |
| 52 | 2 | 65 | A | C2-N3-C4 | -5.28 | 107.96 | 110.60 |
| 52 | 2 | 38 | C | C2-N1-C1' | -5.28 | 113.00 | 118.80 |
| 55 | 5 | 72 | ILE | CG1-CB-CG2 | -5.27 | 99.80 | 111.40 |
| 52 | 2 | 21 | U | C5-C6-N1 | 5.27 | 125.34 | 122.70 |
| 52 | 2 | 1577 | G | N9-C1'-C2' | 5.27 | 120.85 | 114.00 |
| 52 | 2 | 1789 | A | P-O3'-C3' | 5.27 | 126.02 | 119.70 |
| 52 | 2 | 1881 | G | C4-N9-C1' | 5.26 | 133.34 | 126.50 |
| 52 | 2 | 1982 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 52 | 2 | 287 | C | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 1 | A | 967 | G | C4-C5-N7 | 5.25 | 112.90 | 110.80 |
| 52 | 2 | 416 | G | C6-C5-N7 | -5.25 | 127.25 | 130.40 |
| 64 | AI | 135 | HIS | ND1-CG-CD2 | -5.24 | 98.66 | 106.00 |
| 52 | 2 | 56 | U | N1-C2-O2 | 5.24 | 126.47 | 122.80 |
| 52 | 2 | 340 | G | O5'-P-OP1 | -5.24 | 100.99 | 105.70 |
| 52 | 2 | 588 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 52 | 2 | 935 | U | OP1-P-O3' | 5.23 | 116.71 | 105.20 |
| 52 | 2 | 1606 | C | N3-C2-O2 | -5.22 | 118.24 | 121.90 |
| 52 | 2 | 324 | U | N3-C2-O2 | -5.21 | 118.55 | 122.20 |
| 52 | 2 | 1581 | A | O4'-C1'-N9 | -5.21 | 104.03 | 108.20 |
| 52 | 2 | 2095 | G | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 52 | 2 | 124 | A | C8-N9-C4 | 5.21 | 107.88 | 105.80 |
| 52 | 2 | 1978 | G | C4-N9-C1' | -5.20 | 119.74 | 126.50 |
| 52 | 2 | 257 | A | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 3 | C | 101 | C | C5-C6-N1 | 5.18 | 123.59 | 121.00 |
| 52 | 2 | 2047 | A | C4-N9-C1' | -5.18 | 116.98 | 126.30 |
| 55 | 5 | 48 | ALA | C-N-CA | 5.18 | 134.65 | 121.70 |
| 7 | G | 171 | U | C5-C6-N1 | 5.17 | 125.29 | 122.70 |
| 52 | 2 | 1576 | G | N3-C4-N9 | 5.17 | 129.10 | 126.00 |
| 52 | 2 | 550 | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 52 | 2 | 253 | U | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 69 | AN | 43 | GLN | C-N-CA | -5.15 | 108.82 | 121.70 |
| 42 | p | 149 | VAL | C-N-CD | 5.15 | 139.21 | 128.40 |
| 2 | B | 714 | A | N1-C6-N6 | -5.15 | 115.51 | 118.60 |
| 1 | A | 437 | A | C2-N3-C4 | -5.14 | 108.03 | 110.60 |
| 3 | C | 174 | A | C2-N3-C4 | -5.14 | 108.03 | 110.60 |
| 1 | A | 813 | C | C2-N1-C1' | 5.13 | 124.44 | 118.80 |
| 52 | 2 | 1854 | C | OP2-P-O3' | 5.13 | 116.48 | 105.20 |
| 7 | G | 166 | C | N3-C2-O2 | -5.13 | 118.31 | 121.90 |
| 52 | 2 | 1925 | G | N3-C4-N9 | -5.13 | 122.92 | 126.00 |
| 52 | 2 | 1830 | A | P-O3'-C3' | 5.12 | 125.84 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 52 | 2 | 564 | A | OP1-P-O3' | 5.12 | 116.46 | 105.20 |
| 52 | 2 | 950 | U | N3-C2-O2 | -5.12 | 118.62 | 122.20 |
| 8 | H | 7 | C | N3-C2-O2 | -5.12 | 118.32 | 121.90 |
| 52 | 2 | 904 | G | C8-N9-C1' | -5.10 | 120.37 | 127.00 |
| 50 | 0 | 80 | GLU | N-CA-C | 5.10 | 124.77 | 111.00 |
| 52 | 2 | 1816 | U | N1-C2-O2 | 5.10 | 126.37 | 122.80 |
| 52 | 2 | 1957 | G | C8-N9-C4 | -5.10 | 104.36 | 106.40 |
| 1 | A | 276 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 52 | 2 | 1251 | G | N3-C4-C5 | 5.09 | 131.15 | 128.60 |
| 54 | 4 | 134 | TYR | C-N-CD | -5.09 | 109.40 | 120.60 |
| 52 | 2 | 1148 | G | N7-C8-N9 | 5.08 | 115.64 | 113.10 |
| 52 | 2 | 1239 | A | C5-N7-C8 | -5.08 | 101.36 | 103.90 |
| 66 | AK | 69 | LEU | CA-CB-CG | -5.08 | 103.61 | 115.30 |
| 2 | B | 958 | U | N3-C2-O2 | -5.08 | 118.64 | 122.20 |
| 20 | T | 65 | SER | C-N-CA | -5.08 | 109.00 | 121.70 |
| 52 | 2 | 1699 | G | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 46 | t | 23 | SER | C-N-CD | 5.07 | 139.05 | 128.40 |
| 52 | 2 | 1606 | C | P-O3'-C3' | 5.07 | 125.78 | 119.70 |
| 78 | AX | 195 | GLY | N-CA-C | -5.07 | 100.43 | 113.10 |
| 52 | 2 | 2164 | U | OP2-P-O3' | 5.07 | 116.34 | 105.20 |
| 52 | 2 | 1890 | A | N1-C6-N6 | -5.06 | 115.56 | 118.60 |
| 1 | A | 813 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 15 | O | 52 | GLY | C-N-CA | -5.06 | 109.06 | 121.70 |
| 28 | b | 36 | SER | N-CA-C | -5.06 | 97.35 | 111.00 |
| 52 | 2 | 291 | G | O5'-P-OP1 | -5.06 | 101.15 | 105.70 |
| 52 | 2 | 1875 | A | C2-N3-C4 | 5.05 | 113.13 | 110.60 |
| 52 | 2 | 689 | U | N3-C2-O2 | -5.05 | 118.66 | 122.20 |
| 1 | A | 931 | G | C4-N9-C1' | 5.05 | 133.06 | 126.50 |
| 35 | i | 39 | GLY | N-CA-C | 5.05 | 125.72 | 113.10 |
| 52 | 2 | 1661 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 52 | 2 | 1854 | C | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 13 | M | 87 | GLY | C-N-CD | 5.04 | 138.99 | 128.40 |
| 52 | 2 | 580 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 52 | 2 | 1132 | G | N3-C4-N9 | -5.04 | 122.98 | 126.00 |
| 55 | 5 | 62 | THR | C-N-CA | -5.03 | 111.74 | 122.30 |
| 14 | N | 135 | THR | C-N-CD | 5.02 | 138.95 | 128.40 |
| 52 | 2 | 672 | G | C2-N3-C4 | -5.02 | 109.39 | 111.90 |
| 52 | 2 | 1576 | G | C4-N9-C1' | 5.02 | 133.03 | 126.50 |
| 52 | 2 | 1678 | G | N3-C4-C5 | 5.01 | 131.11 | 128.60 |
| 57 | 7 | 27 | ILE | CA-C-N | -5.01 | 106.17 | 117.20 |
| 52 | 2 | 498 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 52 | 2 | 554 | U | P-O3'-C3' | 5.01 | 125.71 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 52 | 2 | 672 | G | C4-C5-N7 | 5.01 | 112.80 | 110.80 |
| 52 | 2 | 1400 | C | C4-C5-C6 | 5.00 | 119.90 | 117.40 |

There are no chirality outliers.

All (58) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 50 | 0 | 82 | GLU | Peptide |
| 53 | 3 | 149 | ASN | Mainchain |
| 54 | 4 | 42 | PRO | Peptide |
| 55 | 5 | 49 | ARG | Mainchain,Peptide |
| 57 | 7 | 2 | ASN | Peptide |
| 58 | 8 | 22 | CYS | Peptide |
| 59 | AC | 199 | CYS | Peptide |
| 59 | AC | 241 | ARG | Peptide |
| 59 | AC | 41 | SER | Peptide |
| 61 | AE | 82 | ARG | Peptide |
| 62 | AG | 131 | ARG | Peptide |
| 62 | AG | 7 | ASN | Peptide |
| 62 | AG | 72 | LEU | Peptide |
| 64 | AI | 107 | HIS | Peptide |
| 64 | AI | 124 | GLY | Peptide |
| 64 | AI | 43 | LEU | Peptide |
| 66 | AK | 32 | GLN | Peptide |
| 67 | AL | 85 | ALA | Peptide |
| 68 | AM | 117 | LYS | Peptide |
| 68 | AM | 118 | ILE | Peptide |
| 68 | AM | 12 | HIS | Peptide |
| 68 | AM | 137 | THR | Peptide |
| 68 | AM | 145 | LYS | Peptide |
| 68 | AM | 148 | GLY | Peptide |
| 68 | AM | 98 | HIS | Peptide |
| 69 | AN | 152 | LEU | Peptide |
| 69 | AN | 26 | ASP | Peptide |
| 69 | AN | 31 | THR | Peptide |
| 69 | AN | 88 | LEU | Peptide |
| 70 | AO | 101 | SER | Peptide |
| 70 | AO | 102 | LYS | Peptide |
| 70 | AO | 130 | LYS | Peptide |
| 70 | AO | 154 | LYS | Peptide |
| 70 | AO | 25 | LYS | Peptide |
| 70 | AO | 56 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 72 | AQ | 24 | ARG | Peptide |
| 75 | AT | 104 | GLY | Peptide |
| 75 | AT | 84 | ASP | Peptide |
| 77 | AW | 68 | THR | Peptide |
| 78 | AX | 198 | GLY | Peptide |
| 9 | I | 180 | THR | Peptide |
| 13 | M | 132 | ARG | Peptide |
| 13 | M | 163 | HIS | Peptide |
| 16 | P | 36 | ILE | Peptide |
| 16 | P | 64 | ASN | Peptide |
| 20 | T | 66 | ASP | Peptide |
| 23 | W | 25 | ALA | Peptide |
| 24 | X | 56 | LYS | Mainchain |
| 28 | b | 35 | GLY | Peptide |
| 29 | c | 195 | CYS | Peptide |
| 31 | e | 78 | ASP | Mainchain |
| 37 | k | 12 | ALA | Peptide |
| 38 | l | 3 | LYS | Peptide |
| 38 | l | 4 | GLY | Peptide |
| 38 | l | 66 | TYR | Mainchain |
| 39 | m | 16 | THR | Peptide |
| 47 | u | 186 | ALA | 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 | |
|---|---|---|---|---|---|---|---|
| 9 | I | 195/198 (98%) | 180 (92%) | 12 (6%) | 3 (2%) | 10 | 34 |
| 10 | J | 209/213 (98%) | 193 (92%) | 13 (6%) | 3 (1%) | 11 | 36 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 11 | K | 165/188 (88%) | 152 (92%) | 12 (7%) | 1 (1%) | 25 | 58 |
| 12 | L | 175/220 (80%) | 159 (91%) | 14 (8%) | 2 (1%) | 14 | 42 |
| 13 | M | 219/222 (99%) | 212 (97%) | 6 (3%) | 1 (0%) | 29 | 61 |
| 14 | N | 166/175 (95%) | 153 (92%) | 12 (7%) | 1 (1%) | 25 | 58 |
| 15 | O | 201/204 (98%) | 192 (96%) | 9 (4%) | 0 | 100 | 100 |
| 16 | P | 153/166 (92%) | 145 (95%) | 7 (5%) | 1 (1%) | 22 | 54 |
| 17 | Q | 176/179 (98%) | 163 (93%) | 11 (6%) | 2 (1%) | 14 | 42 |
| 18 | R | 194/245 (79%) | 193 (100%) | 1 (0%) | 0 | 100 | 100 |
| 19 | S | 156/159 (98%) | 144 (92%) | 11 (7%) | 1 (1%) | 25 | 58 |
| 20 | T | 121/129 (94%) | 116 (96%) | 5 (4%) | 0 | 100 | 100 |
| 21 | U | 135/139 (97%) | 126 (93%) | 9 (7%) | 0 | 100 | 100 |
| 22 | V | 118/145 (81%) | 106 (90%) | 11 (9%) | 1 (1%) | 19 | 51 |
| 23 | W | 63/124 (51%) | 61 (97%) | 2 (3%) | 0 | 100 | 100 |
| 24 | X | 118/143 (82%) | 111 (94%) | 5 (4%) | 2 (2%) | 9 | 31 |
| 25 | Y | 131/134 (98%) | 124 (95%) | 6 (5%) | 1 (1%) | 19 | 51 |
| 26 | Z | 142/145 (98%) | 125 (88%) | 14 (10%) | 3 (2%) | 7 | 26 |
| 27 | a | 144/147 (98%) | 134 (93%) | 9 (6%) | 1 (1%) | 22 | 54 |
| 28 | b | 67/70 (96%) | 64 (96%) | 3 (4%) | 0 | 100 | 100 |
| 29 | c | 251/260 (96%) | 229 (91%) | 20 (8%) | 2 (1%) | 19 | 51 |
| 30 | d | 397/419 (95%) | 376 (95%) | 20 (5%) | 1 (0%) | 41 | 71 |
| 31 | e | 92/104 (88%) | 88 (96%) | 4 (4%) | 0 | 100 | 100 |
| 32 | f | 108/183 (59%) | 102 (94%) | 6 (6%) | 0 | 100 | 100 |
| 33 | g | 127/133 (96%) | 119 (94%) | 8 (6%) | 0 | 100 | 100 |
| 34 | h | 122/168 (73%) | 117 (96%) | 4 (3%) | 1 (1%) | 19 | 51 |
| 35 | i | 124/127 (98%) | 117 (94%) | 6 (5%) | 1 (1%) | 19 | 51 |
| 36 | j | 130/144 (90%) | 119 (92%) | 11 (8%) | 0 | 100 | 100 |
| 37 | k | 97/105 (92%) | 94 (97%) | 3 (3%) | 0 | 100 | 100 |
| 38 | l | 79/83 (95%) | 72 (91%) | 7 (9%) | 0 | 100 | 100 |
| 39 | m | 89/92 (97%) | 82 (92%) | 7 (8%) | 0 | 100 | 100 |
| 40 | n | 73/83 (88%) | 70 (96%) | 3 (4%) | 0 | 100 | 100 |
| 41 | o | 48/51 (94%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 42 | p | 362/373 (97%) | 340 (94%) | 20 (6%) | 2 (1%) | 25 | 58 |
| 43 | q | 50/128 (39%) | 47 (94%) | 3 (6%) | 0 | 100 | 100 |
| 44 | r | 94/106 (89%) | 85 (90%) | 8 (8%) | 1 (1%) | 14 | 42 |
| 45 | s | 258/305 (85%) | 246 (95%) | 12 (5%) | 0 | 100 | 100 |
| 46 | t | 133/195 (68%) | 123 (92%) | 8 (6%) | 2 (2%) | 10 | 34 |
| 47 | u | 226/252 (90%) | 209 (92%) | 16 (7%) | 1 (0%) | 34 | 66 |
| 48 | v | 228/348 (66%) | 218 (96%) | 10 (4%) | 0 | 100 | 100 |
| 49 | w | 185/190 (97%) | 173 (94%) | 11 (6%) | 1 (0%) | 29 | 61 |
| 50 | 0 | 219/264 (83%) | 208 (95%) | 10 (5%) | 1 (0%) | 29 | 61 |
| 51 | 1 | 256/273 (94%) | 231 (90%) | 22 (9%) | 3 (1%) | 13 | 40 |
| 53 | 3 | 247/249 (99%) | 236 (96%) | 10 (4%) | 1 (0%) | 34 | 66 |
| 54 | 4 | 198/200 (99%) | 183 (92%) | 11 (6%) | 4 (2%) | 7 | 27 |
| 55 | 5 | 178/220 (81%) | 160 (90%) | 16 (9%) | 2 (1%) | 14 | 42 |
| 56 | 6 | 162/190 (85%) | 151 (93%) | 9 (6%) | 2 (1%) | 13 | 40 |
| 57 | 7 | 306/312 (98%) | 275 (90%) | 28 (9%) | 3 (1%) | 15 | 45 |
| 58 | 8 | 36/57 (63%) | 30 (83%) | 5 (14%) | 1 (3%) | 5 | 19 |
| 59 | AC | 201/246 (82%) | 193 (96%) | 8 (4%) | 0 | 100 | 100 |
| 60 | AD | 91/153 (60%) | 78 (86%) | 11 (12%) | 2 (2%) | 6 | 24 |
| 61 | AE | 136/173 (79%) | 131 (96%) | 4 (3%) | 1 (1%) | 22 | 54 |
| 62 | AG | 139/151 (92%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 63 | AH | 134/144 (93%) | 126 (94%) | 8 (6%) | 0 | 100 | 100 |
| 64 | AI | 119/152 (78%) | 102 (86%) | 17 (14%) | 0 | 100 | 100 |
| 65 | AJ | 127/130 (98%) | 120 (94%) | 6 (5%) | 1 (1%) | 19 | 51 |
| 66 | AK | 138/149 (93%) | 118 (86%) | 16 (12%) | 4 (3%) | 4 | 18 |
| 67 | AL | 119/143 (83%) | 108 (91%) | 8 (7%) | 3 (2%) | 5 | 21 |
| 68 | AM | 146/153 (95%) | 125 (86%) | 21 (14%) | 0 | 100 | 100 |
| 69 | AN | 188/190 (99%) | 165 (88%) | 21 (11%) | 2 (1%) | 14 | 42 |
| 70 | AO | 143/179 (80%) | 114 (80%) | 25 (18%) | 4 (3%) | 5 | 19 |
| 71 | AP | 222/265 (84%) | 216 (97%) | 6 (3%) | 0 | 100 | 100 |
| 72 | AQ | 100/116 (86%) | 86 (86%) | 13 (13%) | 1 (1%) | 15 | 45 |
| 73 | AR | 81/164 (49%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 74 | AS | 140/143 (98%) | 132 (94%) | 5 (4%) | 3 (2%) | 7 | 26 |
| 75 | AT | 124/137 (90%) | 117 (94%) | 6 (5%) | 1 (1%) | 19 | 51 |
| 76 | AV | 102/112 (91%) | 90 (88%) | 8 (8%) | 4 (4%) | 3 | 12 |
| 77 | AW | 80/86 (93%) | 76 (95%) | 4 (5%) | 0 | 100 | 100 |
| 78 | AX | 201/219 (92%) | 179 (89%) | 17 (8%) | 5 (2%) | 5 | 21 |
| 79 | AY | 54/66 (82%) | 48 (89%) | 6 (11%) | 0 | 100 | 100 |
| 80 | AZ | 66/87 (76%) | 60 (91%) | 4 (6%) | 2 (3%) | 4 | 17 |
| All | All | 10774/12317 (88%) | 9993 (93%) | 696 (6%) | 85 (1%) | 24 | 51 |

