# Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 04:20 PM EST

| | | |
|---|---|---|
| PDB ID | : | 6D9J |
| EMDB ID | : | EMD-7836 |
| Title | : | Mammalian 80S ribosome with a double translocated CrPV-IRES, P-sitetRNA and eRF1. |
| Authors | : | Pisareva, V.P.; Pisarev, A.V.; Fernandez, I.S. |
| Deposited on | : | 2018-04-30 |
| Resolution | : | 3.20 Å(reported) |

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

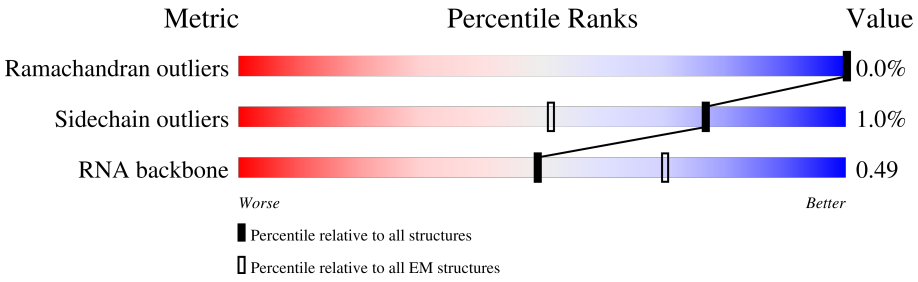
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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 | 257 | 91% · 7% |
| 2 | B | 403 | 97% ·· |
| 3 | C | 392 | 90% · 8% |
| 4 | D | 297 | 98% ·· |
| 5 | E | 291 | 74% · 26% |
| 6 | F | 249 | 90% 10% |
| 7 | G | 242 | 95% ·· |
| 8 | H | 192 | 96% ·· |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | I | 214 | 95% |
| 10 | J | 178 | 95% |
| 11 | L | 211 | 99% |
| 12 | M | 198 | 69% 31% |
| 13 | N | 204 | 100% |
| 14 | O | 198 | 98% |
| 15 | P | 187 | 81% 18% |
| 16 | Q | 187 | 99% |
| 17 | R | 181 | 98% |
| 18 | S | 176 | 100% |
| 19 | T | 160 | 98% |
| 20 | U | 99 | 100% |
| 21 | V | 140 | 91% 8% |
| 22 | W | 157 | 68% 32% |
| 23 | X | 156 | 76% 24% |
| 24 | Y | 145 | 92% 8% |
| 25 | Z | 136 | 99% |
| 26 | a | 148 | 98% |
| 27 | b | 226 | 45% 54% |
| 28 | c | 115 | 85% 15% |
| 29 | d | 125 | 84% 14% |
| 30 | e | 135 | 95% 5% |
| 31 | f | 110 | 96% |
| 32 | g | 126 | 90% 10% |
| 33 | h | 123 | 99% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | i | 105 | 96% |
| 35 | j | 97 | 88% 11% |
| 36 | k | 69 | 100% |
| 37 | l | 51 | 94% |
| 38 | m | 52 | 8% 98% |
| 39 | n | 25 | 100% |
| 40 | o | 106 | 95% |
| 41 | p | 92 | 99% |
| 42 | r | 137 | 90% 9% |
| 43 | s | 303 | 7% 64% 35% |
| 44 | t | 195 | 21% 78% 22% |
| 45 | 5 | 3594 | 72% 26% |
| 46 | 7 | 119 | 84% 16% |
| 47 | 8 | 151 | 72% 27% |
| 48 | K | 217 | 35% 96% |
| 49 | 2 | 1697 | 72% 26% |
| 50 | BB | 217 | 8% 98% |
| 51 | CC | 264 | 79% 19% |
| 52 | DD | 221 | 100% |
| 53 | EE | 281 | 7% 79% 19% |
| 54 | FF | 262 | 100% |
| 55 | GG | 204 | 90% 9% |
| 56 | HH | 249 | 95% 5% |
| 57 | II | 194 | 7% 95% 5% |
| 58 | JJ | 206 | 100% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 59 | KK | 194 | 94% 5% |
| 60 | LL | 149 | 5% 64% 36% |
| 61 | MM | 158 | 7% 89% 9% |
| 62 | NN | 132 | 52% 88% 11% |
| 63 | OO | 151 | 97% |
| 64 | PP | 151 | 6% 90% 10% |
| 65 | QQ | 145 | 6% 79% 21% |
| 66 | RR | 172 | 82% 17% |
| 67 | SS | 135 | 24% 96% |
| 68 | TT | 152 | 12% 93% 5% |
| 69 | UU | 145 | 97% |
| 70 | VV | 119 | 8% 83% 16% |
| 71 | WW | 83 | 5% 98% |
| 72 | XX | 130 | 98% |
| 73 | YY | 143 | 97% |
| 74 | ZZ | 134 | 91% 7% |
| 75 | aa | 125 | 6% 60% 40% |
| 76 | bb | 101 | 100% |
| 77 | cc | 84 | 6% 99% |
| 78 | dd | 69 | 13% 90% 10% |
| 79 | ee | 56 | 98% |
| 80 | ff | 133 | 41% 57% |
| 81 | gg | 156 | 19% 43% 56% |
| 82 | hh | 317 | 5% 98% |
| 83 | 3 | 87 | 7% 70% 30% |

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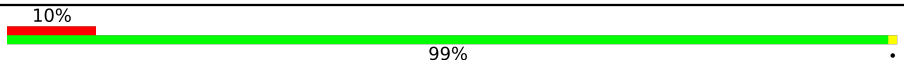
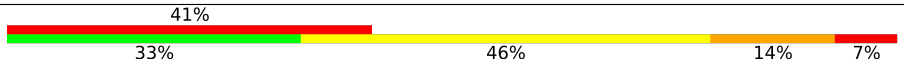
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 84 | 9 | 856 |   |
| 85 | 4 | 190 |   |

# 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 227188 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 239 | 1777 | 1110 | 361 | 300 | 6 | 0 | 0 |

- Molecule 2 is a protein called uL3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 394 | 3172 | 2020 | 597 | 542 | 13 | 0 | 0 |

- Molecule 3 is a protein called uL4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 362 | 2883 | 1812 | 577 | 480 | 14 | 0 | 0 |

- Molecule 4 is a protein called uL18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | D | 293 | 2391 | 1512 | 438 | 427 | 14 | 0 | 0 |

- Molecule 5 is a protein called eL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | E | 216 | 1729 | 1115 | 329 | 282 | 3 | 0 | 0 |

- Molecule 6 is a protein called uL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | F | 225 | 1875 | 1205 | 358 | 303 | 9 | 0 | 0 |

- Molecule 7 is a protein called eL8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 233 | Total | C | N | O | S | 0 | 0 |
| | | | 1879 | 1199 | 361 | 315 | 4 | | |

- Molecule 8 is a protein called uL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1516 | 954 | 284 | 272 | 6 | | |

- Molecule 9 is a protein called uL16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1664 | 1056 | 321 | 274 | 13 | | |

- Molecule 10 is a protein called uL11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 170 | Total | C | N | O | S | 0 | 0 |
| | | | 1362 | 861 | 254 | 241 | 6 | | |

- Molecule 11 is a protein called eL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | L | 210 | Total | C | N | O | S | 0 | 0 |
| | | | 1702 | 1065 | 354 | 279 | 4 | | |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| L | 46 | ILE | - | insertion | UNP G1TPV0 |
| L | 47 | ALA | - | insertion | UNP G1TPV0 |
| L | 48 | PRO | - | insertion | UNP G1TPV0 |
| L | 49 | ARG | - | insertion | UNP G1TPV0 |
| L | 50 | PRO | - | insertion | UNP G1TPV0 |
| L | 51 | ALA | - | insertion | UNP G1TPV0 |
| L | 52 | ALA | - | insertion | UNP G1TPV0 |
| L | 53 | GLY | - | insertion | UNP G1TPV0 |
| L | 54 | PRO | - | insertion | UNP G1TPV0 |

- Molecule 12 is a protein called eL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | M | 137 | Total | C | N | O | S | 0 | 0 |
| | | | 1130 | 722 | 220 | 181 | 7 | | |

- Molecule 13 is a protein called eL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | N | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1701 | 1072 | 359 | 266 | 4 | | |

- Molecule 14 is a protein called uL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | O | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1623 | 1046 | 318 | 254 | 5 | | |

- Molecule 15 is a protein called uL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | P | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1242 | 777 | 241 | 215 | 9 | | |

- Molecule 16 is a protein called eL18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | Q | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1515 | 946 | 315 | 250 | 4 | | |

- Molecule 17 is a protein called eL19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | R | 180 | Total | C | N | O | S | 0 | 0 |
| | | | 1508 | 933 | 328 | 238 | 9 | | |

- Molecule 18 is a protein called eL20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | S | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1462 | 930 | 285 | 236 | 11 | | |

- Molecule 19 is a protein called eL21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | T | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1298 | 823 | 252 | 217 | 6 | | |

- Molecule 20 is a protein called eL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | U | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 809 | 519 | 141 | 147 | 2 | | |

- Molecule 21 is a protein called uL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | V | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 969 | 613 | 182 | 169 | 5 | | |

- Molecule 22 is a protein called eL24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | W | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 860 | 538 | 174 | 144 | 4 | | |

- Molecule 23 is a protein called eL23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | X | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 967 | 618 | 181 | 167 | 1 | | |

- Molecule 24 is a protein called uL24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | Y | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1115 | 700 | 226 | 186 | 3 | | |

- Molecule 25 is a protein called eL27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | Z | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1107 | 714 | 208 | 182 | 3 | | |

- Molecule 26 is a protein called uL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | a | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1162 | 734 | 239 | 185 | 4 | | |

- Molecule 27 is a protein called eL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | b | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 848 | 527 | 189 | 129 | 3 | | |

- Molecule 28 is a protein called eL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | c | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 761 | 481 | 134 | 140 | 6 | | |

- Molecule 29 is a protein called eL31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | d | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 888 | 560 | 171 | 155 | 2 | | |

- Molecule 30 is a protein called eL32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | e | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 667 | 216 | 165 | 5 | | |

- Molecule 31 is a protein called eL33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | f | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 876 | 555 | 174 | 143 | 4 | | |

- Molecule 32 is a protein called eL34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | g | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 906 | 566 | 187 | 147 | 6 | | |

- Molecule 33 is a protein called eL35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | h | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 1013 | 640 | 204 | 168 | 1 | | |

- Molecule 34 is a protein called eL36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | i | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 830 | 520 | 176 | 129 | 5 | | |

- Molecule 35 is a protein called eL37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | j | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 705 | 434 | 155 | 111 | 5 | | |

- Molecule 36 is a protein called eL38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | k | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 569 | 366 | 103 | 99 | 1 | | |

- Molecule 37 is a protein called eL39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | l | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 447 | 286 | 96 | 64 | 1 | | |

- Molecule 38 is a protein called eL40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | m | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 429 | 266 | 90 | 67 | 6 | | |

- Molecule 39 is a protein called eL41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | n | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 239 | 145 | 64 | 27 | 3 | | |

- Molecule 40 is a protein called eL42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | o | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 851 | 533 | 174 | 138 | 6 | | |

- Molecule 41 is a protein called eL43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | p | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 708 | 445 | 136 | 120 | 7 | | |

- Molecule 42 is a protein called eL28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | r | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 994 | 616 | 205 | 167 | 6 | | |

- Molecule 43 is a protein called uL10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | s | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1507 | 959 | 263 | 276 | 9 | | |

- Molecule 44 is a protein called uL11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | t | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1160 | 722 | 218 | 217 | 3 | | |

- Molecule 45 is a RNA chain called 28S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | 5 | 3594 | Total | C | N | O | P | 0 | 0 |
| | | | 77073 | 34324 | 14116 | 25039 | 3594 | | |

- Molecule 46 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | 7 | 119 | Total | C | N | O | P | 0 | 0 |
| | | | 2538 | 1132 | 454 | 834 | 118 | | |

- Molecule 47 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | 8 | 151 | Total | C | N | O | P | 0 | 0 |
| | | | 3208 | 1432 | 564 | 1062 | 150 | | |

- Molecule 48 is a protein called uL1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | K | 212 | Total | C | N | O | S | 0 | 0 |
| | | | 1705 | 1091 | 306 | 300 | 8 | | |

- Molecule 49 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | 2 | 1697 | Total | C | N | O | P | 0 | 0 |
| | | | 36229 | 16171 | 6507 | 11855 | 1696 | | |

- Molecule 50 is a protein called uS2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | BB | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1710 | 1086 | 300 | 316 | 8 | | |

- Molecule 51 is a protein called eS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | CC | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1729 | 1098 | 309 | 308 | 14 | | |

- Molecule 52 is a protein called uS5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | DD | 221 | Total | C | N | O | S | 0 | 0 |
| | | | 1716 | 1111 | 295 | 301 | 9 | | |

- Molecule 53 is a protein called uS3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | EE | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1768 | 1126 | 318 | 316 | 8 | | |

- Molecule 54 is a protein called eS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | FF | 262 | Total | C | N | O | S | 0 | 0 |
| | | | 2076 | 1324 | 386 | 358 | 8 | | |

- Molecule 55 is a protein called uS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | GG | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1471 | 921 | 277 | 266 | 7 | | |

- Molecule 56 is a protein called eS6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | HH | 237 | Total | C | N | O | S | 0 | 0 |
| | | | 1923 | 1200 | 387 | 329 | 7 | | |

- Molecule 57 is a protein called eS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | II | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1488 | 952 | 271 | 264 | 1 | | |

- Molecule 58 is a protein called eS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 58 | JJ | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1686 | 1058 | 332 | 291 | 5 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| JJ | 47 | ARG | GLY | conflict | UNP G1TJW1 |

- Molecule 59 is a protein called uS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 59 | KK | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1525 | 969 | 306 | 248 | 2 | | |

- Molecule 60 is a protein called eS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 60 | LL | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 810 | 530 | 143 | 131 | 6 | | |

- Molecule 61 is a protein called uS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | MM | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1175 | 749 | 222 | 198 | 6 | | |

- Molecule 62 is a protein called eS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | NN | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 908 | 570 | 161 | 169 | 8 | | |

- Molecule 63 is a protein called uS15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 63 | OO | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1202 | 770 | 228 | 203 | 1 | | |

- Molecule 64 is a protein called uS11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 64 | PP | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1016 | 621 | 199 | 190 | 6 | | |

- Molecule 65 is a protein called uS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 65 | QQ | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 956 | 610 | 176 | 163 | 7 | | |

- Molecule 66 is a protein called uS9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 66 | RR | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1128 | 717 | 213 | 195 | 3 | | |

- Molecule 67 is a protein called eS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 67 | SS | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1068 | 670 | 199 | 195 | 4 | | |

- Molecule 68 is a protein called uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 68 | TT | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1190 | 746 | 241 | 202 | 1 | | |

- Molecule 69 is a protein called eS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 69 | UU | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1097 | 688 | 211 | 195 | 3 | | |

- Molecule 70 is a protein called uS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 70 | VV | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 795 | 498 | 152 | 141 | 4 | | |

- Molecule 71 is a protein called eS21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | WW | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 636 | 393 | 117 | 121 | 5 | | |

- Molecule 72 is a protein called uS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | XX | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1034 | 659 | 193 | 176 | 6 | | |

- Molecule 73 is a protein called uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 73 | YY | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 693 | 219 | 183 | 3 | | |

- Molecule 74 is a protein called eS24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 74 | ZZ | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1011 | 640 | 198 | 168 | 5 | | |

- Molecule 75 is a protein called eS25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 75 | aa | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 598 | 382 | 111 | 104 | 1 | | |

- Molecule 76 is a protein called eS26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 76 | bb | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 507 | 170 | 132 | 5 | | |

- Molecule 77 is a protein called eS27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 77 | cc | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 651 | 408 | 121 | 115 | 7 | | |

- Molecule 78 is a protein called eS28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 78 | dd | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 488 | 297 | 97 | 92 | 2 | | |

- Molecule 79 is a protein called eS29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 79 | ee | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 459 | 286 | 94 | 74 | 5 | | |

- Molecule 80 is a protein called eS30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 80 | ff | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 457 | 282 | 101 | 73 | 1 | | |

- Molecule 81 is a protein called eS31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 81 | gg | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 555 | 351 | 103 | 94 | 7 | | |

- Molecule 82 is a protein called RACK1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 82 | hh | 313 | Total | C | N | O | S | 0 | 0 |
| | | | 2436 | 1535 | 424 | 465 | 12 | | |

- Molecule 83 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 83 | 3 | 87 | Total | C | N | O | P | 0 | 0 |
| | | | 1860 | 829 | 333 | 612 | 86 | | |

- Molecule 84 is a protein called eEF2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 84 | 9 | 856 | Total | C | N | O | S | 0 | 0 |
| | | | 6673 | 4234 | 1148 | 1247 | 44 | | |

- Molecule 85 is a RNA chain called CrPV IRES.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 85 | 4 | 190 | Total | C | N | O | P | 0 | 0 |
| | | | 4020 | 1802 | 689 | 1339 | 190 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 4 | 6217 | C | - | insertion | GB 8895506 |
| 4 | 6218 | U | - | insertion | GB 8895506 |
| 4 | 6219 | U | - | insertion | GB 8895506 |

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

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 86 | p | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 86 | 2 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 86 | bb | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

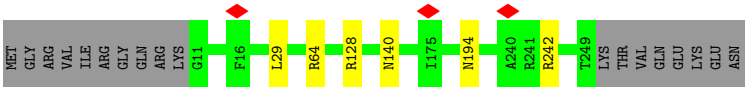
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 87 | 5 | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |

# 3 Residue-property plots (i)

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

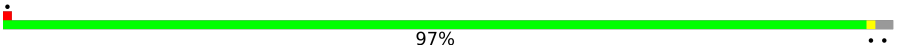
- Molecule 1: uL2

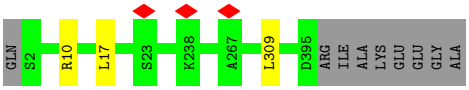
Chain A:


- Molecule 2: uL3

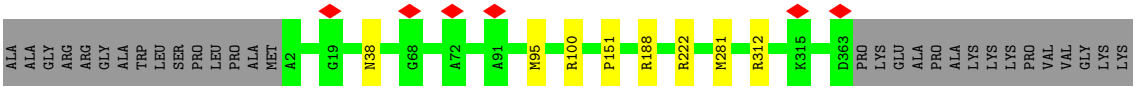
Chain B:



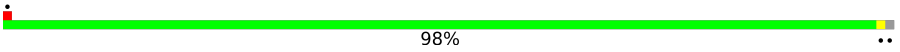

- Molecule 3: uL4

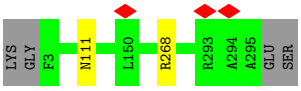
Chain C:


- Molecule 4: uL18

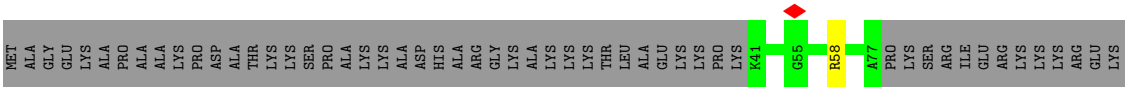
Chain D:

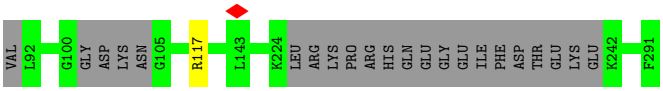



- Molecule 5: eL6

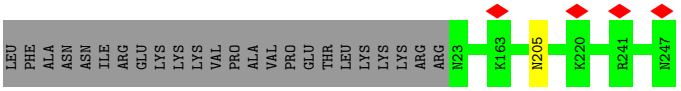
Chain E:



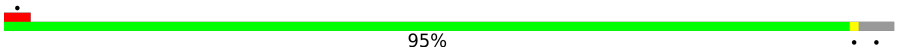

• Molecule 6: uL30

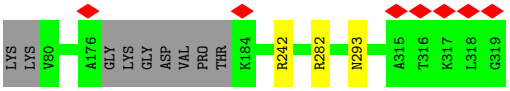
Chain F:


• Molecule 7: eL8

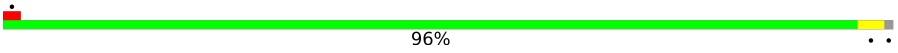
Chain G:

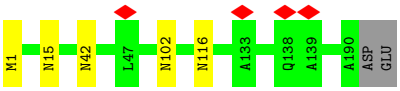



• Molecule 8: uL6

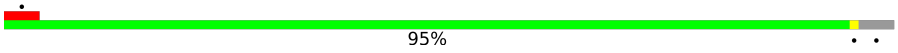
Chain H:

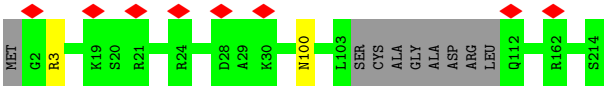



• Molecule 9: uL16

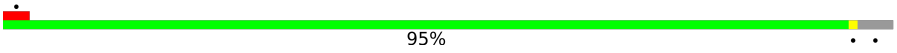
Chain I:

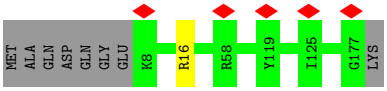



• Molecule 10: uL11

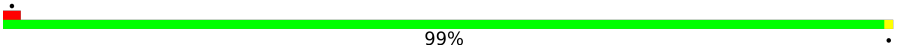
Chain J:

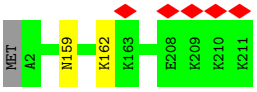



• Molecule 11: eL13

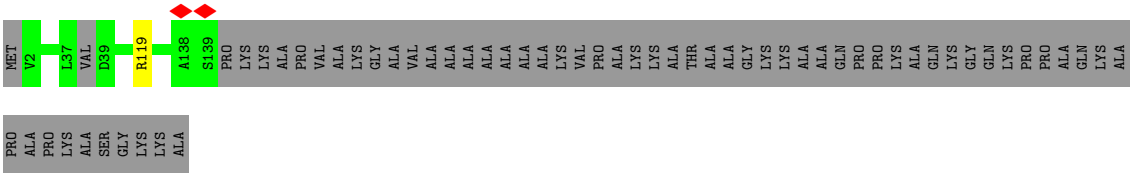
Chain L:



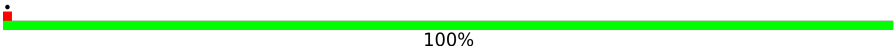

• Molecule 12: eL14

Chain M:


• Molecule 13: eL15

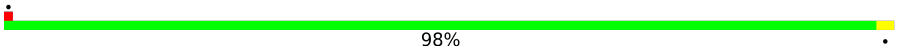
Chain N:

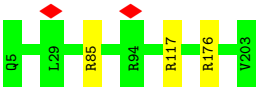




• Molecule 14: uL13

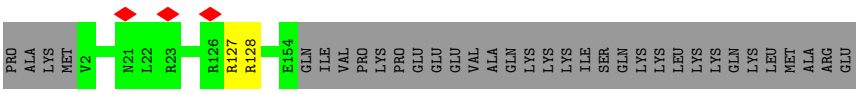
Chain O:



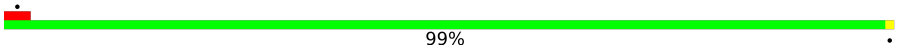

• Molecule 15: uL22

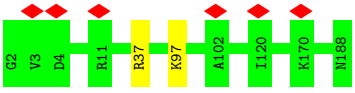
Chain P:


• Molecule 16: eL18

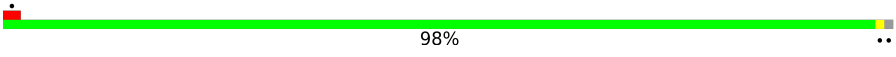
Chain Q:




• Molecule 17: eL19

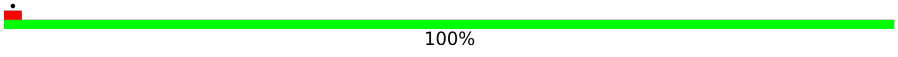
Chain R:

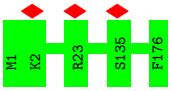




• Molecule 18: eL20

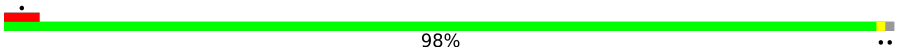
Chain S:

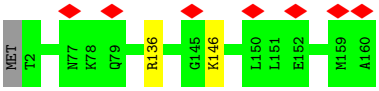





• Molecule 19: eL21

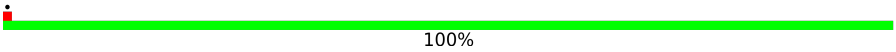
Chain T:




• Molecule 20: eL22

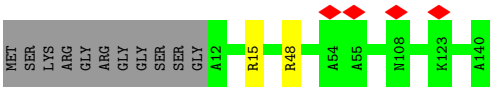
Chain U:





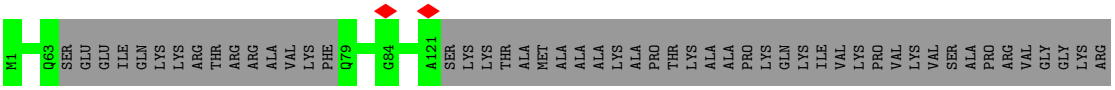
• Molecule 21: uL14

Chain V:

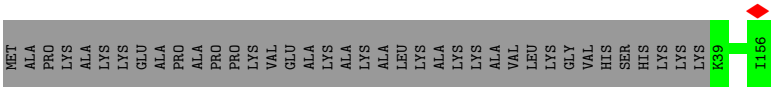

• Molecule 22: eL24

Chain W:

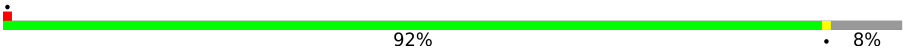

• Molecule 23: eL23

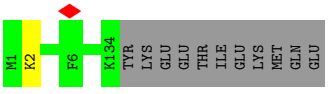
Chain X:


• Molecule 24: uL24

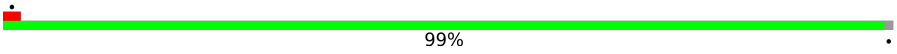
Chain Y:

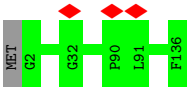



• Molecule 25: eL27

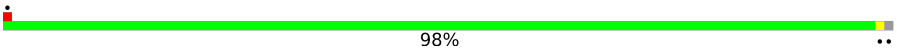
Chain Z:

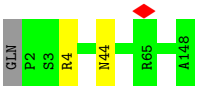



• Molecule 26: uL15

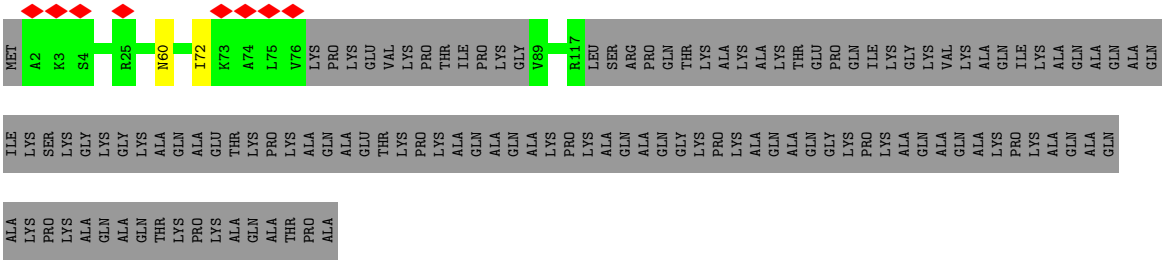
Chain a:



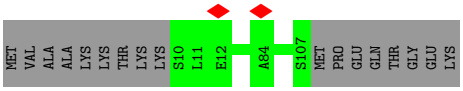

• Molecule 27: eL29

Chain b:

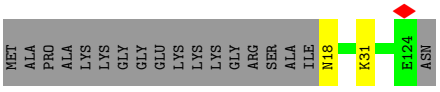

• Molecule 28: eL30

Chain c:

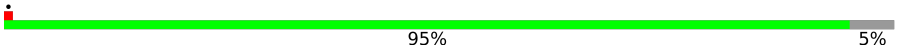

• Molecule 29: eL31

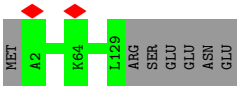
Chain d:


• Molecule 30: eL32

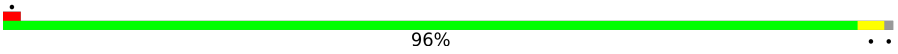
Chain e:

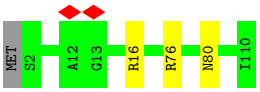



• Molecule 31: eL33

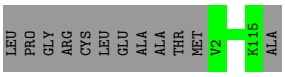
Chain f:



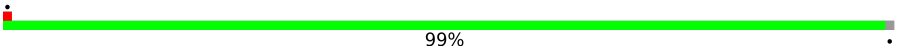

• Molecule 32: eL34

Chain g:


• Molecule 33: eL35

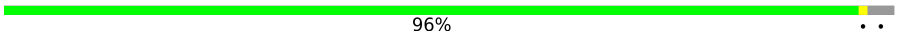
Chain h:

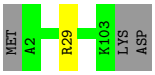




• Molecule 34: eL36

Chain i:



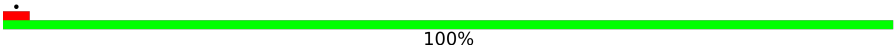

• Molecule 35: eL37

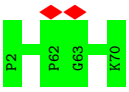
Chain j:



• Molecule 36: eL38

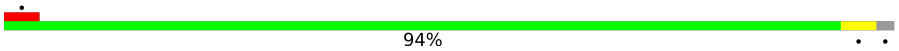
Chain k:

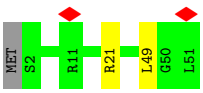



• Molecule 37: eL39

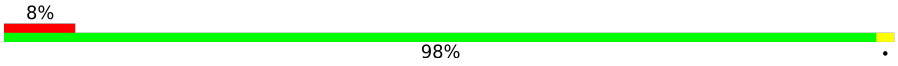
Chain l:

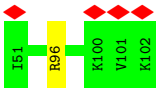



• Molecule 38: eL40

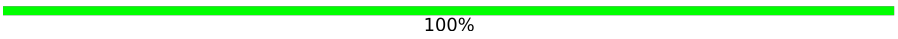
Chain m:




• Molecule 39: eL41

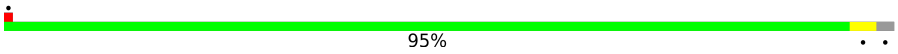
Chain n:

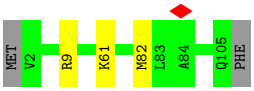



There are no outlier residues recorded for this chain.