All (85) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | J | 142 | GLU |
| 10 | J | 145 | VAL |
| 12 | L | 21 | SER |
| 24 | X | 59 | ALA |
| 26 | Z | 114 | HIS |
| 26 | Z | 115 | ILE |
| 29 | c | 150 | LEU |
| 30 | d | 277 | TYR |
| 34 | h | 63 | ILE |
| 35 | i | 42 | GLU |
| 44 | r | 95 | ASP |
| 46 | t | 69 | MET |
| 47 | u | 226 | GLN |
| 50 | 0 | 242 | VAL |
| 54 | 4 | 192 | PRO |
| 57 | 7 | 28 | LYS |
| 58 | 8 | 27 | ASN |
| 65 | AJ | 29 | PRO |
| 66 | AK | 40 | VAL |
| 66 | AK | 119 | ASP |
| 72 | AQ | 107 | VAL |
| 74 | AS | 27 | TRP |
| 74 | AS | 61 | GLN |
| 75 | AT | 85 | ASP |
| 78 | AX | 187 | ILE |
| 78 | AX | 191 | SER |
| 78 | AX | 197 | ASN |
| 80 | AZ | 86 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | I | 190 | TYR |
| 14 | N | 136 | PRO |
| 17 | Q | 120 | TYR |
| 26 | Z | 73 | ILE |
| 27 | a | 57 | LYS |
| 61 | AE | 67 | LYS |
| 66 | AK | 61 | VAL |
| 69 | AN | 64 | PHE |
| 70 | AO | 23 | ILE |
| 80 | AZ | 85 | ARG |
| 19 | S | 124 | ALA |
| 29 | c | 214 | GLY |
| 46 | t | 24 | PRO |
| 51 | 1 | 240 | GLN |
| 57 | 7 | 75 | HIS |
| 60 | AD | 41 | ARG |
| 66 | AK | 37 | VAL |
| 70 | AO | 134 | LYS |
| 22 | V | 53 | VAL |
| 55 | 5 | 32 | LEU |
| 60 | AD | 123 | SER |
| 67 | AL | 118 | ARG |
| 70 | AO | 29 | ALA |
| 70 | AO | 85 | VAL |
| 76 | AV | 17 | ARG |
| 9 | I | 6 | THR |
| 9 | I | 8 | ILE |
| 12 | L | 180 | GLU |
| 51 | 1 | 213 | ALA |
| 53 | 3 | 80 | ARG |
| 56 | 6 | 120 | SER |
| 74 | AS | 134 | TYR |
| 42 | p | 218 | ALA |
| 56 | 6 | 155 | ILE |
| 24 | X | 67 | VAL |
| 54 | 4 | 42 | PRO |
| 54 | 4 | 191 | ASN |
| 57 | 7 | 269 | ILE |
| 67 | AL | 95 | ILE |
| 76 | AV | 20 | VAL |
| 76 | AV | 67 | PRO |
| 78 | AX | 47 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | w | 120 | VAL |
| 54 | 4 | 16 | PRO |
| 11 | K | 113 | ILE |
| 25 | Y | 68 | VAL |
| 42 | p | 143 | ILE |
| 67 | AL | 85 | ALA |
| 76 | AV | 43 | VAL |
| 78 | AX | 92 | VAL |
| 10 | J | 159 | PHE |
| 13 | M | 131 | VAL |
| 17 | Q | 26 | VAL |
| 51 | 1 | 167 | VAL |
| 55 | 5 | 175 | ILE |
| 69 | AN | 133 | VAL |
| 16 | P | 10 | VAL |

### 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 | |
|---|---|---|---|---|---|---|
| 9 | I | 163/164 (99%) | 158 (97%) | 5 (3%) | 40 | 74 |
| 10 | J | 178/179 (99%) | 175 (98%) | 3 (2%) | 60 | 86 |
| 11 | K | 145/163 (89%) | 144 (99%) | 1 (1%) | 84 | 95 |
| 12 | L | 152/182 (84%) | 151 (99%) | 1 (1%) | 84 | 95 |
| 13 | M | 188/189 (100%) | 187 (100%) | 1 (0%) | 88 | 96 |
| 14 | N | 139/144 (96%) | 136 (98%) | 3 (2%) | 52 | 81 |
| 15 | O | 179/180 (99%) | 178 (99%) | 1 (1%) | 86 | 96 |
| 16 | P | 133/144 (92%) | 133 (100%) | 0 | 100 | 100 |
| 17 | Q | 156/158 (99%) | 156 (100%) | 0 | 100 | 100 |
| 18 | R | 168/196 (86%) | 166 (99%) | 2 (1%) | 71 | 91 |
| 19 | S | 132/133 (99%) | 131 (99%) | 1 (1%) | 81 | 94 |
| 20 | T | 107/114 (94%) | 107 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 21 | U | 110/111 (99%) | 110 (100%) | 0 | 100 | 100 |
| 22 | V | 103/123 (84%) | 103 (100%) | 0 | 100 | 100 |
| 23 | W | 60/104 (58%) | 59 (98%) | 1 (2%) | 60 | 86 |
| 24 | X | 103/121 (85%) | 103 (100%) | 0 | 100 | 100 |
| 25 | Y | 114/115 (99%) | 113 (99%) | 1 (1%) | 78 | 93 |
| 26 | Z | 114/115 (99%) | 114 (100%) | 0 | 100 | 100 |
| 27 | a | 118/119 (99%) | 116 (98%) | 2 (2%) | 60 | 86 |
| 28 | b | 57/58 (98%) | 57 (100%) | 0 | 100 | 100 |
| 29 | c | 198/204 (97%) | 193 (98%) | 5 (2%) | 47 | 78 |
| 30 | d | 337/351 (96%) | 336 (100%) | 1 (0%) | 92 | 98 |
| 31 | e | 82/90 (91%) | 77 (94%) | 5 (6%) | 18 | 48 |
| 32 | f | 97/156 (62%) | 97 (100%) | 0 | 100 | 100 |
| 33 | g | 113/117 (97%) | 111 (98%) | 2 (2%) | 59 | 85 |
| 34 | h | 107/145 (74%) | 107 (100%) | 0 | 100 | 100 |
| 35 | i | 116/117 (99%) | 116 (100%) | 0 | 100 | 100 |
| 36 | j | 109/121 (90%) | 107 (98%) | 2 (2%) | 59 | 85 |
| 37 | k | 81/87 (93%) | 81 (100%) | 0 | 100 | 100 |
| 38 | l | 69/70 (99%) | 69 (100%) | 0 | 100 | 100 |
| 39 | m | 73/74 (99%) | 73 (100%) | 0 | 100 | 100 |
| 40 | n | 68/74 (92%) | 68 (100%) | 0 | 100 | 100 |
| 41 | o | 46/47 (98%) | 46 (100%) | 0 | 100 | 100 |
| 42 | p | 295/302 (98%) | 293 (99%) | 2 (1%) | 84 | 95 |
| 43 | q | 46/113 (41%) | 46 (100%) | 0 | 100 | 100 |
| 44 | r | 83/92 (90%) | 80 (96%) | 3 (4%) | 35 | 69 |
| 45 | s | 209/242 (86%) | 208 (100%) | 1 (0%) | 88 | 96 |
| 46 | t | 111/152 (73%) | 110 (99%) | 1 (1%) | 78 | 93 |
| 47 | u | 190/209 (91%) | 187 (98%) | 3 (2%) | 62 | 86 |
| 48 | v | 196/292 (67%) | 196 (100%) | 0 | 100 | 100 |
| 49 | w | 169/172 (98%) | 168 (99%) | 1 (1%) | 86 | 96 |
| 50 | 0 | 194/222 (87%) | 189 (97%) | 5 (3%) | 46 | 77 |
| 51 | 1 | 215/225 (96%) | 212 (99%) | 3 (1%) | 67 | 89 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 53 | 3 | 208/208 (100%) | 206 (99%) | 2 (1%) | 76 | 92 |
| 54 | 4 | 186/186 (100%) | 185 (100%) | 1 (0%) | 88 | 96 |
| 55 | 5 | 149/176 (85%) | 147 (99%) | 2 (1%) | 69 | 90 |
| 56 | 6 | 147/164 (90%) | 145 (99%) | 2 (1%) | 67 | 89 |
| 57 | 7 | 263/266 (99%) | 259 (98%) | 4 (2%) | 65 | 87 |
| 58 | 8 | 35/49 (71%) | 35 (100%) | 0 | 100 | 100 |
| 59 | AC | 177/202 (88%) | 177 (100%) | 0 | 100 | 100 |
| 60 | AD | 82/129 (64%) | 81 (99%) | 1 (1%) | 71 | 91 |
| 61 | AE | 124/150 (83%) | 122 (98%) | 2 (2%) | 62 | 86 |
| 62 | AG | 125/132 (95%) | 125 (100%) | 0 | 100 | 100 |
| 63 | AH | 105/113 (93%) | 105 (100%) | 0 | 100 | 100 |
| 64 | AI | 104/130 (80%) | 102 (98%) | 2 (2%) | 57 | 84 |
| 65 | AJ | 110/111 (99%) | 105 (96%) | 5 (4%) | 27 | 61 |
| 66 | AK | 113/120 (94%) | 108 (96%) | 5 (4%) | 28 | 61 |
| 67 | AL | 107/123 (87%) | 107 (100%) | 0 | 100 | 100 |
| 68 | AM | 125/130 (96%) | 121 (97%) | 4 (3%) | 39 | 73 |
| 69 | AN | 159/159 (100%) | 158 (99%) | 1 (1%) | 86 | 96 |
| 70 | AO | 118/147 (80%) | 118 (100%) | 0 | 100 | 100 |
| 71 | AP | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 72 | AQ | 94/104 (90%) | 94 (100%) | 0 | 100 | 100 |
| 73 | AR | 68/119 (57%) | 68 (100%) | 0 | 100 | 100 |
| 74 | AS | 115/116 (99%) | 110 (96%) | 5 (4%) | 29 | 62 |
| 75 | AT | 111/120 (92%) | 111 (100%) | 0 | 100 | 100 |
| 76 | AV | 87/93 (94%) | 86 (99%) | 1 (1%) | 73 | 92 |
| 77 | AW | 72/75 (96%) | 71 (99%) | 1 (1%) | 67 | 89 |
| 78 | AX | 171/185 (92%) | 167 (98%) | 4 (2%) | 50 | 80 |
| 79 | AY | 49/54 (91%) | 49 (100%) | 0 | 100 | 100 |
| 80 | AZ | 57/74 (77%) | 54 (95%) | 3 (5%) | 22 | 54 |
| All | All | 9268/10330 (90%) | 9167 (99%) | 101 (1%) | 74 | 92 |

All (101) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | I | 9 | SER |
| 9 | I | 19 | THR |
| 9 | I | 20 | TYR |
| 9 | I | 188 | ARG |
| 9 | I | 189 | SER |
| 10 | J | 141 | LYS |
| 10 | J | 142 | GLU |
| 10 | J | 203 | LYS |
| 11 | K | 122 | LYS |
| 12 | L | 180 | GLU |
| 13 | M | 167 | LYS |
| 14 | N | 46 | MET |
| 14 | N | 134 | LYS |
| 14 | N | 137 | VAL |
| 15 | O | 90 | LEU |
| 18 | R | 19 | ARG |
| 18 | R | 62 | ARG |
| 19 | S | 9 | SER |
| 23 | W | 62 | ILE |
| 25 | Y | 58 | SER |
| 27 | a | 69 | SER |
| 27 | a | 75 | ARG |
| 29 | c | 136 | ILE |
| 29 | c | 149 | LYS |
| 29 | c | 150 | LEU |
| 29 | c | 174 | ARG |
| 29 | c | 187 | TYR |
| 30 | d | 274 | GLN |
| 31 | e | 24 | LYS |
| 31 | e | 79 | LEU |
| 31 | e | 83 | CYS |
| 31 | e | 100 | SER |
| 31 | e | 101 | ASP |
| 33 | g | 129 | LYS |
| 33 | g | 130 | LEU |
| 36 | j | 14 | LEU |
| 36 | j | 126 | VAL |
| 42 | p | 139 | ARG |
| 42 | p | 320 | ILE |
| 44 | r | 77 | CYS |
| 44 | r | 95 | ASP |
| 44 | r | 96 | LYS |
| 45 | s | 126 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | t | 107 | GLN |
| 47 | u | 25 | ARG |
| 47 | u | 224 | MET |
| 47 | u | 225 | ARG |
| 49 | w | 137 | SER |
| 50 | 0 | 77 | SER |
| 50 | 0 | 80 | GLU |
| 50 | 0 | 97 | ARG |
| 50 | 0 | 134 | ASP |
| 50 | 0 | 184 | ILE |
| 51 | 1 | 39 | LEU |
| 51 | 1 | 98 | LEU |
| 51 | 1 | 179 | ILE |
| 53 | 3 | 44 | SER |
| 53 | 3 | 150 | LEU |
| 54 | 4 | 190 | TRP |
| 55 | 5 | 49 | ARG |
| 55 | 5 | 163 | ILE |
| 56 | 6 | 18 | PHE |
| 56 | 6 | 120 | SER |
| 57 | 7 | 25 | SER |
| 57 | 7 | 26 | TYR |
| 57 | 7 | 27 | ILE |
| 57 | 7 | 149 | HIS |
| 60 | AD | 41 | ARG |
| 61 | AE | 65 | ASN |
| 61 | AE | 99 | ILE |
| 64 | AI | 84 | LYS |
| 64 | AI | 134 | LEU |
| 65 | AJ | 5 | SER |
| 65 | AJ | 28 | ARG |
| 65 | AJ | 47 | ILE |
| 65 | AJ | 50 | PHE |
| 65 | AJ | 130 | TYR |
| 66 | AK | 36 | LYS |
| 66 | AK | 37 | VAL |
| 66 | AK | 46 | LEU |
| 66 | AK | 119 | ASP |
| 66 | AK | 122 | LEU |
| 68 | AM | 44 | LEU |
| 68 | AM | 59 | THR |
| 68 | AM | 60 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 68 | AM | 65 | LEU |
| 69 | AN | 63 | MET |
| 74 | AS | 28 | LYS |
| 74 | AS | 36 | LYS |
| 74 | AS | 37 | LYS |
| 74 | AS | 81 | ILE |
| 74 | AS | 105 | PHE |
| 76 | AV | 83 | ILE |
| 77 | AW | 81 | ARG |
| 78 | AX | 189 | LEU |
| 78 | AX | 194 | THR |
| 78 | AX | 196 | ARG |
| 78 | AX | 201 | GLU |
| 80 | AZ | 48 | MET |
| 80 | AZ | 84 | ARG |
| 80 | AZ | 87 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | I | 45 | ASN |
| 10 | J | 71 | GLN |
| 10 | J | 100 | ASN |
| 11 | K | 157 | HIS |
| 12 | L | 6 | ASN |
| 12 | L | 117 | ASN |
| 13 | M | 129 | ASN |
| 14 | N | 49 | HIS |
| 14 | N | 51 | GLN |
| 15 | O | 95 | ASN |
| 15 | O | 196 | ASN |
| 16 | P | 3 | HIS |
| 16 | P | 97 | ASN |
| 17 | Q | 110 | HIS |
| 17 | Q | 145 | HIS |
| 17 | Q | 155 | GLN |
| 18 | R | 137 | ASN |
| 18 | R | 169 | ASN |
| 20 | T | 75 | ASN |
| 21 | U | 49 | ASN |
| 23 | W | 14 | HIS |
| 24 | X | 111 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | Y | 21 | HIS |
| 25 | Y | 77 | HIS |
| 25 | Y | 117 | GLN |
| 26 | Z | 11 | GLN |
| 26 | Z | 60 | HIS |
| 26 | Z | 114 | HIS |
| 27 | a | 33 | ASN |
| 27 | a | 42 | HIS |
| 28 | b | 6 | ASN |
| 29 | c | 139 | HIS |
| 29 | c | 215 | ASN |
| 30 | d | 261 | HIS |
| 30 | d | 274 | GLN |
| 30 | d | 352 | GLN |
| 30 | d | 378 | GLN |
| 32 | f | 120 | ASN |
| 33 | g | 28 | GLN |
| 34 | h | 7 | GLN |
| 34 | h | 13 | HIS |
| 34 | h | 123 | ASN |
| 39 | m | 37 | HIS |
| 40 | n | 74 | HIS |
| 42 | p | 145 | ASN |
| 42 | p | 237 | HIS |
| 42 | p | 306 | GLN |
| 43 | q | 90 | ASN |
| 43 | q | 109 | ASN |
| 44 | r | 59 | HIS |
| 44 | r | 82 | GLN |
| 45 | s | 35 | GLN |
| 45 | s | 39 | GLN |
| 45 | s | 201 | HIS |
| 46 | t | 60 | ASN |
| 47 | u | 120 | GLN |
| 47 | u | 185 | ASN |
| 47 | u | 226 | GLN |
| 47 | u | 245 | ASN |
| 48 | v | 111 | HIS |
| 48 | v | 123 | GLN |
| 49 | w | 77 | GLN |
| 50 | 0 | 75 | ASN |
| 50 | 0 | 102 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 0 | 104 | HIS |
| 50 | 0 | 151 | ASN |
| 51 | 1 | 5 | HIS |
| 51 | 1 | 33 | HIS |
| 51 | 1 | 68 | HIS |
| 51 | 1 | 142 | HIS |
| 51 | 1 | 230 | ASN |
| 51 | 1 | 231 | HIS |
| 53 | 3 | 10 | ASN |
| 53 | 3 | 15 | GLN |
| 53 | 3 | 180 | GLN |
| 54 | 4 | 34 | HIS |
| 54 | 4 | 178 | GLN |
| 54 | 4 | 196 | GLN |
| 55 | 5 | 88 | ASN |
| 56 | 6 | 3 | ASN |
| 56 | 6 | 122 | HIS |
| 56 | 6 | 130 | GLN |
| 57 | 7 | 10 | HIS |
| 57 | 7 | 75 | HIS |
| 57 | 7 | 149 | HIS |
| 57 | 7 | 195 | ASN |
| 57 | 7 | 233 | ASN |
| 57 | 7 | 298 | HIS |
| 57 | 7 | 301 | ASN |
| 58 | 8 | 27 | ASN |
| 58 | 8 | 47 | ASN |
| 58 | 8 | 50 | HIS |
| 59 | AC | 129 | HIS |
| 59 | AC | 149 | GLN |
| 59 | AC | 168 | GLN |
| 59 | AC | 200 | ASN |
| 60 | AD | 101 | HIS |
| 61 | AE | 20 | GLN |
| 61 | AE | 65 | ASN |
| 61 | AE | 107 | HIS |
| 62 | AG | 78 | ASN |
| 62 | AG | 123 | HIS |
| 63 | AH | 13 | ASN |
| 63 | AH | 36 | HIS |
| 63 | AH | 84 | ASN |
| 63 | AH | 87 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 64 | AI | 51 | ASN |
| 64 | AI | 55 | HIS |
| 64 | AI | 86 | HIS |
| 65 | AJ | 56 | HIS |
| 66 | AK | 38 | ASN |
| 66 | AK | 80 | GLN |
| 66 | AK | 100 | GLN |
| 66 | AK | 103 | HIS |
| 68 | AM | 12 | HIS |
| 68 | AM | 86 | ASN |
| 68 | AM | 126 | HIS |
| 68 | AM | 136 | HIS |
| 69 | AN | 165 | ASN |
| 70 | AO | 46 | HIS |
| 70 | AO | 66 | HIS |
| 71 | AP | 112 | ASN |
| 71 | AP | 217 | HIS |
| 72 | AQ | 89 | HIS |
| 73 | AR | 23 | HIS |
| 74 | AS | 73 | GLN |
| 74 | AS | 77 | ASN |
| 74 | AS | 110 | HIS |
| 75 | AT | 4 | GLN |
| 75 | AT | 27 | GLN |
| 75 | AT | 95 | ASN |
| 77 | AW | 86 | HIS |
| 78 | AX | 111 | ASN |
| 78 | AX | 144 | GLN |
| 80 | AZ | 39 | ASN |
| 80 | AZ | 42 | GLN |
| 80 | AZ | 63 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | A | 1591/1781 (89%) | 282 (17%) | 1 (0%) |
| 2 | B | 1058/1465 (72%) | 162 (15%) | 7 (0%) |
| 3 | C | 160/262 (61%) | 24 (15%) | 1 (0%) |
| 4 | D | 118/120 (98%) | 10 (8%) | 0 |
| 5 | E | 163/213 (76%) | 20 (12%) | 0 |
| 52 | 2 | 1801/2205 (81%) | 656 (36%) | 162 (8%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 6 | F | 70/73 (95%) | 16 (22%) | 1 (1%) |
| 7 | G | 182/183 (99%) | 18 (9%) | 1 (0%) |
| 8 | H | 89/127 (70%) | 13 (14%) | 0 |
| All | All | 5232/6429 (81%) | 1201 (22%) | 173 (3%) |