• Molecule 40: eL42

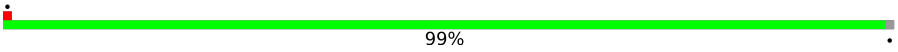
Chain o:




• Molecule 41: eL43

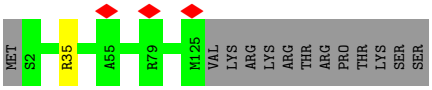
Chain p:





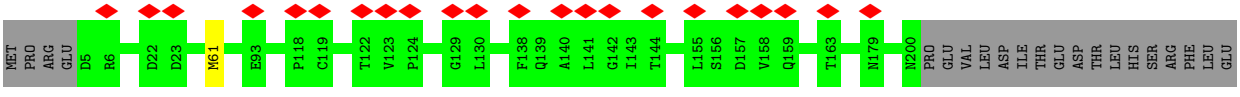
• Molecule 42: eL28

Chain r:


• Molecule 43: uL10

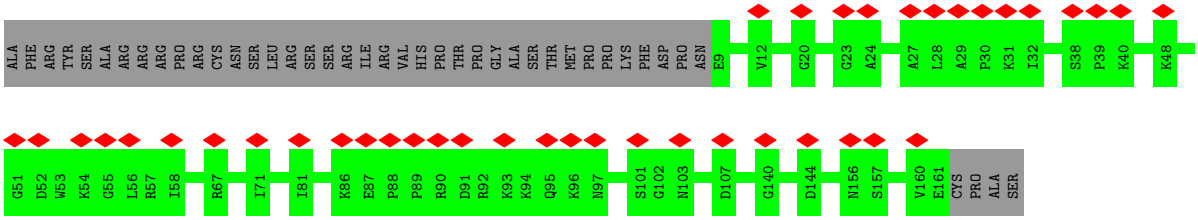
Chain s:



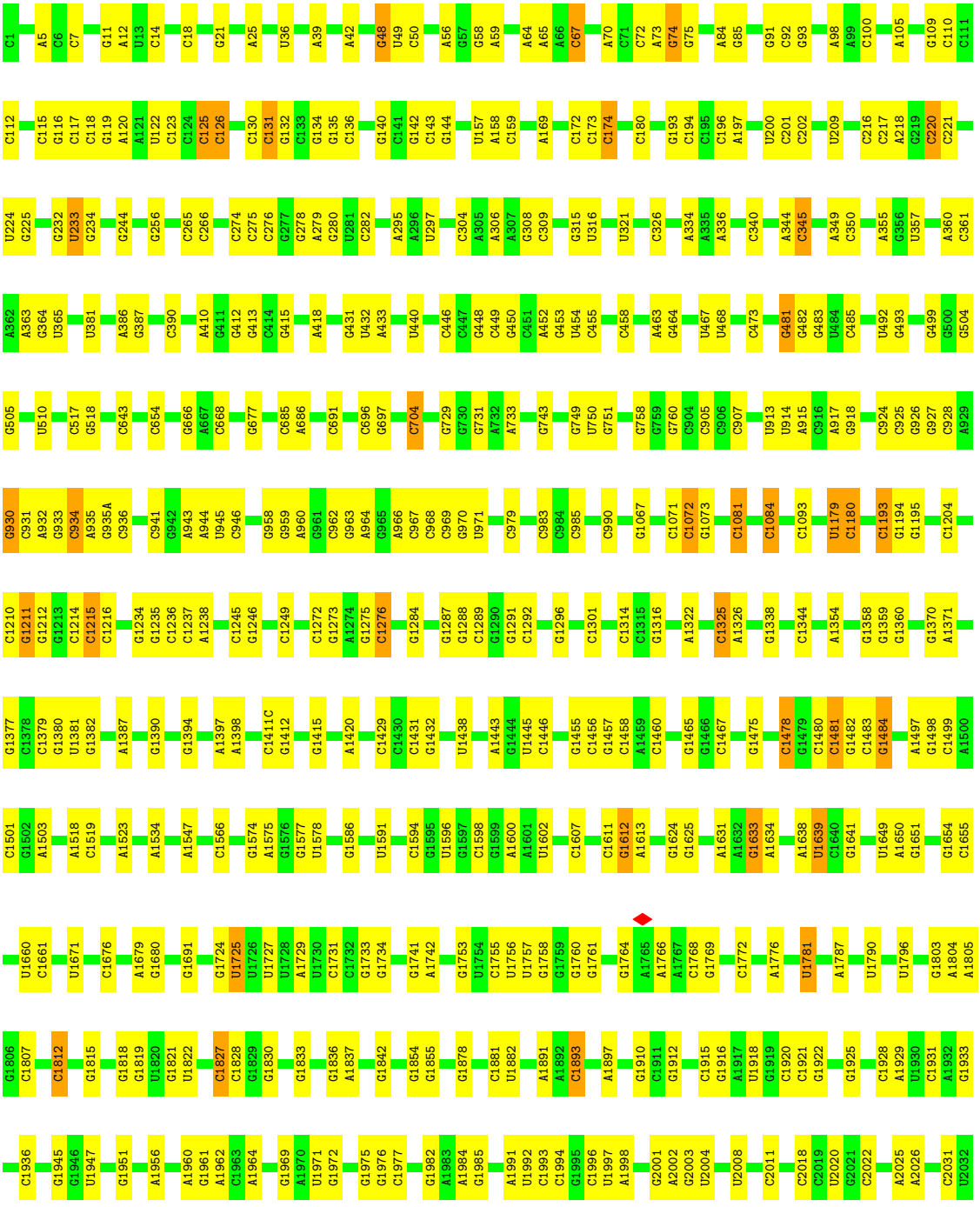

• Molecule 44: uL11

Chain t:



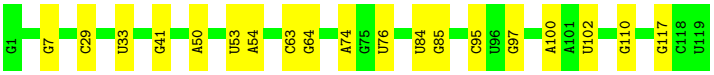

• Molecule 45: 28S rRNA

Chain 5: 72% 26%



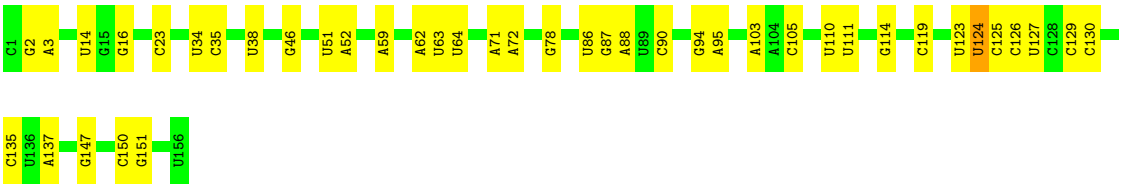
• Molecule 46: 5S rRNA

Chain 7:

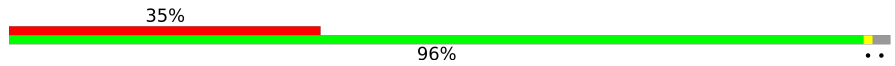

• Molecule 47: 5.8S rRNA

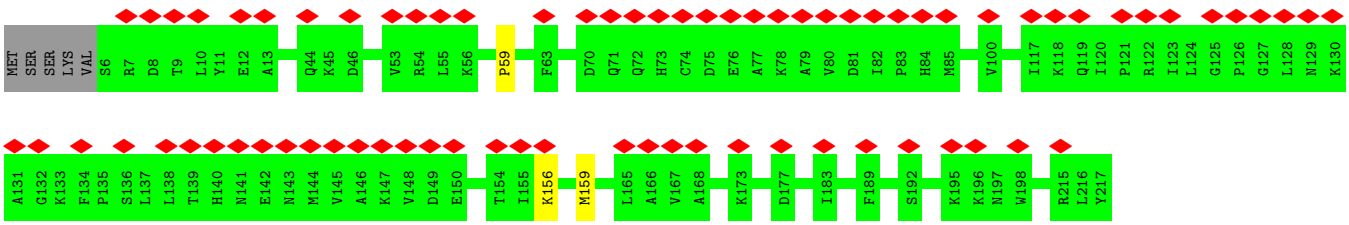
Chain 8:


• Molecule 48: uL1

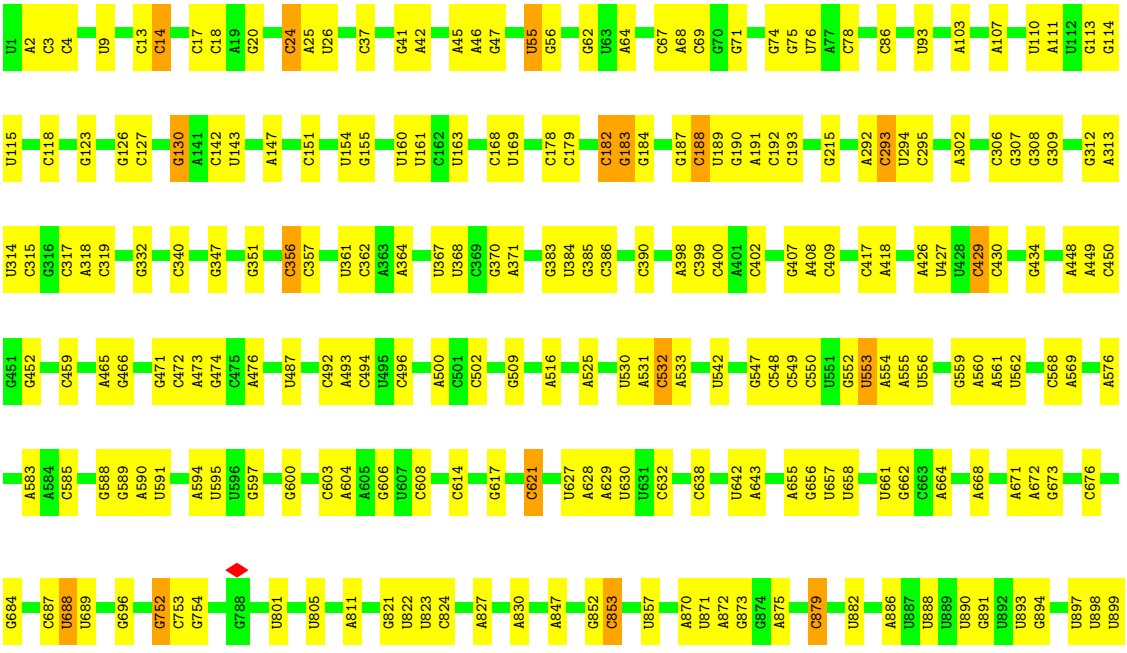
Chain K:

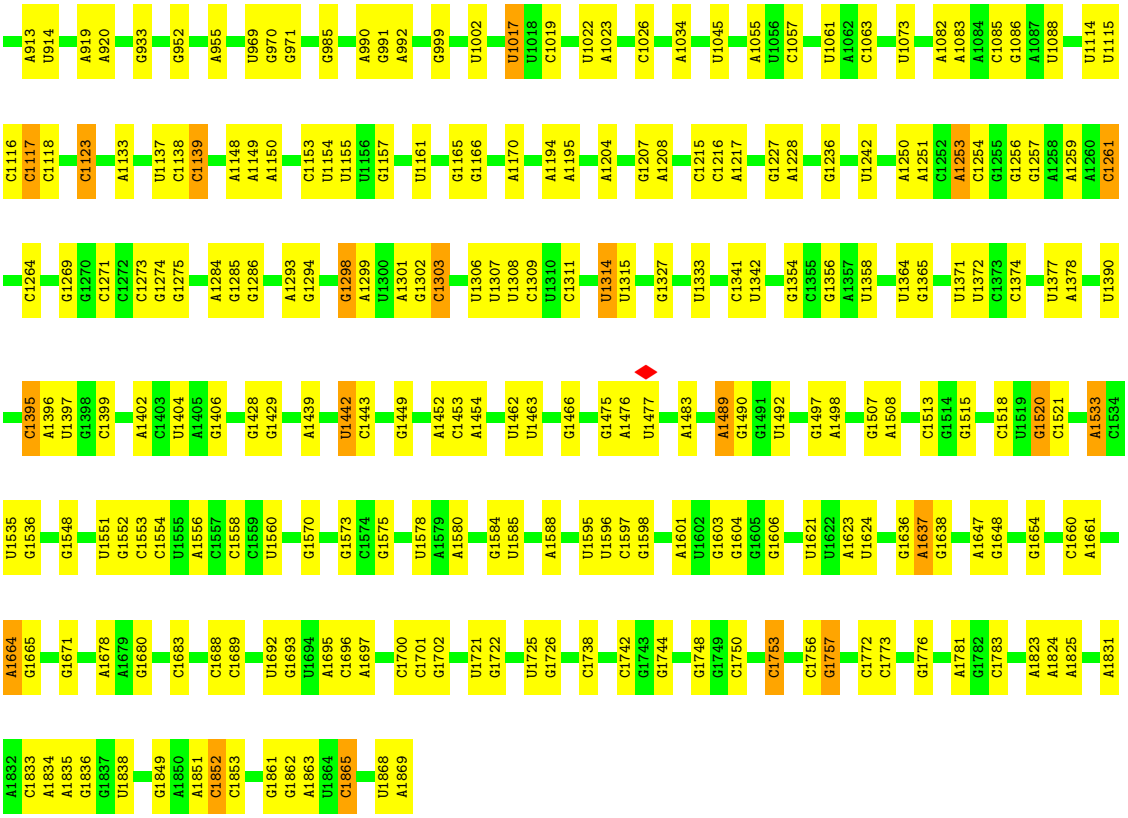



• Molecule 49: 18S rRNA

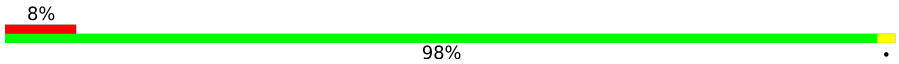
Chain 2:




- Molecule 50: uS2

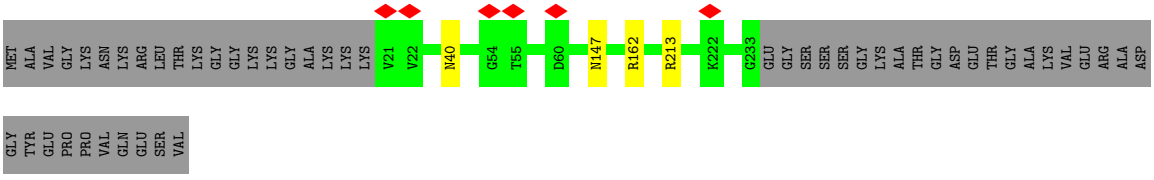
Chain BB:





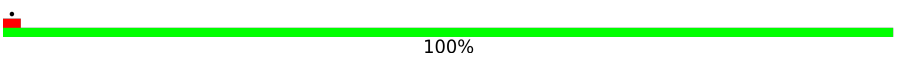
- Molecule 51: eS1

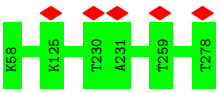
Chain CC:


- Molecule 52: uS5

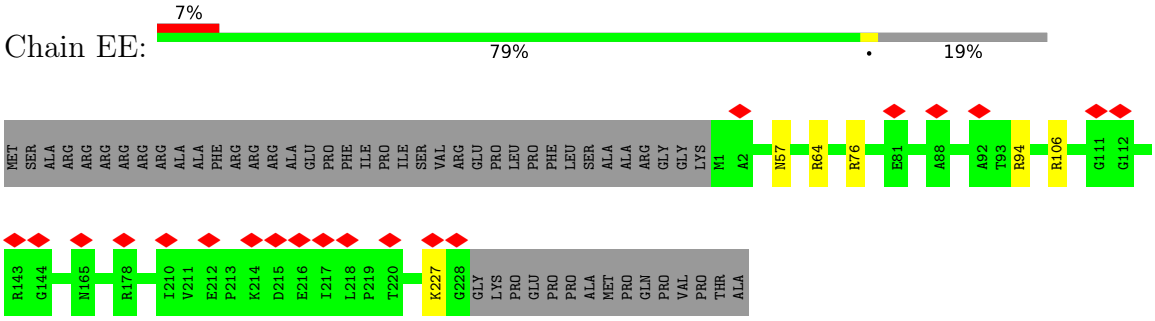
Chain DD:



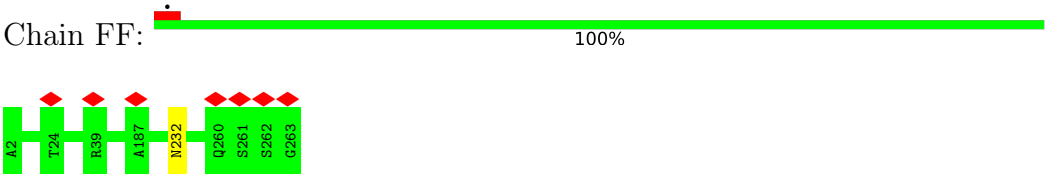

- Molecule 53: uS3

Chain EE:



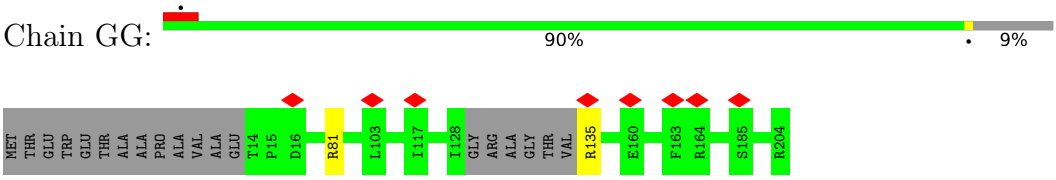

• Molecule 54: eS4

Chain FF:



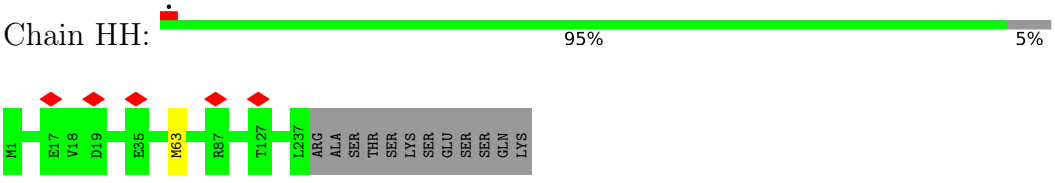

• Molecule 55: uS7

Chain GG:



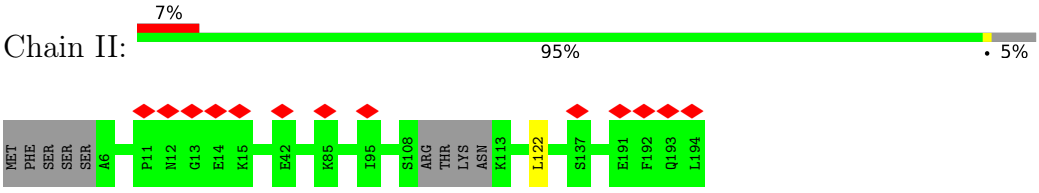

• Molecule 56: eS6

Chain HH:



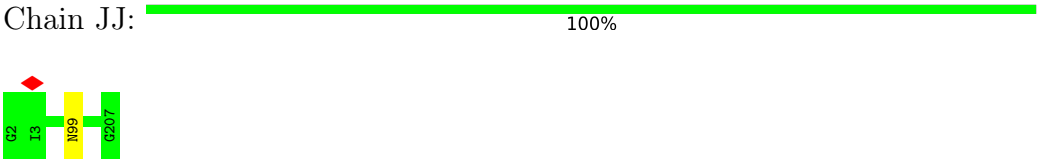

• Molecule 57: eS7

Chain II:



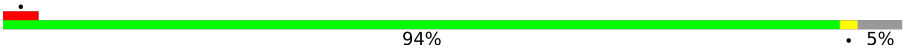

• Molecule 58: eS8

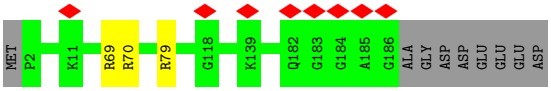
Chain JJ:




• Molecule 59: uS4

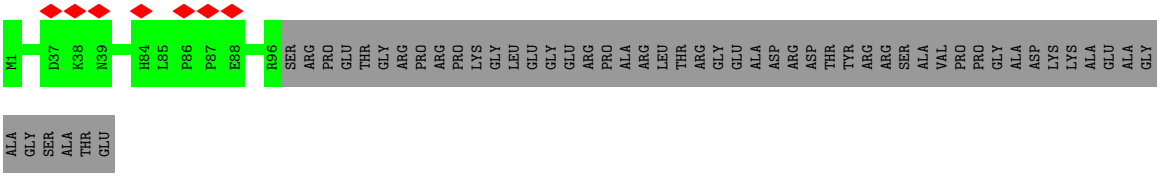
Chain KK:





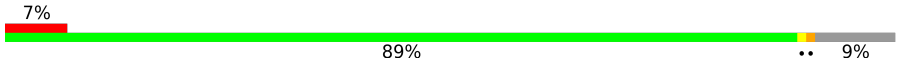

• Molecule 60: eS10

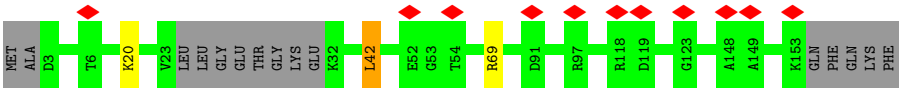
Chain LL:


• Molecule 61: uS17

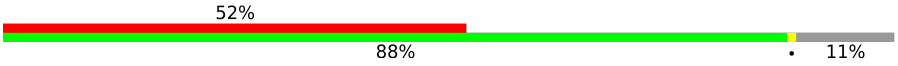
Chain MM:

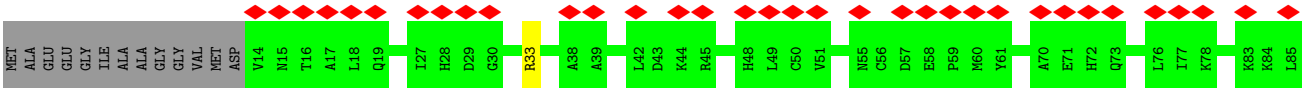


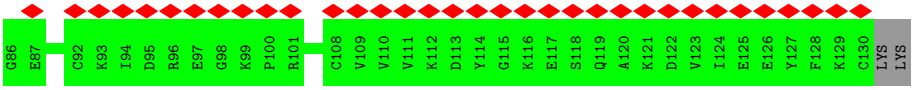




• Molecule 62: eS12

Chain NN:

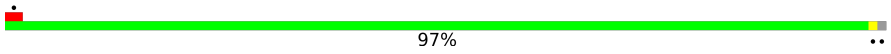


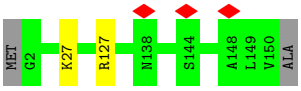




• Molecule 63: uS15

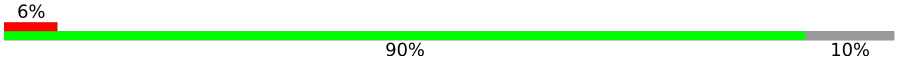
Chain OO:

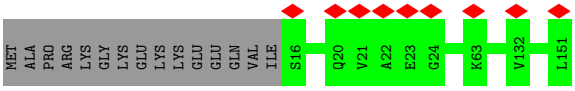



• Molecule 64: uS11

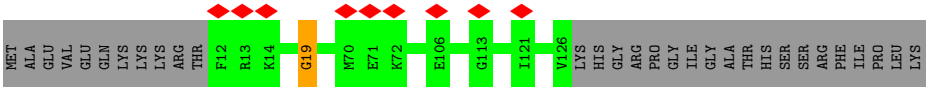
Chain PP:



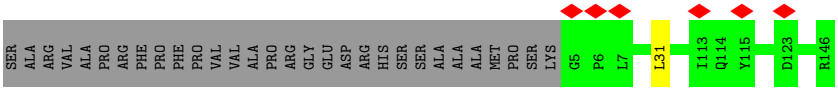

• Molecule 65: uS19

Chain QQ:



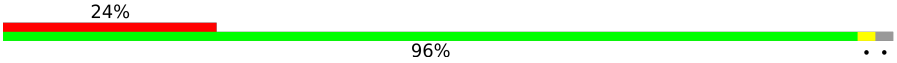

• Molecule 66: uS9

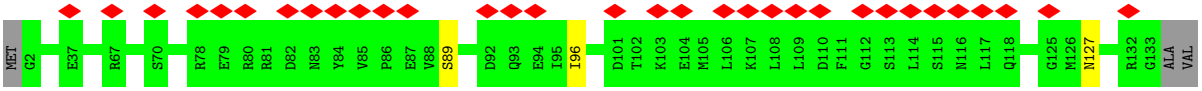
Chain RR:


• Molecule 67: eS17

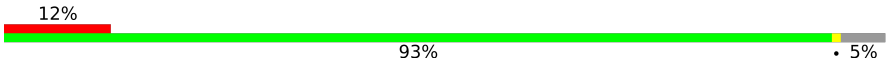
Chain SS:

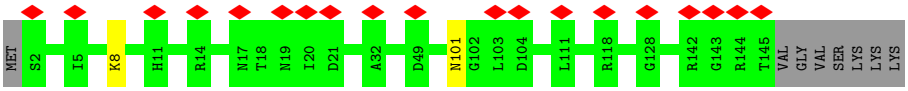



• Molecule 68: uS13

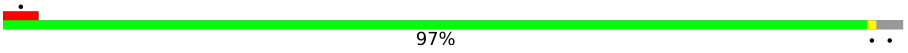
Chain TT:

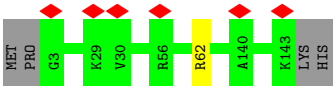



• Molecule 69: eS19

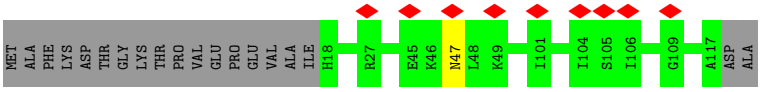
Chain UU:



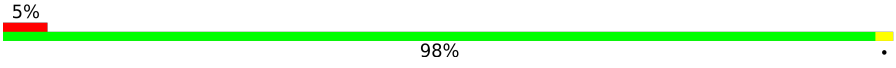

• Molecule 70: uS10

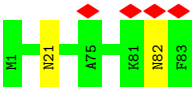
Chain VV:


• Molecule 71: eS21

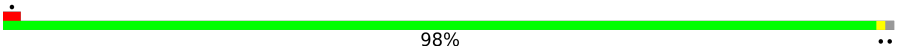
Chain WW:

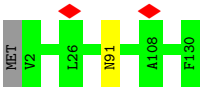



• Molecule 72: uS8

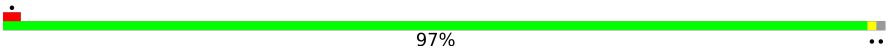
Chain XX:

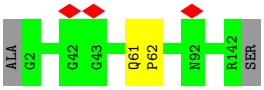



• Molecule 73: uS12

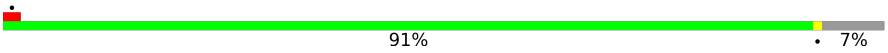
Chain YY:

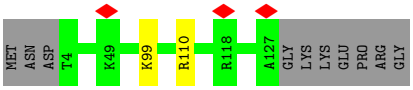



• Molecule 74: eS24

Chain ZZ:



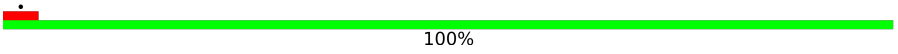

• Molecule 75: eS25

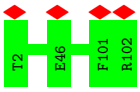
Chain aa:



• Molecule 76: eS26

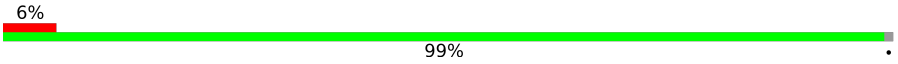
Chain bb:

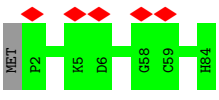



• Molecule 77: eS27

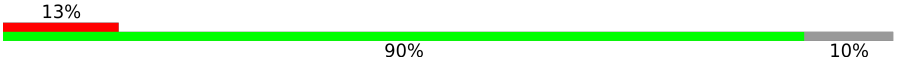
Chain cc:

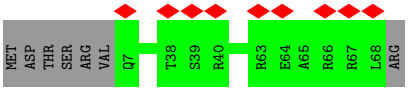



• Molecule 78: eS28

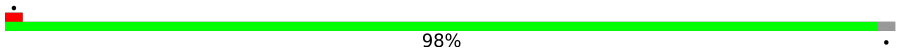
Chain dd:

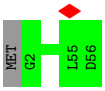





• Molecule 79: eS29

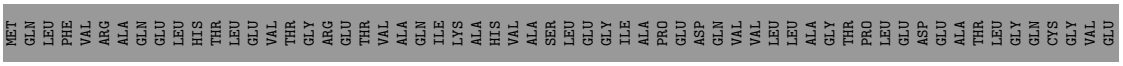
Chain ee:

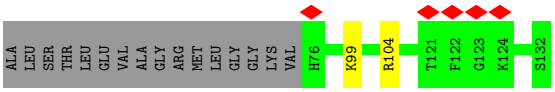



• Molecule 80: eS30

Chain ff:

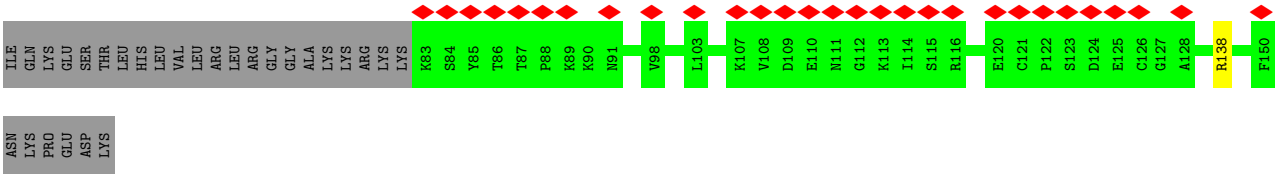




• Molecule 81: eS31

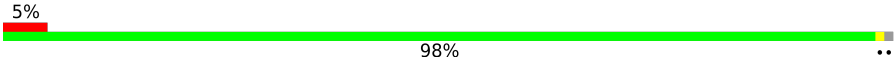
Chain gg:

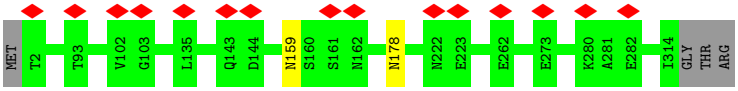





• Molecule 82: RACK1

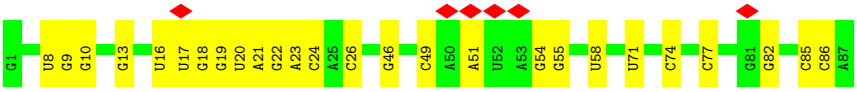
Chain hh:



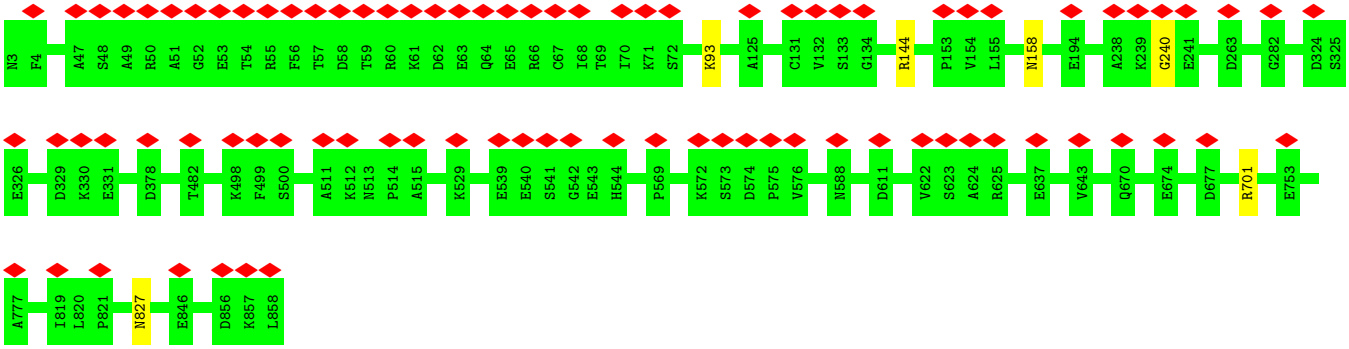

• Molecule 83: P-site tRNA

Chain 3:

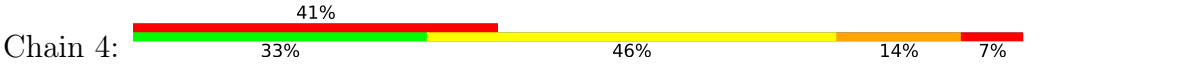

• Molecule 84: eEF2

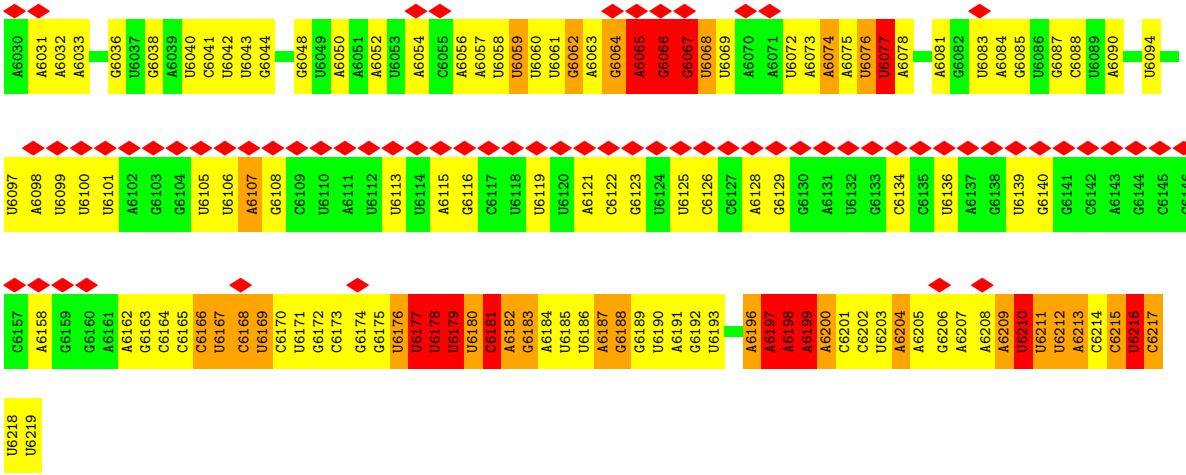
Chain 9:


• Molecule 85: CrPV IRES

Chain 4:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 75654 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 64 | 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 | 0.076 | Depositor |
| Minimum map value | -0.013 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.008 | Depositor |
| Recommended contour level | 0.02 | Depositor |
| Map size (Å) | 432.00003, 432.00003, 432.00003 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.08, 1.08, 1.08 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.26 | 0/1812 | 0.50 | 1/2439 (0.0%) |
| 2 | B | 0.25 | 0/3240 | 0.51 | 2/4339 (0.0%) |
| 3 | C | 0.24 | 0/2936 | 0.45 | 0/3943 |
| 4 | D | 0.26 | 0/2437 | 0.44 | 0/3264 |
| 5 | E | 0.25 | 0/1762 | 0.48 | 0/2362 |
| 6 | F | 0.25 | 0/1911 | 0.44 | 0/2549 |
| 7 | G | 0.25 | 0/1910 | 0.49 | 0/2569 |
| 8 | H | 0.25 | 0/1535 | 0.50 | 0/2063 |
| 9 | I | 0.26 | 0/1702 | 0.45 | 0/2272 |
| 10 | J | 0.25 | 0/1385 | 0.47 | 0/1852 |
| 11 | L | 0.27 | 0/1733 | 0.46 | 0/2316 |
| 12 | M | 0.25 | 0/1150 | 0.44 | 0/1534 |
| 13 | N | 0.24 | 0/1746 | 0.43 | 0/2338 |
| 14 | O | 0.25 | 0/1653 | 0.44 | 0/2206 |
| 15 | P | 0.24 | 0/1268 | 0.47 | 0/1700 |
| 16 | Q | 0.24 | 0/1539 | 0.48 | 0/2054 |
| 17 | R | 0.24 | 0/1524 | 0.44 | 0/2013 |
| 18 | S | 0.25 | 0/1501 | 0.48 | 0/2012 |
| 19 | T | 0.25 | 0/1326 | 0.44 | 0/1770 |
| 20 | U | 0.26 | 0/823 | 0.45 | 0/1104 |
| 21 | V | 0.26 | 0/983 | 0.46 | 0/1319 |
| 22 | W | 0.25 | 0/873 | 0.43 | 0/1158 |
| 23 | X | 0.24 | 0/984 | 0.46 | 0/1323 |
| 24 | Y | 0.24 | 0/1132 | 0.44 | 0/1504 |
| 25 | Z | 0.26 | 0/1130 | 0.46 | 0/1507 |
| 26 | a | 0.23 | 0/1191 | 0.42 | 0/1590 |
| 27 | b | 0.24 | 0/861 | 0.40 | 0/1138 |
| 28 | c | 0.25 | 0/771 | 0.45 | 0/1034 |
| 29 | d | 0.26 | 0/903 | 0.49 | 0/1216 |
| 30 | e | 0.24 | 0/1071 | 0.47 | 0/1429 |
| 31 | f | 0.25 | 0/895 | 0.49 | 0/1198 |
| 32 | g | 0.25 | 0/916 | 0.48 | 0/1220 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | h | 0.25 | 0/1021 | 0.42 | 0/1348 |
| 34 | i | 0.25 | 0/841 | 0.43 | 0/1112 |
| 35 | j | 0.26 | 0/720 | 0.45 | 0/952 |
| 36 | k | 0.24 | 0/575 | 0.47 | 0/761 |
| 37 | l | 0.24 | 0/459 | 0.47 | 1/608 (0.2%) |
| 38 | m | 0.25 | 0/435 | 0.46 | 0/575 |
| 39 | n | 0.23 | 0/240 | 0.40 | 0/305 |
| 40 | o | 0.24 | 0/864 | 0.46 | 0/1140 |
| 41 | p | 0.24 | 0/718 | 0.44 | 0/953 |
| 42 | r | 0.24 | 0/1010 | 0.47 | 0/1354 |
| 43 | s | 0.27 | 0/1530 | 0.47 | 0/2064 |
| 44 | t | 0.25 | 0/1174 | 0.52 | 0/1582 |
| 45 | 5 | 0.27 | 1/86202 (0.0%) | 1.01 | 331/134412 (0.2%) |
| 46 | 7 | 0.27 | 0/2836 | 1.00 | 5/4421 (0.1%) |
| 47 | 8 | 0.27 | 0/3581 | 1.00 | 10/5577 (0.2%) |
| 48 | K | 0.28 | 0/1730 | 0.55 | 0/2315 |
| 49 | 2 | 0.28 | 0/40500 | 1.03 | 194/63092 (0.3%) |
| 50 | BB | 0.26 | 0/1747 | 0.51 | 0/2374 |
| 51 | CC | 0.26 | 0/1756 | 0.50 | 0/2350 |
| 52 | DD | 0.25 | 0/1753 | 0.48 | 0/2369 |
| 53 | EE | 0.26 | 0/1796 | 0.51 | 0/2417 |
| 54 | FF | 0.25 | 0/2118 | 0.47 | 0/2849 |
| 55 | GG | 0.25 | 0/1492 | 0.46 | 0/2005 |
| 56 | HH | 0.25 | 0/1946 | 0.48 | 0/2590 |
| 57 | II | 0.26 | 0/1510 | 0.50 | 1/2022 (0.0%) |
| 58 | JJ | 0.25 | 0/1715 | 0.46 | 0/2287 |
| 59 | KK | 0.25 | 0/1550 | 0.48 | 0/2069 |
| 60 | LL | 0.25 | 0/834 | 0.48 | 0/1125 |
| 61 | MM | 0.25 | 0/1195 | 0.51 | 1/1597 (0.1%) |
| 62 | NN | 0.26 | 0/918 | 0.54 | 0/1233 |
| 63 | OO | 0.24 | 0/1226 | 0.45 | 0/1649 |
| 64 | PP | 0.25 | 0/1029 | 0.49 | 0/1380 |
| 65 | QQ | 0.25 | 0/974 | 0.49 | 0/1301 |
| 66 | RR | 0.25 | 0/1146 | 0.48 | 1/1534 (0.1%) |
| 67 | SS | 0.25 | 0/1082 | 0.50 | 1/1452 (0.1%) |
| 68 | TT | 0.25 | 0/1208 | 0.47 | 0/1618 |
| 69 | UU | 0.25 | 0/1115 | 0.44 | 0/1493 |
| 70 | VV | 0.24 | 0/805 | 0.48 | 0/1081 |
| 71 | WW | 0.26 | 0/643 | 0.48 | 0/860 |
| 72 | XX | 0.26 | 0/1051 | 0.49 | 0/1406 |
| 73 | YY | 0.26 | 0/1116 | 0.48 | 0/1490 |
| 74 | ZZ | 0.25 | 0/1028 | 0.47 | 0/1366 |
| 75 | aa | 0.24 | 0/604 | 0.50 | 0/810 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 76 | bb | 0.24 | 0/828 | 0.44 | 0/1109 |
| 77 | cc | 0.24 | 0/665 | 0.47 | 0/891 |
| 78 | dd | 0.23 | 0/490 | 0.45 | 0/656 |
| 79 | ee | 0.25 | 0/470 | 0.41 | 0/623 |
| 80 | ff | 0.25 | 0/462 | 0.44 | 0/607 |
| 81 | gg | 0.24 | 0/567 | 0.46 | 0/753 |
| 82 | hh | 0.25 | 0/2492 | 0.52 | 0/3391 |
| 83 | 3 | 0.26 | 0/2077 | 0.96 | 2/3238 (0.1%) |
| 84 | 9 | 0.26 | 0/6804 | 0.52 | 0/9189 |
| 85 | 4 | 0.69 | 16/4490 (0.4%) | 1.54 | 125/6984 (1.8%) |
| All | All | 0.28 | 17/243741 (0.0%) | 0.86 | 675/357074 (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 |
|---|---|---|---|
| 3 | C | 0 | 1 |
| 50 | BB | 0 | 1 |
| 65 | QQ | 0 | 1 |
| 67 | SS | 0 | 1 |
| 73 | YY | 0 | 1 |
| 84 | 9 | 0 | 1 |
| 85 | 4 | 1 | 14 |
| All | All | 1 | 20 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 85 | 4 | 6178 | U | C2-O2 | 9.15 | 1.30 | 1.22 |
| 85 | 4 | 6065 | A | O3'-P | 8.59 | 1.71 | 1.61 |
| 85 | 4 | 6078 | A | O3'-P | -8.35 | 1.51 | 1.61 |
| 85 | 4 | 6217 | C | O3'-P | 8.15 | 1.71 | 1.61 |
| 85 | 4 | 6187 | A | O3'-P | 7.84 | 1.70 | 1.61 |
| 85 | 4 | 6077 | U | C4-O4 | 7.79 | 1.29 | 1.23 |
| 85 | 4 | 6210 | U | O3'-P | 7.62 | 1.70 | 1.61 |
| 85 | 4 | 6166 | C | O3'-P | 7.58 | 1.70 | 1.61 |
| 85 | 4 | 6181 | C | O3'-P | 7.49 | 1.70 | 1.61 |
| 85 | 4 | 6218 | U | C1'-N1 | 6.91 | 1.59 | 1.48 |
| 85 | 4 | 6219 | U | C1'-N1 | 6.85 | 1.59 | 1.48 |
| 85 | 4 | 6212 | U | O3'-P | 6.57 | 1.69 | 1.61 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 85 | 4 | 6218 | U | O3'-P | -5.81 | 1.54 | 1.61 |
| 85 | 4 | 6217 | C | C3'-O3' | 5.80 | 1.50 | 1.42 |
| 85 | 4 | 6197 | A | O3'-P | 5.37 | 1.67 | 1.61 |
| 45 | 5 | 4893 | A | N9-C4 | 5.19 | 1.41 | 1.37 |
| 85 | 4 | 6181 | C | C1'-N1 | 5.11 | 1.56 | 1.48 |