All (1201) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4 | G |
| 1 | A | 20 | G |
| 1 | A | 24 | A |
| 1 | A | 28 | G |
| 1 | A | 38 | A |
| 1 | A | 41 | A |
| 1 | A | 43 | A |
| 1 | A | 47 | C |
| 1 | A | 58 | A |
| 1 | A | 62 | G |
| 1 | A | 63 | A |
| 1 | A | 64 | A |
| 1 | A | 65 | A |
| 1 | A | 66 | A |
| 1 | A | 70 | C |
| 1 | A | 71 | C |
| 1 | A | 72 | G |
| 1 | A | 73 | U |
| 1 | A | 82 | C |
| 1 | A | 84 | G |
| 1 | A | 85 | U |
| 1 | A | 87 | A |
| 1 | A | 91 | G |
| 1 | A | 103 | G |
| 1 | A | 108 | G |
| 1 | A | 114 | G |
| 1 | A | 119 | C |
| 1 | A | 122 | A |
| 1 | A | 127 | G |
| 1 | A | 131 | U |
| 1 | A | 140 | U |
| 1 | A | 141 | U |
| 1 | A | 154 | A |
| 1 | A | 158 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 188 | A |
| 1 | A | 189 | A |
| 1 | A | 190 | U |
| 1 | A | 191 | U |
| 1 | A | 192 | C |
| 1 | A | 196 | C |
| 1 | A | 203 | C |
| 1 | A | 205 | A |
| 1 | A | 206 | A |
| 1 | A | 216 | G |
| 1 | A | 219 | U |
| 1 | A | 220 | A |
| 1 | A | 223 | A |
| 1 | A | 234 | G |
| 1 | A | 236 | G |
| 1 | A | 248 | A |
| 1 | A | 251 | A |
| 1 | A | 255 | G |
| 1 | A | 256 | U |
| 1 | A | 258 | A |
| 1 | A | 267 | A |
| 1 | A | 279 | G |
| 1 | A | 280 | A |
| 1 | A | 281 | G |
| 1 | A | 323 | U |
| 1 | A | 332 | A |
| 1 | A | 336 | U |
| 1 | A | 342 | G |
| 1 | A | 343 | U |
| 1 | A | 367 | A |
| 1 | A | 368 | G |
| 1 | A | 369 | A |
| 1 | A | 372 | A |
| 1 | A | 376 | A |
| 1 | A | 391 | A |
| 1 | A | 410 | U |
| 1 | A | 411 | U |
| 1 | A | 413 | A |
| 1 | A | 415 | A |
| 1 | A | 417 | G |
| 1 | A | 426 | A |
| 1 | A | 428 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 440 | A |
| 1 | A | 443 | A |
| 1 | A | 444 | C |
| 1 | A | 454 | U |
| 1 | A | 463 | C |
| 1 | A | 464 | A |
| 1 | A | 477 | C |
| 1 | A | 485 | A |
| 1 | A | 486 | C |
| 1 | A | 488 | G |
| 1 | A | 493 | A |
| 1 | A | 494 | A |
| 1 | A | 506 | G |
| 1 | A | 520 | G |
| 1 | A | 523 | G |
| 1 | A | 536 | G |
| 1 | A | 539 | C |
| 1 | A | 541 | A |
| 1 | A | 546 | G |
| 1 | A | 547 | U |
| 1 | A | 551 | A |
| 1 | A | 554 | A |
| 1 | A | 555 | U |
| 1 | A | 557 | U |
| 1 | A | 558 | U |
| 1 | A | 569 | G |
| 1 | A | 570 | A |
| 1 | A | 571 | A |
| 1 | A | 572 | A |
| 1 | A | 573 | U |
| 1 | A | 575 | A |
| 1 | A | 582 | U |
| 1 | A | 583 | A |
| 1 | A | 584 | U |
| 1 | A | 588 | A |
| 1 | A | 611 | C |
| 1 | A | 612 | G |
| 1 | A | 617 | G |
| 1 | A | 621 | U |
| 1 | A | 625 | C |
| 1 | A | 632 | A |
| 1 | A | 641 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 644 | G |
| 1 | A | 668 | C |
| 1 | A | 681 | A |
| 1 | A | 692 | A |
| 1 | A | 709 | A |
| 1 | A | 716 | A |
| 1 | A | 719 | U |
| 1 | A | 720 | A |
| 1 | A | 721 | U |
| 1 | A | 726 | G |
| 1 | A | 729 | A |
| 1 | A | 735 | U |
| 1 | A | 748 | A |
| 1 | A | 750 | G |
| 1 | A | 753 | A |
| 1 | A | 754 | G |
| 1 | A | 759 | A |
| 1 | A | 760 | A |
| 1 | A | 761 | U |
| 1 | A | 762 | A |
| 1 | A | 763 | U |
| 1 | A | 769 | U |
| 1 | A | 770 | G |
| 1 | A | 771 | U |
| 1 | A | 800 | U |
| 1 | A | 803 | C |
| 1 | A | 828 | U |
| 1 | A | 832 | G |
| 1 | A | 836 | G |
| 1 | A | 850 | G |
| 1 | A | 868 | A |
| 1 | A | 888 | A |
| 1 | A | 902 | C |
| 1 | A | 912 | C |
| 1 | A | 925 | U |
| 1 | A | 930 | U |
| 1 | A | 931 | G |
| 1 | A | 948 | U |
| 1 | A | 958 | G |
| 1 | A | 959 | G |
| 1 | A | 960 | A |
| 1 | A | 965 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 966 | A |
| 1 | A | 967 | G |
| 1 | A | 968 | A |
| 1 | A | 975 | G |
| 1 | A | 988 | G |
| 1 | A | 995 | C |
| 1 | A | 1004 | G |
| 1 | A | 1005 | U |
| 1 | A | 1011 | U |
| 1 | A | 1012 | C |
| 1 | A | 1025 | G |
| 1 | A | 1029 | G |
| 1 | A | 1030 | U |
| 1 | A | 1031 | A |
| 1 | A | 1032 | G |
| 1 | A | 1033 | A |
| 1 | A | 1045 | G |
| 1 | A | 1092 | U |
| 1 | A | 1098 | A |
| 1 | A | 1114 | A |
| 1 | A | 1116 | A |
| 1 | A | 1122 | U |
| 1 | A | 1123 | G |
| 1 | A | 1128 | A |
| 1 | A | 1132 | A |
| 1 | A | 1133 | A |
| 1 | A | 1134 | C |
| 1 | A | 1135 | U |
| 1 | A | 1141 | G |
| 1 | A | 1148 | A |
| 1 | A | 1150 | A |
| 1 | A | 1151 | A |
| 1 | A | 1155 | A |
| 1 | A | 1156 | A |
| 1 | A | 1160 | G |
| 1 | A | 1161 | A |
| 1 | A | 1174 | G |
| 1 | A | 1188 | G |
| 1 | A | 1200 | A |
| 1 | A | 1201 | U |
| 1 | A | 1211 | A |
| 1 | A | 1217 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1218 | A |
| 1 | A | 1225 | U |
| 1 | A | 1235 | A |
| 1 | A | 1238 | C |
| 1 | A | 1240 | U |
| 1 | A | 1242 | U |
| 1 | A | 1254 | C |
| 1 | A | 1257 | U |
| 1 | A | 1261 | U |
| 1 | A | 1263 | A |
| 1 | A | 1270 | U |
| 1 | A | 1271 | G |
| 1 | A | 1349 | A |
| 1 | A | 1367 | U |
| 1 | A | 1369 | G |
| 1 | A | 1371 | U |
| 1 | A | 1375 | G |
| 1 | A | 1378 | U |
| 1 | A | 1379 | A |
| 1 | A | 1389 | A |
| 1 | A | 1390 | G |
| 1 | A | 1392 | G |
| 1 | A | 1393 | G |
| 1 | A | 1394 | U |
| 1 | A | 1401 | U |
| 1 | A | 1404 | U |
| 1 | A | 1412 | G |
| 1 | A | 1413 | U |
| 1 | A | 1420 | G |
| 1 | A | 1422 | A |
| 1 | A | 1426 | A |
| 1 | A | 1440 | A |
| 1 | A | 1445 | U |
| 1 | A | 1446 | A |
| 1 | A | 1447 | G |
| 1 | A | 1466 | G |
| 1 | A | 1467 | G |
| 1 | A | 1468 | C |
| 1 | A | 1472 | G |
| 1 | A | 1490 | A |
| 1 | A | 1492 | G |
| 1 | A | 1506 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1509 | G |
| 1 | A | 1521 | G |
| 1 | A | 1523 | G |
| 1 | A | 1525 | A |
| 1 | A | 1526 | G |
| 1 | A | 1528 | U |
| 1 | A | 1529 | C |
| 1 | A | 1542 | G |
| 1 | A | 1547 | G |
| 1 | A | 1559 | A |
| 1 | A | 1571 | U |
| 1 | A | 1588 | G |
| 1 | A | 1591 | C |
| 1 | A | 1617 | C |
| 1 | A | 1618 | U |
| 1 | A | 1630 | U |
| 1 | A | 1633 | U |
| 1 | A | 1634 | C |
| 1 | A | 1647 | C |
| 1 | A | 1656 | A |
| 1 | A | 1663 | U |
| 1 | A | 1664 | G |
| 1 | A | 1665 | U |
| 1 | A | 1668 | G |
| 1 | A | 1669 | G |
| 1 | A | 1670 | A |
| 1 | A | 1671 | A |
| 1 | A | 1679 | G |
| 1 | A | 1680 | U |
| 1 | A | 1726 | C |
| 1 | A | 1727 | U |
| 1 | A | 1741 | A |
| 1 | A | 1746 | A |
| 1 | A | 1747 | C |
| 1 | A | 1749 | U |
| 1 | A | 1764 | A |
| 1 | A | 1766 | A |
| 1 | A | 1768 | G |
| 2 | B | 22 | U |
| 2 | B | 24 | A |
| 2 | B | 28 | C |
| 2 | B | 30 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 60 | C |
| 2 | B | 61 | A |
| 2 | B | 62 | U |
| 2 | B | 68 | A |
| 2 | B | 71 | G |
| 2 | B | 74 | C |
| 2 | B | 79 | A |
| 2 | B | 89 | G |
| 2 | B | 96 | A |
| 2 | B | 283 | C |
| 2 | B | 297 | U |
| 2 | B | 300 | C |
| 2 | B | 305 | G |
| 2 | B | 314 | A |
| 2 | B | 327 | A |
| 2 | B | 328 | A |
| 2 | B | 332 | A |
| 2 | B | 341 | A |
| 2 | B | 352 | U |
| 2 | B | 353 | G |
| 2 | B | 390 | A |
| 2 | B | 391 | A |
| 2 | B | 408 | U |
| 2 | B | 427 | A |
| 2 | B | 432 | G |
| 2 | B | 439 | A |
| 2 | B | 455 | G |
| 2 | B | 456 | G |
| 2 | B | 462 | A |
| 2 | B | 464 | A |
| 2 | B | 481 | U |
| 2 | B | 490 | G |
| 2 | B | 491 | C |
| 2 | B | 493 | U |
| 2 | B | 496 | A |
| 2 | B | 498 | G |
| 2 | B | 517 | U |
| 2 | B | 519 | U |
| 2 | B | 530 | U |
| 2 | B | 548 | U |
| 2 | B | 556 | A |
| 2 | B | 558 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 576 | G |
| 2 | B | 580 | A |
| 2 | B | 585 | A |
| 2 | B | 586 | G |
| 2 | B | 587 | A |
| 2 | B | 594 | U |
| 2 | B | 595 | G |
| 2 | B | 598 | U |
| 2 | B | 607 | A |
| 2 | B | 618 | G |
| 2 | B | 625 | G |
| 2 | B | 697 | U |
| 2 | B | 698 | A |
| 2 | B | 706 | A |
| 2 | B | 714 | A |
| 2 | B | 739 | G |
| 2 | B | 740 | C |
| 2 | B | 741 | U |
| 2 | B | 742 | G |
| 2 | B | 900 | A |
| 2 | B | 942 | G |
| 2 | B | 946 | U |
| 2 | B | 947 | G |
| 2 | B | 948 | U |
| 2 | B | 949 | U |
| 2 | B | 955 | A |
| 2 | B | 969 | G |
| 2 | B | 970 | G |
| 2 | B | 977 | G |
| 2 | B | 1014 | G |
| 2 | B | 1015 | U |
| 2 | B | 1018 | U |
| 2 | B | 1019 | A |
| 2 | B | 1020 | A |
| 2 | B | 1037 | A |
| 2 | B | 1039 | A |
| 2 | B | 1040 | G |
| 2 | B | 1044 | U |
| 2 | B | 1052 | A |
| 2 | B | 1054 | A |
| 2 | B | 1059 | A |
| 2 | B | 1067 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 1068 | A |
| 2 | B | 1075 | U |
| 2 | B | 1077 | G |
| 2 | B | 1082 | A |
| 2 | B | 1083 | C |
| 2 | B | 1092 | G |
| 2 | B | 1093 | U |
| 2 | B | 1117 | G |
| 2 | B | 1119 | C |
| 2 | B | 1125 | A |
| 2 | B | 1135 | A |
| 2 | B | 1143 | G |
| 2 | B | 1152 | A |
| 2 | B | 1170 | G |
| 2 | B | 1173 | A |
| 2 | B | 1174 | G |
| 2 | B | 1175 | A |
| 2 | B | 1177 | U |
| 2 | B | 1184 | C |
| 2 | B | 1188 | G |
| 2 | B | 1191 | A |
| 2 | B | 1195 | C |
| 2 | B | 1213 | G |
| 2 | B | 1218 | C |
| 2 | B | 1219 | A |
| 2 | B | 1234 | U |
| 2 | B | 1245 | G |
| 2 | B | 1246 | A |
| 2 | B | 1249 | U |
| 2 | B | 1261 | A |
| 2 | B | 1268 | C |
| 2 | B | 1273 | C |
| 2 | B | 1278 | G |
| 2 | B | 1309 | C |
| 2 | B | 1310 | A |
| 2 | B | 1316 | C |
| 2 | B | 1321 | G |
| 2 | B | 1322 | C |
| 2 | B | 1328 | U |
| 2 | B | 1345 | A |
| 2 | B | 1357 | C |
| 2 | B | 1364 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 1366 | G |
| 2 | B | 1369 | G |
| 2 | B | 1372 | A |
| 2 | B | 1373 | A |
| 2 | B | 1377 | C |
| 2 | B | 1379 | A |
| 2 | B | 1382 | A |
| 2 | B | 1384 | A |
| 2 | B | 1385 | A |
| 2 | B | 1386 | G |
| 2 | B | 1387 | A |
| 2 | B | 1388 | U |
| 2 | B | 1389 | U |
| 2 | B | 1390 | A |
| 2 | B | 1391 | U |
| 2 | B | 1392 | C |
| 2 | B | 1398 | A |
| 2 | B | 1399 | A |
| 2 | B | 1404 | G |
| 2 | B | 1410 | G |
| 2 | B | 1412 | C |
| 2 | B | 1414 | G |
| 2 | B | 1423 | U |
| 2 | B | 1436 | C |
| 2 | B | 1437 | G |
| 2 | B | 1439 | U |
| 2 | B | 1440 | G |
| 2 | B | 1449 | U |
| 2 | B | 1450 | U |
| 2 | B | 1451 | G |
| 2 | B | 1452 | G |
| 2 | B | 1456 | U |
| 3 | C | 103 | A |
| 3 | C | 113 | U |
| 3 | C | 137 | G |
| 3 | C | 138 | C |
| 3 | C | 140 | G |
| 3 | C | 150 | A |
| 3 | C | 153 | A |
| 3 | C | 154 | G |
| 3 | C | 162 | A |
| 3 | C | 173 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 175 | U |
| 3 | C | 177 | U |
| 3 | C | 178 | A |
| 3 | C | 179 | A |
| 3 | C | 185 | C |
| 3 | C | 187 | A |
| 3 | C | 194 | A |
| 3 | C | 196 | C |
| 3 | C | 201 | A |
| 3 | C | 202 | C |
| 3 | C | 210 | G |
| 3 | C | 215 | A |
| 3 | C | 226 | A |
| 3 | C | 248 | U |
| 4 | D | 8 | G |
| 4 | D | 34 | U |
| 4 | D | 50 | A |
| 4 | D | 51 | A |
| 4 | D | 54 | U |
| 4 | D | 65 | A |
| 4 | D | 98 | G |
| 4 | D | 101 | A |
| 4 | D | 111 | G |
| 4 | D | 120 | C |
| 5 | E | 31 | C |
| 5 | E | 49 | G |
| 5 | E | 99 | G |
| 5 | E | 106 | U |
| 5 | E | 107 | U |
| 5 | E | 108 | A |
| 5 | E | 121 | U |
| 5 | E | 122 | U |
| 5 | E | 146 | A |
| 5 | E | 147 | A |
| 5 | E | 148 | A |
| 5 | E | 179 | U |
| 5 | E | 180 | G |
| 5 | E | 189 | G |
| 5 | E | 192 | U |
| 5 | E | 193 | U |
| 5 | E | 196 | A |
| 5 | E | 199 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | E | 207 | G |
| 5 | E | 210 | G |
| 6 | F | 15 | C |
| 6 | F | 24 | C |
| 6 | F | 31 | U |
| 6 | F | 33 | G |
| 6 | F | 42 | A |
| 6 | F | 43 | A |
| 6 | F | 44 | G |
| 6 | F | 52 | G |
| 6 | F | 53 | U |
| 6 | F | 55 | U |
| 6 | F | 64 | U |
| 6 | F | 67 | C |
| 6 | F | 68 | A |
| 6 | F | 69 | A |
| 6 | F | 72 | A |
| 6 | F | 73 | A |
| 7 | G | 8 | U |
| 7 | G | 40 | G |
| 7 | G | 77 | U |
| 7 | G | 84 | U |
| 7 | G | 86 | U |
| 7 | G | 102 | G |
| 7 | G | 106 | G |
| 7 | G | 107 | U |
| 7 | G | 120 | U |
| 7 | G | 121 | C |
| 7 | G | 122 | G |
| 7 | G | 128 | U |
| 7 | G | 144 | G |
| 7 | G | 158 | A |
| 7 | G | 159 | G |
| 7 | G | 170 | G |
| 7 | G | 171 | U |
| 7 | G | 173 | C |
| 8 | H | 10 | C |
| 8 | H | 14 | C |
| 8 | H | 19 | G |
| 8 | H | 23 | A |
| 8 | H | 24 | U |
| 8 | H | 25 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | H | 33 | U |
| 8 | H | 70 | G |
| 8 | H | 93 | U |
| 8 | H | 94 | G |
| 8 | H | 101 | G |
| 8 | H | 104 | G |
| 8 | H | 117 | U |
| 52 | 2 | 2 | A |
| 52 | 2 | 3 | U |
| 52 | 2 | 4 | C |
| 52 | 2 | 6 | G |
| 52 | 2 | 11 | A |
| 52 | 2 | 14 | C |
| 52 | 2 | 15 | U |
| 52 | 2 | 17 | C |
| 52 | 2 | 18 | C |
| 52 | 2 | 22 | A |
| 52 | 2 | 23 | G |
| 52 | 2 | 26 | A |
| 52 | 2 | 33 | U |
| 52 | 2 | 34 | G |
| 52 | 2 | 39 | A |
| 52 | 2 | 42 | G |
| 52 | 2 | 43 | A |
| 52 | 2 | 44 | C |
| 52 | 2 | 45 | U |
| 52 | 2 | 46 | U |
| 52 | 2 | 47 | A |
| 52 | 2 | 48 | G |
| 52 | 2 | 56 | U |
| 52 | 2 | 57 | G |
| 52 | 2 | 59 | C |
| 52 | 2 | 61 | C |
| 52 | 2 | 62 | A |
| 52 | 2 | 65 | A |
| 52 | 2 | 66 | U |
| 52 | 2 | 67 | C |
| 52 | 2 | 68 | A |
| 52 | 2 | 69 | C |
| 52 | 2 | 72 | C |
| 52 | 2 | 74 | U |
| 52 | 2 | 75 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 77 | G |
| 52 | 2 | 78 | C |
| 52 | 2 | 79 | A |
| 52 | 2 | 80 | G |
| 52 | 2 | 81 | G |
| 52 | 2 | 82 | A |
| 52 | 2 | 83 | A |
| 52 | 2 | 84 | U |
| 52 | 2 | 85 | C |
| 52 | 2 | 90 | C |
| 52 | 2 | 91 | A |
| 52 | 2 | 97 | C |
| 52 | 2 | 101 | A |
| 52 | 2 | 102 | C |
| 52 | 2 | 112 | A |
| 52 | 2 | 113 | A |
| 52 | 2 | 115 | C |
| 52 | 2 | 117 | G |
| 52 | 2 | 122 | A |
| 52 | 2 | 125 | A |
| 52 | 2 | 126 | A |
| 52 | 2 | 128 | C |
| 52 | 2 | 129 | U |
| 52 | 2 | 138 | C |
| 52 | 2 | 141 | C |
| 52 | 2 | 144 | A |
| 52 | 2 | 145 | A |
| 52 | 2 | 146 | U |
| 52 | 2 | 147 | U |
| 52 | 2 | 150 | A |
| 52 | 2 | 151 | U |
| 52 | 2 | 158 | G |
| 52 | 2 | 161 | A |
| 52 | 2 | 163 | A |
| 52 | 2 | 164 | C |
| 52 | 2 | 165 | G |
| 52 | 2 | 168 | A |
| 52 | 2 | 171 | C |
| 52 | 2 | 183 | C |
| 52 | 2 | 184 | C |
| 52 | 2 | 185 | A |
| 52 | 2 | 189 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 192 | U |
| 52 | 2 | 194 | U |
| 52 | 2 | 195 | U |
| 52 | 2 | 197 | U |
| 52 | 2 | 198 | C |
| 52 | 2 | 199 | C |
| 52 | 2 | 200 | A |
| 52 | 2 | 227 | U |
| 52 | 2 | 228 | G |
| 52 | 2 | 230 | G |
| 52 | 2 | 238 | G |
| 52 | 2 | 249 | A |
| 52 | 2 | 250 | C |
| 52 | 2 | 251 | A |
| 52 | 2 | 252 | G |
| 52 | 2 | 253 | U |
| 52 | 2 | 254 | A |
| 52 | 2 | 255 | A |
| 52 | 2 | 256 | A |
| 52 | 2 | 257 | A |
| 52 | 2 | 258 | C |
| 52 | 2 | 268 | C |
| 52 | 2 | 269 | A |
| 52 | 2 | 270 | C |
| 52 | 2 | 271 | U |
| 52 | 2 | 275 | A |
| 52 | 2 | 277 | U |
| 52 | 2 | 278 | A |
| 52 | 2 | 281 | A |
| 52 | 2 | 285 | A |
| 52 | 2 | 287 | C |
| 52 | 2 | 288 | A |
| 52 | 2 | 290 | U |
| 52 | 2 | 291 | G |
| 52 | 2 | 294 | G |
| 52 | 2 | 308 | C |
| 52 | 2 | 309 | G |
| 52 | 2 | 310 | U |
| 52 | 2 | 311 | G |
| 52 | 2 | 313 | G |
| 52 | 2 | 314 | A |
| 52 | 2 | 317 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 320 | G |
| 52 | 2 | 321 | G |
| 52 | 2 | 322 | C |
| 52 | 2 | 323 | U |
| 52 | 2 | 324 | U |
| 52 | 2 | 326 | U |
| 52 | 2 | 327 | U |
| 52 | 2 | 328 | C |
| 52 | 2 | 332 | C |
| 52 | 2 | 346 | C |
| 52 | 2 | 348 | A |
| 52 | 2 | 349 | C |
| 52 | 2 | 352 | C |
| 52 | 2 | 355 | U |
| 52 | 2 | 358 | C |
| 52 | 2 | 360 | G |
| 52 | 2 | 363 | G |
| 52 | 2 | 364 | G |
| 52 | 2 | 365 | U |
| 52 | 2 | 366 | G |
| 52 | 2 | 367 | A |
| 52 | 2 | 381 | G |
| 52 | 2 | 382 | A |
| 52 | 2 | 395 | U |
| 52 | 2 | 403 | G |
| 52 | 2 | 404 | C |
| 52 | 2 | 413 | A |
| 52 | 2 | 417 | U |
| 52 | 2 | 418 | U |
| 52 | 2 | 431 | G |
| 52 | 2 | 433 | G |
| 52 | 2 | 442 | A |
| 52 | 2 | 443 | A |
| 52 | 2 | 445 | U |
| 52 | 2 | 447 | G |
| 52 | 2 | 449 | U |
| 52 | 2 | 459 | A |
| 52 | 2 | 461 | G |
| 52 | 2 | 464 | G |
| 52 | 2 | 467 | C |
| 52 | 2 | 468 | A |
| 52 | 2 | 469 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 477 | G |
| 52 | 2 | 478 | C |
| 52 | 2 | 482 | U |
| 52 | 2 | 484 | G |
| 52 | 2 | 485 | C |
| 52 | 2 | 487 | C |
| 52 | 2 | 497 | A |
| 52 | 2 | 498 | C |
| 52 | 2 | 501 | A |
| 52 | 2 | 502 | A |
| 52 | 2 | 503 | C |
| 52 | 2 | 504 | G |
| 52 | 2 | 512 | A |
| 52 | 2 | 516 | A |
| 52 | 2 | 518 | A |
| 52 | 2 | 523 | A |
| 52 | 2 | 524 | U |
| 52 | 2 | 525 | A |
| 52 | 2 | 552 | U |
| 52 | 2 | 553 | U |
| 52 | 2 | 555 | C |
| 52 | 2 | 558 | U |
| 52 | 2 | 559 | G |
| 52 | 2 | 560 | G |
| 52 | 2 | 565 | U |
| 52 | 2 | 566 | A |
| 52 | 2 | 570 | A |
| 52 | 2 | 577 | U |
| 52 | 2 | 578 | C |
| 52 | 2 | 579 | C |
| 52 | 2 | 580 | A |
| 52 | 2 | 581 | A |
| 52 | 2 | 582 | U |
| 52 | 2 | 585 | C |
| 52 | 2 | 587 | A |
| 52 | 2 | 588 | G |
| 52 | 2 | 589 | U |
| 52 | 2 | 590 | A |
| 52 | 2 | 591 | A |
| 52 | 2 | 592 | C |
| 52 | 2 | 600 | G |
| 52 | 2 | 604 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 605 | A |
| 52 | 2 | 606 | G |
| 52 | 2 | 607 | U |
| 52 | 2 | 608 | C |
| 52 | 2 | 610 | G |
| 52 | 2 | 613 | G |
| 52 | 2 | 614 | C |
| 52 | 2 | 615 | C |
| 52 | 2 | 617 | G |
| 52 | 2 | 623 | G |
| 52 | 2 | 627 | U |
| 52 | 2 | 628 | A |
| 52 | 2 | 629 | A |
| 52 | 2 | 631 | U |
| 52 | 2 | 633 | C |
| 52 | 2 | 643 | A |
| 52 | 2 | 644 | G |
| 52 | 2 | 657 | C |
| 52 | 2 | 659 | G |
| 52 | 2 | 660 | U |
| 52 | 2 | 662 | G |
| 52 | 2 | 668 | A |
| 52 | 2 | 669 | A |
| 52 | 2 | 671 | G |
| 52 | 2 | 672 | G |
| 52 | 2 | 673 | G |
| 52 | 2 | 688 | G |
| 52 | 2 | 689 | U |
| 52 | 2 | 690 | G |
| 52 | 2 | 697 | G |
| 52 | 2 | 710 | U |
| 52 | 2 | 717 | C |
| 52 | 2 | 723 | C |
| 52 | 2 | 724 | A |
| 52 | 2 | 725 | U |
| 52 | 2 | 726 | G |
| 52 | 2 | 727 | U |
| 52 | 2 | 728 | C |
| 52 | 2 | 729 | G |
| 52 | 2 | 730 | G |
| 52 | 2 | 733 | U |
| 52 | 2 | 734 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 735 | G |
| 52 | 2 | 736 | G |
| 52 | 2 | 737 | U |
| 52 | 2 | 738 | G |
| 52 | 2 | 739 | A |
| 52 | 2 | 742 | C |
| 52 | 2 | 743 | A |
| 52 | 2 | 745 | G |
| 52 | 2 | 746 | C |
| 52 | 2 | 747 | C |
| 52 | 2 | 748 | C |
| 52 | 2 | 749 | U |
| 52 | 2 | 750 | U |
| 52 | 2 | 751 | G |
| 52 | 2 | 760 | G |
| 52 | 2 | 761 | A |
| 52 | 2 | 762 | A |
| 52 | 2 | 763 | C |
| 52 | 2 | 768 | A |
| 52 | 2 | 769 | A |
| 52 | 2 | 770 | A |
| 52 | 2 | 771 | G |
| 52 | 2 | 772 | A |
| 52 | 2 | 773 | A |
| 52 | 2 | 778 | G |
| 52 | 2 | 780 | A |
| 52 | 2 | 781 | A |
| 52 | 2 | 784 | C |
| 52 | 2 | 788 | A |
| 52 | 2 | 790 | U |
| 52 | 2 | 791 | G |
| 52 | 2 | 793 | U |
| 52 | 2 | 794 | U |
| 52 | 2 | 832 | C |
| 52 | 2 | 839 | G |
| 52 | 2 | 844 | U |
| 52 | 2 | 853 | A |
| 52 | 2 | 854 | C |
| 52 | 2 | 856 | A |
| 52 | 2 | 866 | G |
| 52 | 2 | 867 | A |
| 52 | 2 | 872 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 875 | A |
| 52 | 2 | 876 | G |
| 52 | 2 | 879 | A |
| 52 | 2 | 881 | U |
| 52 | 2 | 882 | U |
| 52 | 2 | 883 | G |
| 52 | 2 | 884 | A |
| 52 | 2 | 886 | U |
| 52 | 2 | 887 | U |
| 52 | 2 | 888 | G |
| 52 | 2 | 890 | A |
| 52 | 2 | 912 | A |
| 52 | 2 | 913 | G |
| 52 | 2 | 914 | G |
| 52 | 2 | 915 | A |
| 52 | 2 | 916 | G |
| 52 | 2 | 917 | C |
| 52 | 2 | 918 | A |
| 52 | 2 | 919 | G |
| 52 | 2 | 920 | C |
| 52 | 2 | 930 | A |
| 52 | 2 | 931 | C |
| 52 | 2 | 936 | U |
| 52 | 2 | 937 | C |
| 52 | 2 | 938 | G |
| 52 | 2 | 939 | G |
| 52 | 2 | 940 | C |
| 52 | 2 | 941 | U |
| 52 | 2 | 942 | U |
| 52 | 2 | 945 | G |
| 52 | 2 | 961 | U |
| 52 | 2 | 964 | U |
| 52 | 2 | 970 | U |
| 52 | 2 | 971 | U |
| 52 | 2 | 972 | A |
| 52 | 2 | 974 | G |
| 52 | 2 | 975 | G |
| 52 | 2 | 1093 | C |
| 52 | 2 | 1097 | C |
| 52 | 2 | 1099 | C |
| 52 | 2 | 1101 | A |
| 52 | 2 | 1103 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 1104 | A |
| 52 | 2 | 1105 | A |
| 52 | 2 | 1106 | U |
| 52 | 2 | 1107 | G |
| 52 | 2 | 1109 | A |
| 52 | 2 | 1119 | U |
| 52 | 2 | 1120 | U |
| 52 | 2 | 1121 | C |
| 52 | 2 | 1123 | G |
| 52 | 2 | 1129 | A |
| 52 | 2 | 1130 | A |
| 52 | 2 | 1133 | U |
| 52 | 2 | 1139 | G |
| 52 | 2 | 1145 | A |
| 52 | 2 | 1159 | U |
| 52 | 2 | 1160 | A |
| 52 | 2 | 1161 | G |
| 52 | 2 | 1162 | A |
| 52 | 2 | 1165 | G |
| 52 | 2 | 1166 | C |
| 52 | 2 | 1168 | C |
| 52 | 2 | 1173 | A |
| 52 | 2 | 1175 | G |
| 52 | 2 | 1180 | A |
| 52 | 2 | 1181 | C |
| 52 | 2 | 1182 | A |
| 52 | 2 | 1187 | A |
| 52 | 2 | 1189 | G |
| 52 | 2 | 1191 | A |
| 52 | 2 | 1192 | U |
| 52 | 2 | 1197 | C |
| 52 | 2 | 1198 | A |
| 52 | 2 | 1199 | A |
| 52 | 2 | 1206 | C |
| 52 | 2 | 1207 | U |
| 52 | 2 | 1213 | A |
| 52 | 2 | 1239 | A |
| 52 | 2 | 1240 | A |
| 52 | 2 | 1242 | A |
| 52 | 2 | 1244 | G |
| 52 | 2 | 1250 | A |
| 52 | 2 | 1251 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 1252 | A |
| 52 | 2 | 1268 | C |
| 52 | 2 | 1272 | A |
| 52 | 2 | 1273 | A |
| 52 | 2 | 1275 | C |
| 52 | 2 | 1279 | G |
| 52 | 2 | 1287 | U |
| 52 | 2 | 1293 | G |
| 52 | 2 | 1299 | C |
| 52 | 2 | 1378 | U |
| 52 | 2 | 1379 | A |
| 52 | 2 | 1399 | A |
| 52 | 2 | 1402 | G |
| 52 | 2 | 1416 | A |
| 52 | 2 | 1434 | C |
| 52 | 2 | 1438 | A |
| 52 | 2 | 1443 | U |
| 52 | 2 | 1444 | U |
| 52 | 2 | 1445 | U |
| 52 | 2 | 1446 | G |
| 52 | 2 | 1447 | A |
| 52 | 2 | 1450 | U |
| 52 | 2 | 1451 | U |
| 52 | 2 | 1452 | A |
| 52 | 2 | 1454 | A |
| 52 | 2 | 1462 | G |
| 52 | 2 | 1463 | G |
| 52 | 2 | 1466 | G |
| 52 | 2 | 1467 | A |
| 52 | 2 | 1492 | A |
| 52 | 2 | 1504 | G |
| 52 | 2 | 1508 | G |
| 52 | 2 | 1509 | G |
| 52 | 2 | 1512 | C |
| 52 | 2 | 1514 | A |
| 52 | 2 | 1516 | A |
| 52 | 2 | 1517 | A |
| 52 | 2 | 1518 | G |
| 52 | 2 | 1519 | A |
| 52 | 2 | 1522 | U |
| 52 | 2 | 1524 | G |
| 52 | 2 | 1525 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 1528 | G |
| 52 | 2 | 1529 | U |
| 52 | 2 | 1530 | G |
| 52 | 2 | 1531 | C |
| 52 | 2 | 1536 | U |
| 52 | 2 | 1537 | A |
| 52 | 2 | 1539 | U |
| 52 | 2 | 1540 | U |
| 52 | 2 | 1545 | U |
| 52 | 2 | 1547 | A |
| 52 | 2 | 1548 | A |
| 52 | 2 | 1549 | C |
| 52 | 2 | 1550 | A |
| 52 | 2 | 1551 | C |
| 52 | 2 | 1552 | G |
| 52 | 2 | 1553 | G |
| 52 | 2 | 1554 | G |
| 52 | 2 | 1555 | G |
| 52 | 2 | 1556 | A |
| 52 | 2 | 1557 | A |
| 52 | 2 | 1558 | C |
| 52 | 2 | 1559 | U |
| 52 | 2 | 1560 | U |
| 52 | 2 | 1562 | A |
| 52 | 2 | 1568 | U |
| 52 | 2 | 1571 | G |
| 52 | 2 | 1573 | A |
| 52 | 2 | 1575 | A |
| 52 | 2 | 1576 | G |
| 52 | 2 | 1577 | G |
| 52 | 2 | 1580 | G |
| 52 | 2 | 1581 | A |
| 52 | 2 | 1582 | G |
| 52 | 2 | 1583 | G |
| 52 | 2 | 1584 | A |
| 52 | 2 | 1585 | U |
| 52 | 2 | 1587 | G |
| 52 | 2 | 1597 | G |
| 52 | 2 | 1598 | U |
| 52 | 2 | 1599 | G |
| 52 | 2 | 1601 | U |
| 52 | 2 | 1605 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 1607 | U |
| 52 | 2 | 1608 | C |
| 52 | 2 | 1609 | G |
| 52 | 2 | 1610 | A |
| 52 | 2 | 1611 | U |
| 52 | 2 | 1612 | U |
| 52 | 2 | 1619 | A |
| 52 | 2 | 1622 | G |
| 52 | 2 | 1623 | U |
| 52 | 2 | 1624 | G |
| 52 | 2 | 1627 | G |
| 52 | 2 | 1628 | C |
| 52 | 2 | 1629 | A |
| 52 | 2 | 1638 | U |
| 52 | 2 | 1639 | U |
| 52 | 2 | 1640 | U |
| 52 | 2 | 1655 | U |
| 52 | 2 | 1660 | U |
| 52 | 2 | 1661 | U |
| 52 | 2 | 1668 | U |
| 52 | 2 | 1669 | U |
| 52 | 2 | 1675 | A |
| 52 | 2 | 1686 | U |
| 52 | 2 | 1687 | C |
| 52 | 2 | 1700 | U |
| 52 | 2 | 1701 | A |
| 52 | 2 | 1711 | A |
| 52 | 2 | 1712 | U |
| 52 | 2 | 1774 | A |
| 52 | 2 | 1776 | U |
| 52 | 2 | 1777 | C |
| 52 | 2 | 1783 | U |
| 52 | 2 | 1786 | G |
| 52 | 2 | 1790 | U |
| 52 | 2 | 1791 | U |
| 52 | 2 | 1792 | C |
| 52 | 2 | 1793 | C |
| 52 | 2 | 1795 | U |
| 52 | 2 | 1796 | U |
| 52 | 2 | 1797 | G |
| 52 | 2 | 1801 | U |
| 52 | 2 | 1802 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 1809 | G |
| 52 | 2 | 1812 | G |
| 52 | 2 | 1813 | A |
| 52 | 2 | 1814 | A |
| 52 | 2 | 1815 | A |
| 52 | 2 | 1816 | U |
| 52 | 2 | 1817 | U |
| 52 | 2 | 1818 | U |
| 52 | 2 | 1826 | C |
| 52 | 2 | 1828 | G |
| 52 | 2 | 1830 | A |
| 52 | 2 | 1831 | G |
| 52 | 2 | 1835 | U |
| 52 | 2 | 1836 | G |
| 52 | 2 | 1838 | G |
| 52 | 2 | 1839 | A |
| 52 | 2 | 1842 | C |
| 52 | 2 | 1844 | C |
| 52 | 2 | 1846 | U |
| 52 | 2 | 1847 | C |
| 52 | 2 | 1848 | A |
| 52 | 2 | 1849 | A |
| 52 | 2 | 1850 | U |
| 52 | 2 | 1851 | G |
| 52 | 2 | 1854 | C |
| 52 | 2 | 1855 | U |
| 52 | 2 | 1861 | A |
| 52 | 2 | 1862 | C |
| 52 | 2 | 1863 | A |
| 52 | 2 | 1864 | C |
| 52 | 2 | 1865 | G |
| 52 | 2 | 1866 | C |
| 52 | 2 | 1867 | G |
| 52 | 2 | 1874 | A |
| 52 | 2 | 1875 | A |
| 52 | 2 | 1876 | U |
| 52 | 2 | 1877 | G |
| 52 | 2 | 1878 | U |
| 52 | 2 | 1879 | C |
| 52 | 2 | 1880 | A |
| 52 | 2 | 1881 | G |
| 52 | 2 | 1882 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 1883 | G |
| 52 | 2 | 1884 | A |
| 52 | 2 | 1885 | G |
| 52 | 2 | 1887 | A |
| 52 | 2 | 1888 | C |
| 52 | 2 | 1890 | A |
| 52 | 2 | 1895 | A |
| 52 | 2 | 1896 | A |
| 52 | 2 | 1897 | C |
| 52 | 2 | 1898 | G |
| 52 | 2 | 1899 | A |
| 52 | 2 | 1908 | C |
| 52 | 2 | 1909 | C |
| 52 | 2 | 1912 | C |
| 52 | 2 | 1913 | U |
| 52 | 2 | 1914 | U |
| 52 | 2 | 1915 | G |
| 52 | 2 | 1916 | A |
| 52 | 2 | 1917 | U |
| 52 | 2 | 1918 | C |
| 52 | 2 | 1919 | A |
| 52 | 2 | 1920 | A |
| 52 | 2 | 1921 | A |
| 52 | 2 | 1929 | G |
| 52 | 2 | 1931 | A |
| 52 | 2 | 1932 | A |
| 52 | 2 | 1933 | A |
| 52 | 2 | 1934 | C |
| 52 | 2 | 1935 | C |
| 52 | 2 | 1936 | C |
| 52 | 2 | 1938 | G |
| 52 | 2 | 1942 | C |
| 52 | 2 | 1943 | A |
| 52 | 2 | 1944 | U |
| 52 | 2 | 1945 | A |
| 52 | 2 | 1946 | G |
| 52 | 2 | 1947 | A |
| 52 | 2 | 1948 | C |
| 52 | 2 | 1949 | U |
| 52 | 2 | 1950 | C |
| 52 | 2 | 1951 | A |
| 52 | 2 | 1952 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 1953 | U |
| 52 | 2 | 1954 | U |
| 52 | 2 | 1955 | G |
| 52 | 2 | 1957 | G |
| 52 | 2 | 1959 | C |
| 52 | 2 | 1962 | A |
| 52 | 2 | 1963 | G |
| 52 | 2 | 1968 | G |
| 52 | 2 | 1969 | C |
| 52 | 2 | 1971 | A |
| 52 | 2 | 1974 | A |
| 52 | 2 | 1976 | U |
| 52 | 2 | 1977 | G |
| 52 | 2 | 1978 | G |
| 52 | 2 | 1979 | U |
| 52 | 2 | 1980 | C |
| 52 | 2 | 1981 | G |
| 52 | 2 | 1982 | C |
| 52 | 2 | 1984 | C |
| 52 | 2 | 1985 | A |
| 52 | 2 | 1986 | A |
| 52 | 2 | 1988 | G |
| 52 | 2 | 1989 | A |
| 52 | 2 | 1990 | G |
| 52 | 2 | 1991 | G |
| 52 | 2 | 1997 | C |
| 52 | 2 | 1998 | U |
| 52 | 2 | 2000 | G |
| 52 | 2 | 2001 | U |
| 52 | 2 | 2007 | C |
| 52 | 2 | 2010 | C |
| 52 | 2 | 2011 | U |
| 52 | 2 | 2012 | C |
| 52 | 2 | 2013 | A |
| 52 | 2 | 2017 | A |
| 52 | 2 | 2018 | A |
| 52 | 2 | 2025 | C |
| 52 | 2 | 2028 | U |
| 52 | 2 | 2032 | G |
| 52 | 2 | 2035 | C |
| 52 | 2 | 2038 | G |
| 52 | 2 | 2042 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 2045 | G |
| 52 | 2 | 2047 | A |
| 52 | 2 | 2048 | C |
| 52 | 2 | 2049 | A |
| 52 | 2 | 2050 | C |
| 52 | 2 | 2051 | A |
| 52 | 2 | 2053 | C |
| 52 | 2 | 2054 | G |
| 52 | 2 | 2067 | U |
| 52 | 2 | 2074 | A |
| 52 | 2 | 2093 | C |
| 52 | 2 | 2095 | G |
| 52 | 2 | 2096 | A |
| 52 | 2 | 2098 | A |
| 52 | 2 | 2133 | G |
| 52 | 2 | 2158 | A |
| 52 | 2 | 2159 | A |
| 52 | 2 | 2160 | G |
| 52 | 2 | 2163 | G |
| 52 | 2 | 2164 | U |
| 52 | 2 | 2165 | A |
| 52 | 2 | 2169 | A |
| 52 | 2 | 2171 | G |
| 52 | 2 | 2172 | U |
| 52 | 2 | 2183 | G |
| 52 | 2 | 2185 | A |
| 52 | 2 | 2186 | C |
| 52 | 2 | 2195 | G |
| 52 | 2 | 2196 | G |
| 52 | 2 | 2197 | A |
| 52 | 2 | 2199 | C |
| 52 | 2 | 2202 | U |
| 52 | 2 | 2203 | U |

All (173) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1010 | C |
| 2 | B | 78 | C |
| 2 | B | 946 | U |
| 2 | B | 1173 | A |
| 2 | B | 1385 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 1390 | A |
| 2 | B | 1391 | U |
| 2 | B | 1450 | U |
| 3 | C | 174 | A |
| 6 | F | 72 | A |
| 7 | G | 143 | C |
| 52 | 2 | 42 | G |
| 52 | 2 | 44 | C |
| 52 | 2 | 46 | U |
| 52 | 2 | 47 | A |
| 52 | 2 | 56 | U |
| 52 | 2 | 65 | A |
| 52 | 2 | 68 | A |
| 52 | 2 | 74 | U |
| 52 | 2 | 78 | C |
| 52 | 2 | 83 | A |
| 52 | 2 | 91 | A |
| 52 | 2 | 112 | A |
| 52 | 2 | 114 | U |
| 52 | 2 | 125 | A |
| 52 | 2 | 128 | C |
| 52 | 2 | 144 | A |
| 52 | 2 | 146 | U |
| 52 | 2 | 182 | A |
| 52 | 2 | 194 | U |
| 52 | 2 | 196 | C |
| 52 | 2 | 198 | C |
| 52 | 2 | 226 | G |
| 52 | 2 | 250 | C |
| 52 | 2 | 251 | A |
| 52 | 2 | 252 | G |
| 52 | 2 | 253 | U |
| 52 | 2 | 254 | A |
| 52 | 2 | 256 | A |
| 52 | 2 | 257 | A |
| 52 | 2 | 268 | C |
| 52 | 2 | 270 | C |
| 52 | 2 | 274 | C |
| 52 | 2 | 276 | G |
| 52 | 2 | 277 | U |
| 52 | 2 | 287 | C |
| 52 | 2 | 289 | G |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 290 | U |
| 52 | 2 | 297 | U |
| 52 | 2 | 325 | G |
| 52 | 2 | 348 | A |
| 52 | 2 | 363 | G |
| 52 | 2 | 364 | G |
| 52 | 2 | 366 | G |
| 52 | 2 | 402 | A |
| 52 | 2 | 460 | C |
| 52 | 2 | 554 | U |
| 52 | 2 | 564 | A |
| 52 | 2 | 579 | C |
| 52 | 2 | 580 | A |
| 52 | 2 | 581 | A |
| 52 | 2 | 586 | G |
| 52 | 2 | 591 | A |
| 52 | 2 | 604 | A |
| 52 | 2 | 709 | C |
| 52 | 2 | 716 | U |
| 52 | 2 | 724 | A |
| 52 | 2 | 726 | G |
| 52 | 2 | 761 | A |
| 52 | 2 | 762 | A |
| 52 | 2 | 767 | C |
| 52 | 2 | 770 | A |
| 52 | 2 | 772 | A |
| 52 | 2 | 780 | A |
| 52 | 2 | 783 | A |
| 52 | 2 | 787 | G |
| 52 | 2 | 790 | U |
| 52 | 2 | 880 | U |
| 52 | 2 | 885 | C |
| 52 | 2 | 886 | U |
| 52 | 2 | 887 | U |
| 52 | 2 | 913 | G |
| 52 | 2 | 914 | G |
| 52 | 2 | 915 | A |
| 52 | 2 | 917 | C |
| 52 | 2 | 918 | A |
| 52 | 2 | 930 | A |
| 52 | 2 | 935 | U |
| 52 | 2 | 937 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 963 | U |
| 52 | 2 | 970 | U |
| 52 | 2 | 1092 | A |
| 52 | 2 | 1098 | U |
| 52 | 2 | 1100 | U |
| 52 | 2 | 1103 | G |
| 52 | 2 | 1104 | A |
| 52 | 2 | 1106 | U |
| 52 | 2 | 1165 | G |
| 52 | 2 | 1271 | C |
| 52 | 2 | 1378 | U |
| 52 | 2 | 1443 | U |
| 52 | 2 | 1445 | U |
| 52 | 2 | 1516 | A |
| 52 | 2 | 1517 | A |
| 52 | 2 | 1521 | G |
| 52 | 2 | 1529 | U |
| 52 | 2 | 1536 | U |
| 52 | 2 | 1539 | U |
| 52 | 2 | 1547 | A |
| 52 | 2 | 1550 | A |
| 52 | 2 | 1553 | G |
| 52 | 2 | 1554 | G |
| 52 | 2 | 1555 | G |
| 52 | 2 | 1556 | A |
| 52 | 2 | 1572 | G |
| 52 | 2 | 1575 | A |
| 52 | 2 | 1576 | G |
| 52 | 2 | 1577 | G |
| 52 | 2 | 1580 | G |
| 52 | 2 | 1581 | A |
| 52 | 2 | 1606 | C |
| 52 | 2 | 1611 | U |
| 52 | 2 | 1623 | U |
| 52 | 2 | 1627 | G |
| 52 | 2 | 1628 | C |
| 52 | 2 | 1639 | U |
| 52 | 2 | 1699 | G |
| 52 | 2 | 1700 | U |
| 52 | 2 | 1789 | A |
| 52 | 2 | 1791 | U |
| 52 | 2 | 1792 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 2 | 1813 | A |
| 52 | 2 | 1816 | U |
| 52 | 2 | 1817 | U |
| 52 | 2 | 1829 | C |
| 52 | 2 | 1830 | A |
| 52 | 2 | 1835 | U |
| 52 | 2 | 1837 | U |
| 52 | 2 | 1841 | G |
| 52 | 2 | 1846 | U |
| 52 | 2 | 1849 | A |
| 52 | 2 | 1854 | C |
| 52 | 2 | 1861 | A |
| 52 | 2 | 1882 | U |
| 52 | 2 | 1889 | A |
| 52 | 2 | 1896 | A |
| 52 | 2 | 1897 | C |
| 52 | 2 | 1898 | G |
| 52 | 2 | 1917 | U |
| 52 | 2 | 1928 | G |
| 52 | 2 | 1930 | G |
| 52 | 2 | 1931 | A |
| 52 | 2 | 1937 | C |
| 52 | 2 | 1950 | C |
| 52 | 2 | 1952 | C |
| 52 | 2 | 1968 | G |
| 52 | 2 | 1981 | G |
| 52 | 2 | 1996 | U |
| 52 | 2 | 1997 | C |
| 52 | 2 | 2000 | G |
| 52 | 2 | 2006 | G |
| 52 | 2 | 2009 | G |
| 52 | 2 | 2011 | U |
| 52 | 2 | 2012 | C |
| 52 | 2 | 2024 | C |
| 52 | 2 | 2034 | C |
| 52 | 2 | 2046 | U |
| 52 | 2 | 2047 | A |
| 52 | 2 | 2050 | C |
| 52 | 2 | 2052 | C |
| 52 | 2 | 2053 | C |
| 52 | 2 | 2095 | G |
| 52 | 2 | 2164 | U |

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 52 | 2 | 2 |
| 77 | AW | 2 |
| 38 | l | 1 |
| 15 | O | 1 |
| 29 | c | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | 2 | 1972:U | O3' | 1973:U | P | 6.52 |
| 1 | 2 | 1954:U | O3' | 1955:G | P | 2.07 |
| 1 | AW | 79:GLY | C | 80:TYR | N | 1.68 |
| 1 | l | 66:TYR | C | 67:LEU | N | 1.18 |
| 1 | O | 50:MET | C | 51:LEU | N | 1.15 |
| 1 | c | 246:ILE | C | 247:ARG | N | 1.01 |
| 1 | AW | 80:TYR | C | 81:ARG | N | 0.87 |

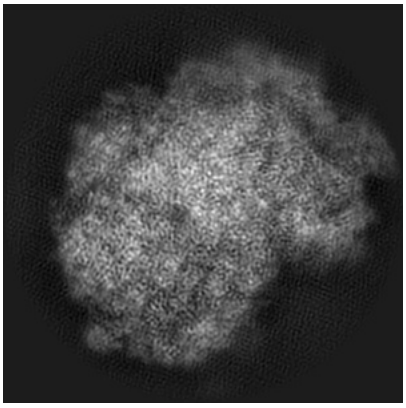
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8343. These allow visual inspection of the internal detail of the map and identification of artifacts.

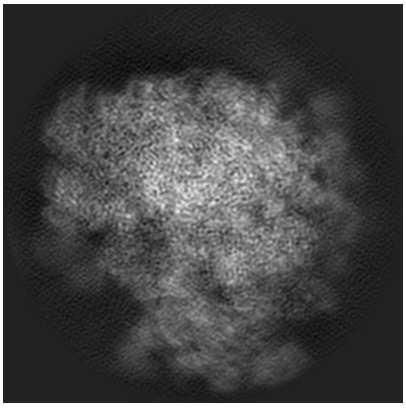
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

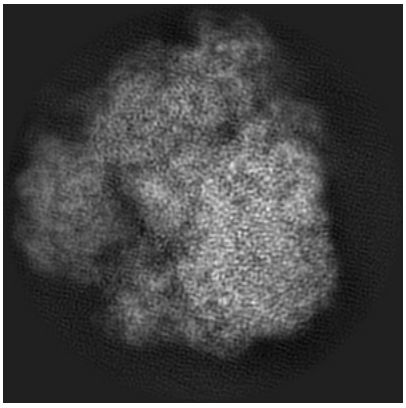
### 6.1.1 Primary map



X



Y

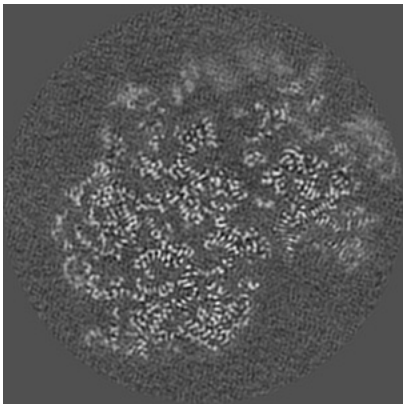


Z

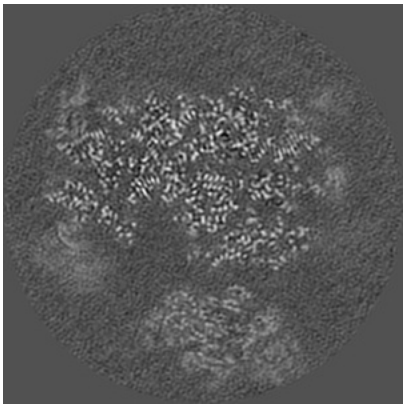
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

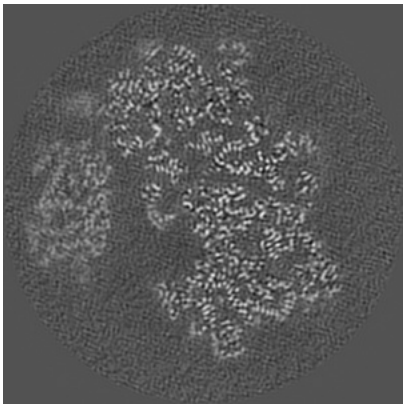
### 6.2.1 Primary map



X Index: 200



Y Index: 200

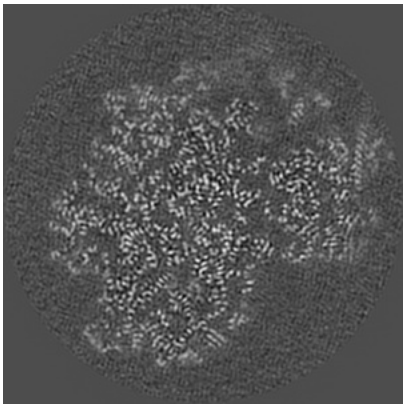


Z Index: 200

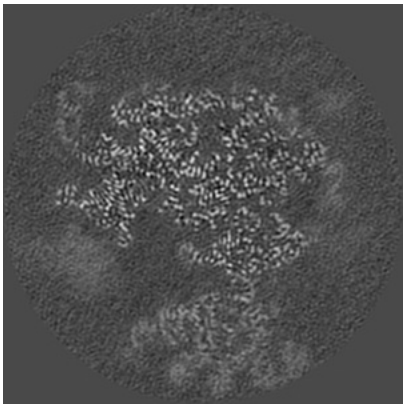
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

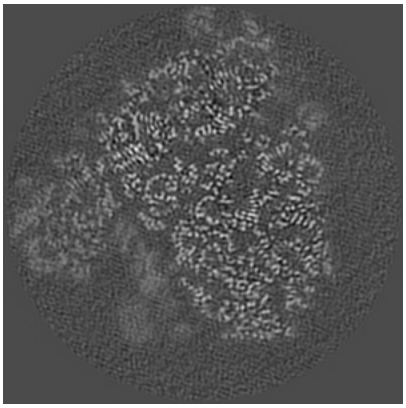
### 6.3.1 Primary map



X Index: 214



Y Index: 211

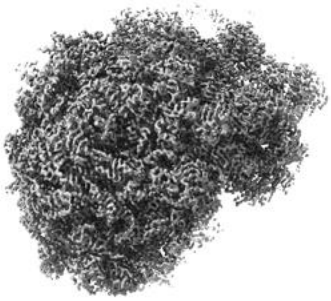


Z Index: 231

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

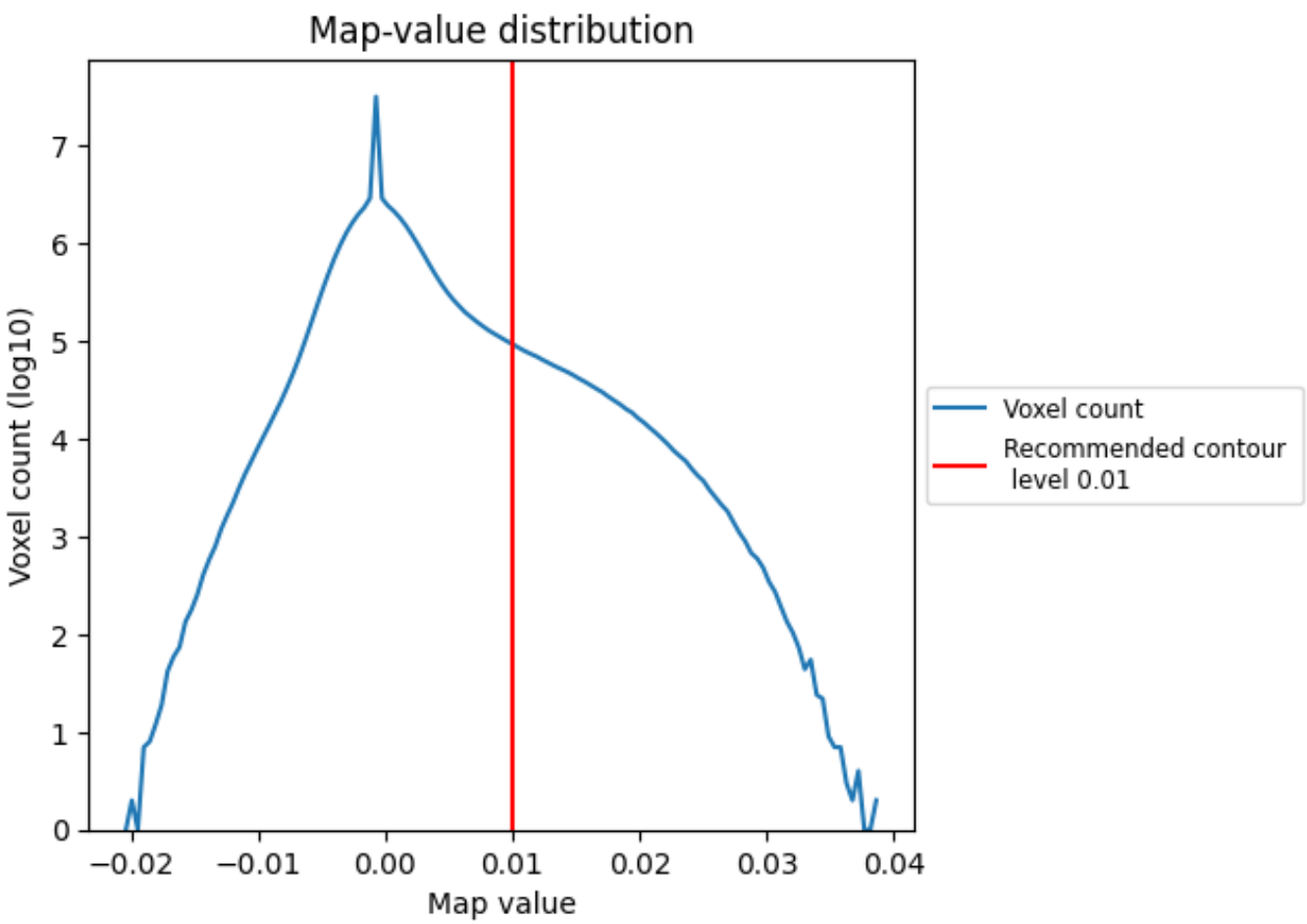
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

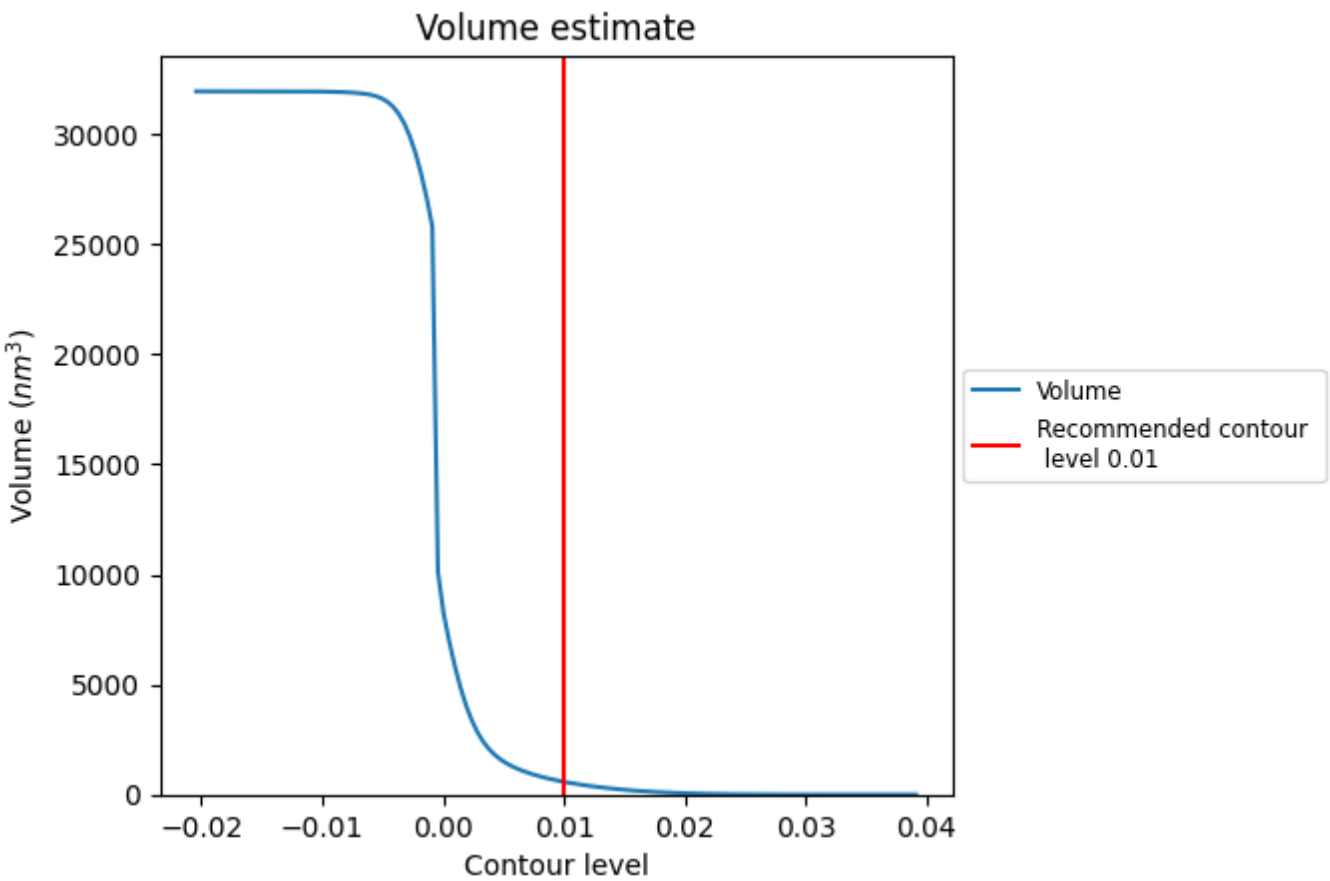
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

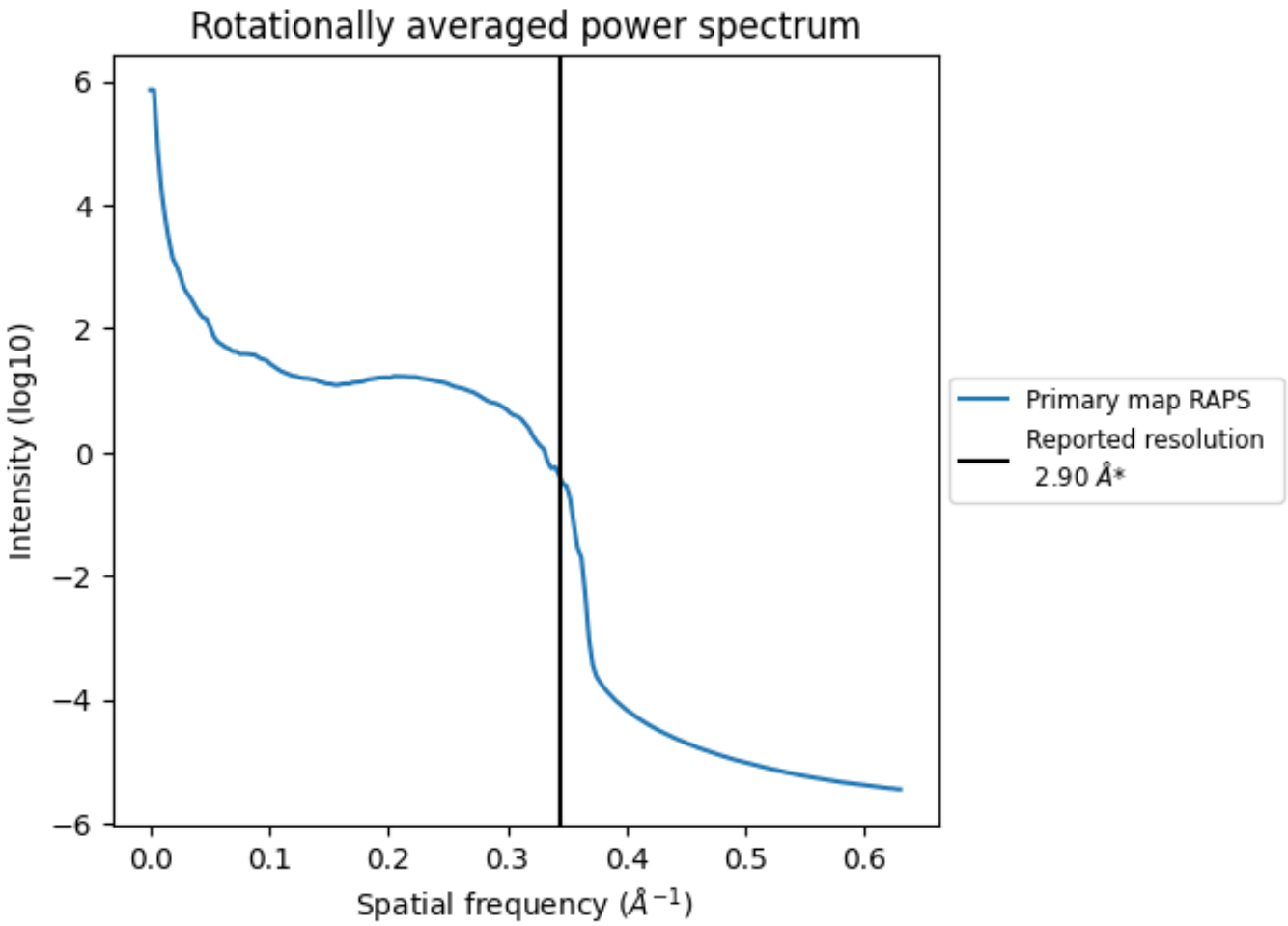
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 580 $nm^3$; this corresponds to an approximate mass of 524 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 0.345 Å$^{-1}$

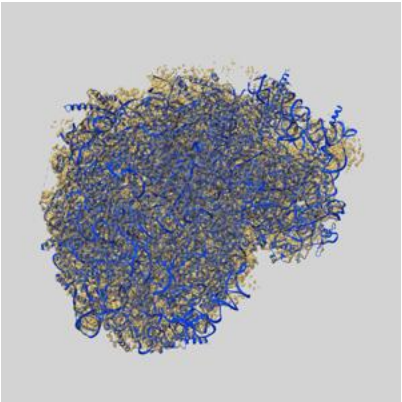
# 8 Fourier-Shell correlation (i)

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

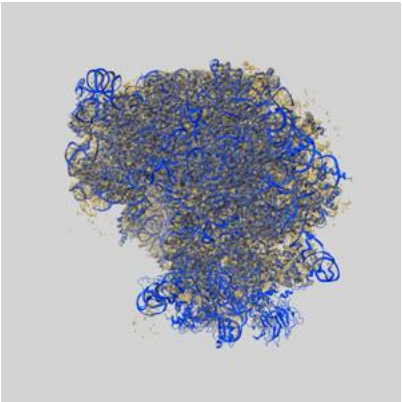
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8343 and PDB model 5T2A. Per-residue inclusion information can be found in section 3 on page 19.

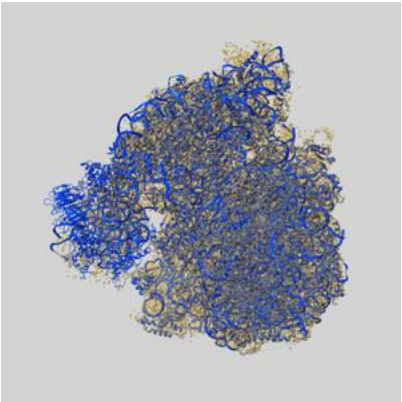
## 9.1 Map-model overlay (i)



X



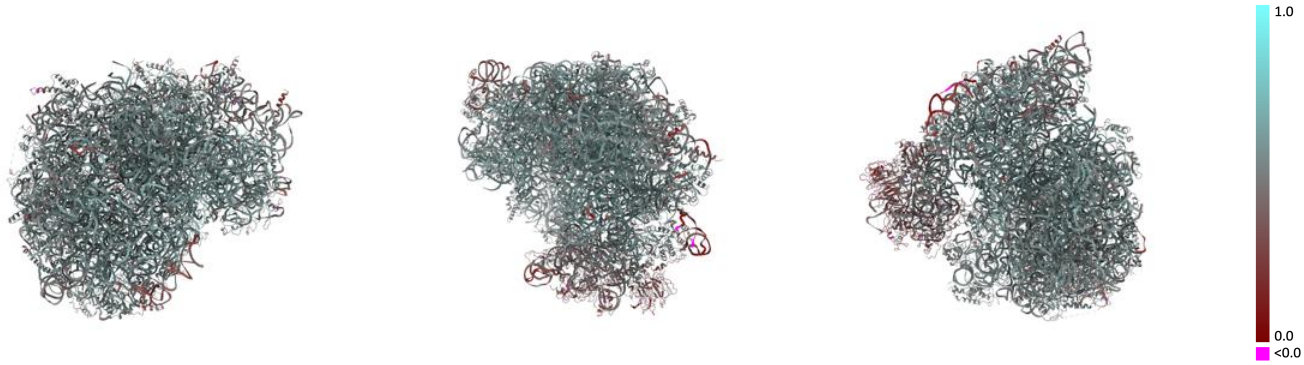
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

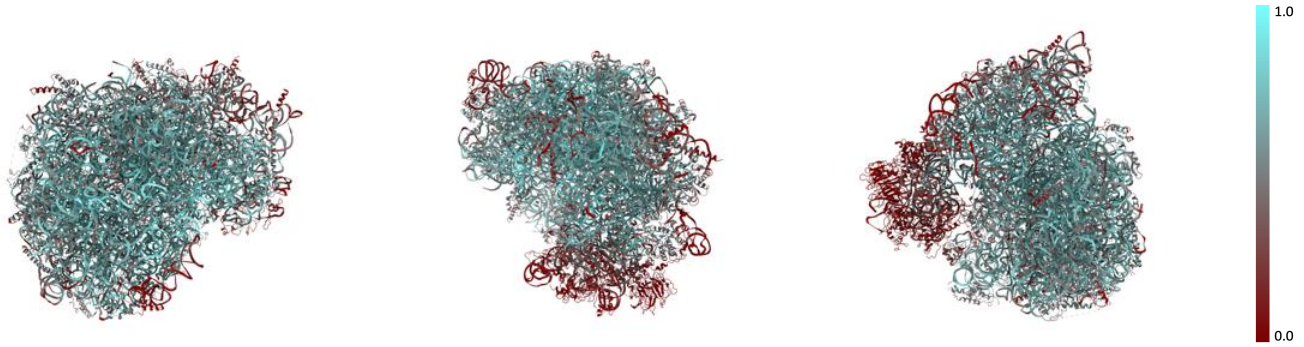
## 9.2 Q-score mapped to coordinate model (i)




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.

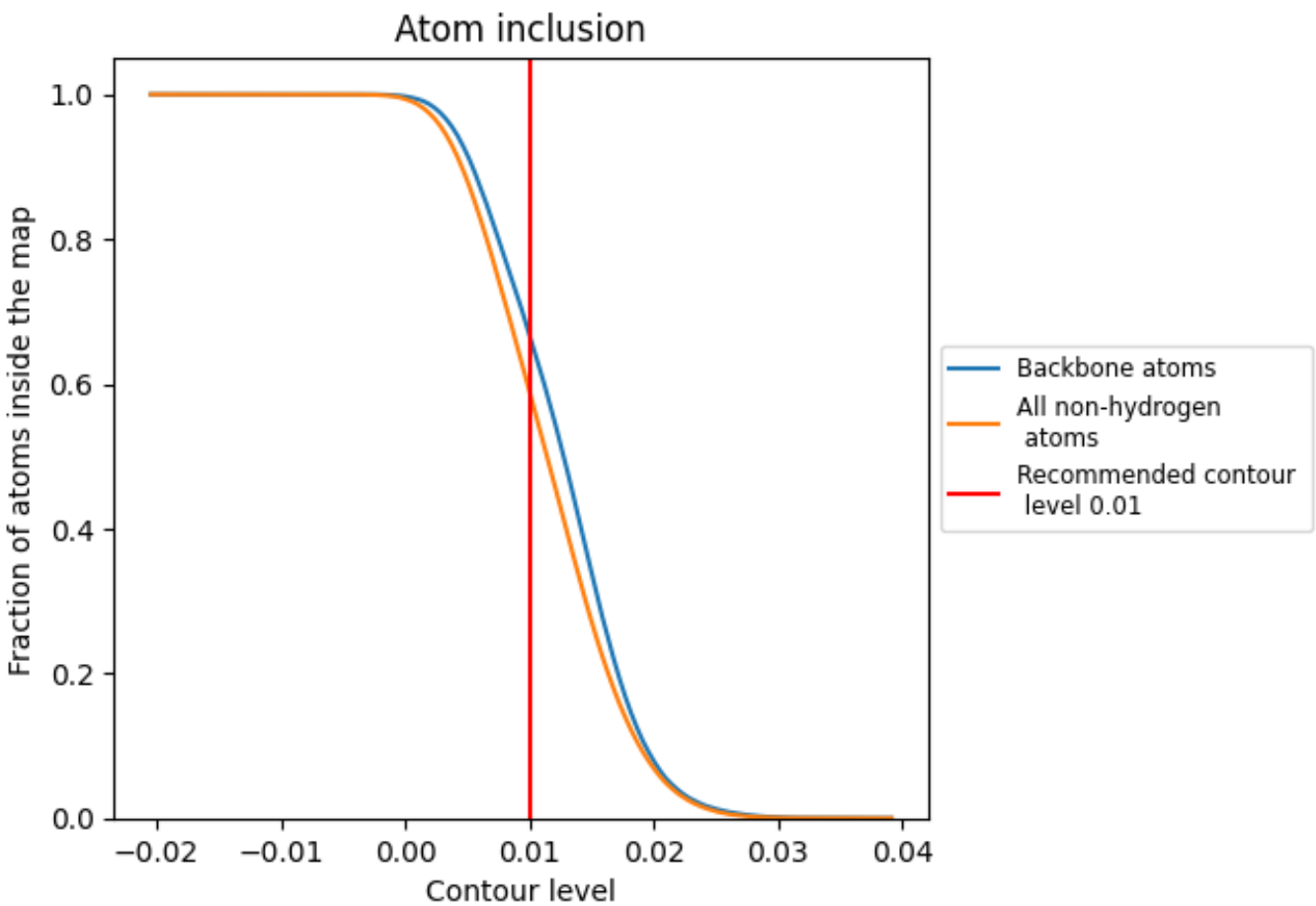
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.01).

## 9.4 Atom inclusion (i)




At the recommended contour level, 67% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5906 | 0.5270 |
| 0 | 0.4870 | 0.5380 |
| 1 | 0.5749 | 0.5500 |
| 2 | 0.5652 | 0.5170 |
| 3 | 0.3751 | 0.4970 |
| 4 | 0.4882 | 0.5230 |
| 5 | 0.6080 | 0.5580 |
| 6 | 0.5709 | 0.5410 |
| 7 | 0.0120 | 0.3000 |
| 8 | 0.1848 | 0.4210 |
| A | 0.7310 | 0.5530 |
| AC | 0.4354 | 0.5100 |
| AD | 0.0417 | 0.3510 |
| AE | 0.6514 | 0.5800 |
| AG | 0.6002 | 0.5550 |
| AH | 0.5066 | 0.5350 |
| AI | 0.0251 | 0.3360 |
| AJ | 0.6247 | 0.5560 |
| AK | 0.0971 | 0.3800 |
| AL | 0.1209 | 0.4060 |
| AM | 0.0602 | 0.2810 |
| AN | 0.0663 | 0.4100 |
| AO | 0.0933 | 0.3020 |
| AP | 0.5462 | 0.5370 |
| AQ | 0.0953 | 0.3610 |
| AR | 0.5048 | 0.5220 |
| AS | 0.5747 | 0.5450 |
| AT | 0.3946 | 0.5170 |
| AV | 0.4817 | 0.5210 |
| AW | 0.5064 | 0.5350 |
| AX | 0.1402 | 0.4060 |
| AY | 0.2779 | 0.4900 |
| AZ | 0.0828 | 0.3970 |
| B | 0.7220 | 0.5550 |
| C | 0.6959 | 0.5260 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| D | 0.7294 | 0.5450 |
| E | 0.7225 | 0.5630 |
| F | 0.6247 | 0.5290 |
| G | 0.8077 | 0.5870 |
| H | 0.8136 | 0.5920 |
| I | 0.5681 | 0.5280 |
| J | 0.5369 | 0.5240 |
| K | 0.3566 | 0.4740 |
| L | 0.5427 | 0.5060 |
| M | 0.5964 | 0.5520 |
| N | 0.4571 | 0.4860 |
| O | 0.6253 | 0.5490 |
| P | 0.6678 | 0.5560 |
| Q | 0.6303 | 0.5640 |
| R | 0.5434 | 0.5340 |
| S | 0.5566 | 0.5280 |
| T | 0.4897 | 0.5240 |
| U | 0.6660 | 0.5740 |
| V | 0.5545 | 0.5270 |
| W | 0.6660 | 0.5680 |
| X | 0.5785 | 0.5310 |
| Y | 0.5476 | 0.5340 |
| Z | 0.6171 | 0.5510 |
| a | 0.5314 | 0.5130 |
| b | 0.5605 | 0.5210 |
| c | 0.6439 | 0.5610 |
| d | 0.6572 | 0.5620 |
| e | 0.5467 | 0.5370 |
| f | 0.6414 | 0.5550 |
| g | 0.5905 | 0.5430 |
| h | 0.5864 | 0.5450 |
| i | 0.5084 | 0.5100 |
| j | 0.6245 | 0.5510 |
| k | 0.4423 | 0.4950 |
| l | 0.6751 | 0.5540 |
| m | 0.6111 | 0.5560 |
| n | 0.5212 | 0.5150 |
| o | 0.6098 | 0.5530 |
| p | 0.5512 | 0.5170 |
| q | 0.6348 | 0.5550 |
| r | 0.5507 | 0.5370 |
| s | 0.4956 | 0.5110 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| t | 0.5391 | 0.5230 |
| u | 0.5777 | 0.5330 |
| v | 0.4810 | 0.5010 |
| w | 0.6073 | 0.5500 |