All (675) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 85 | 4 | 6068 | U | OP1-P-O3' | 25.71 | 161.75 | 105.20 |
| 85 | 4 | 6068 | U | O3'-P-O5' | -20.16 | 65.70 | 104.00 |
| 85 | 4 | 6218 | U | O3'-P-O5' | -18.73 | 68.41 | 104.00 |
| 85 | 4 | 6188 | G | O5'-P-OP2 | 16.39 | 130.37 | 110.70 |
| 85 | 4 | 6218 | U | P-O3'-C3' | 15.72 | 138.56 | 119.70 |
| 85 | 4 | 6215 | C | C4'-C3'-O3' | 14.53 | 142.05 | 113.00 |
| 85 | 4 | 6188 | G | O5'-P-OP1 | -14.40 | 92.74 | 105.70 |
| 85 | 4 | 6065 | A | O4'-C1'-N9 | 14.02 | 119.42 | 108.20 |
| 85 | 4 | 6204 | A | O3'-P-O5' | -13.97 | 77.46 | 104.00 |
| 85 | 4 | 6077 | U | C5-C4-O4 | -13.70 | 117.68 | 125.90 |
| 85 | 4 | 6212 | U | N1-C1'-C2' | 12.71 | 130.52 | 114.00 |
| 85 | 4 | 6210 | U | O4'-C1'-N1 | 12.54 | 118.23 | 108.20 |
| 85 | 4 | 6068 | U | OP2-P-O3' | -12.18 | 78.40 | 105.20 |
| 85 | 4 | 6218 | U | OP1-P-O3' | 11.97 | 131.53 | 105.20 |
| 85 | 4 | 6077 | U | N1-C1'-C2' | -11.54 | 99.00 | 114.00 |
| 85 | 4 | 6197 | A | N9-C1'-C2' | 11.49 | 128.93 | 114.00 |
| 85 | 4 | 6177 | U | N1-C1'-C2' | 11.39 | 128.80 | 114.00 |
| 85 | 4 | 6176 | U | C1'-C2'-O2' | -11.23 | 76.91 | 110.60 |
| 85 | 4 | 6211 | U | N1-C1'-C2' | 11.11 | 128.44 | 114.00 |
| 85 | 4 | 6199 | A | C4-N9-C1' | -10.68 | 107.08 | 126.30 |
| 85 | 4 | 6199 | A | O4'-C1'-N9 | 10.67 | 116.73 | 108.20 |
| 85 | 4 | 6179 | U | N1-C1'-C2' | 10.64 | 127.83 | 114.00 |
| 85 | 4 | 6166 | C | C4'-C3'-O3' | 10.44 | 133.87 | 113.00 |
| 85 | 4 | 6181 | C | C6-N1-C1' | -10.29 | 108.45 | 120.80 |
| 49 | 2 | 1852 | C | N1-C2-O2 | 9.99 | 124.89 | 118.90 |
| 85 | 4 | 6211 | U | O4'-C1'-N1 | 9.89 | 116.11 | 108.20 |
| 85 | 4 | 6181 | C | C3'-C2'-C1' | 9.87 | 109.40 | 101.50 |
| 85 | 4 | 6199 | A | C8-N9-C1' | 9.85 | 145.43 | 127.70 |
| 85 | 4 | 6168 | C | N1-C1'-C2' | 9.78 | 126.71 | 114.00 |
| 85 | 4 | 6065 | A | C8-N9-C1' | -9.73 | 110.18 | 127.70 |
| 49 | 2 | 1261 | C | N1-C2-O2 | 9.73 | 124.74 | 118.90 |
| 85 | 4 | 6151 | A | O4'-C1'-N9 | 9.67 | 115.94 | 108.20 |
| 85 | 4 | 6210 | U | N1-C1'-C2' | 9.46 | 126.30 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 2655 | C | N1-C2-O2 | 9.44 | 124.56 | 118.90 |
| 85 | 4 | 6199 | A | N9-C1'-C2' | 9.43 | 126.26 | 114.00 |
| 49 | 2 | 1063 | C | N1-C2-O2 | 9.43 | 124.56 | 118.90 |
| 85 | 4 | 6216 | U | O4'-C1'-N1 | 9.42 | 115.73 | 108.20 |
| 85 | 4 | 6064 | G | N9-C1'-C2' | -9.35 | 101.72 | 112.00 |
| 49 | 2 | 178 | C | N1-C2-O2 | 9.08 | 124.35 | 118.90 |
| 45 | 5 | 220 | C | N1-C2-O2 | 9.01 | 124.30 | 118.90 |
| 85 | 4 | 6178 | U | C4'-C3'-O3' | 8.93 | 130.85 | 113.00 |
| 85 | 4 | 6201 | C | N1-C1'-C2' | -8.88 | 102.23 | 112.00 |
| 45 | 5 | 2499 | C | N1-C2-O2 | 8.86 | 124.22 | 118.90 |
| 85 | 4 | 6197 | A | C8-N9-C1' | -8.84 | 111.78 | 127.70 |
| 45 | 5 | 2819 | U | N3-C2-O2 | -8.83 | 116.02 | 122.20 |
| 85 | 4 | 6150 | C | C2'-C3'-O3' | 8.82 | 128.90 | 109.50 |
| 85 | 4 | 6187 | A | C1'-C2'-O2' | -8.59 | 84.84 | 110.60 |
| 49 | 2 | 494 | C | N1-C2-O2 | 8.57 | 124.04 | 118.90 |
| 49 | 2 | 1442 | U | N1-C2-O2 | 8.52 | 128.76 | 122.80 |
| 45 | 5 | 3909 | C | N1-C2-O2 | 8.47 | 123.98 | 118.90 |
| 45 | 5 | 4958 | C | N1-C2-O2 | 8.45 | 123.97 | 118.90 |
| 85 | 4 | 6215 | C | N1-C1'-C2' | -8.44 | 102.72 | 112.00 |
| 85 | 4 | 6200 | A | N9-C1'-C2' | -8.43 | 102.73 | 112.00 |
| 49 | 2 | 1865 | C | N1-C2-O2 | 8.42 | 123.95 | 118.90 |
| 85 | 4 | 6176 | U | N1-C1'-C2' | -8.40 | 102.76 | 112.00 |
| 49 | 2 | 1750 | C | N1-C2-O2 | 8.38 | 123.93 | 118.90 |
| 45 | 5 | 112 | C | N1-C2-O2 | 8.38 | 123.93 | 118.90 |
| 49 | 2 | 1261 | C | C2-N1-C1' | 8.37 | 128.00 | 118.80 |
| 49 | 2 | 1442 | U | N3-C2-O2 | -8.29 | 116.40 | 122.20 |
| 45 | 5 | 2819 | U | N1-C2-O2 | 8.26 | 128.58 | 122.80 |
| 85 | 4 | 6074 | A | N9-C1'-C2' | -8.21 | 102.97 | 112.00 |
| 45 | 5 | 1193 | C | C2-N1-C1' | 8.20 | 127.82 | 118.80 |
| 85 | 4 | 6181 | C | N1-C1'-C2' | 8.19 | 124.64 | 114.00 |
| 45 | 5 | 473 | C | N1-C2-O2 | 8.17 | 123.80 | 118.90 |
| 85 | 4 | 6181 | C | C1'-C2'-O2' | -8.17 | 86.10 | 110.60 |
| 49 | 2 | 1624 | U | C2-N1-C1' | 8.07 | 127.39 | 117.70 |
| 49 | 2 | 1261 | C | N3-C2-O2 | -8.05 | 116.26 | 121.90 |
| 45 | 5 | 2655 | C | N3-C2-O2 | -7.93 | 116.35 | 121.90 |
| 85 | 4 | 6197 | A | C4-N9-C1' | 7.92 | 140.55 | 126.30 |
| 85 | 4 | 6151 | A | C1'-O4'-C4' | -7.84 | 103.62 | 109.90 |
| 45 | 5 | 1276 | C | N1-C2-O2 | 7.82 | 123.59 | 118.90 |
| 45 | 5 | 282 | C | N1-C2-O2 | 7.81 | 123.59 | 118.90 |
| 45 | 5 | 3810 | C | C2-N1-C1' | 7.80 | 127.38 | 118.80 |
| 49 | 2 | 632 | C | N1-C2-O2 | 7.79 | 123.58 | 118.90 |
| 49 | 2 | 1688 | C | N3-C2-O2 | -7.78 | 116.45 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 2499 | C | N3-C2-O2 | -7.78 | 116.46 | 121.90 |
| 49 | 2 | 1520 | G | C4-N9-C1' | 7.73 | 136.55 | 126.50 |
| 47 | 8 | 119 | C | N1-C2-O2 | 7.71 | 123.53 | 118.90 |
| 49 | 2 | 1852 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 49 | 2 | 178 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 85 | 4 | 6077 | U | N3-C4-O4 | -7.71 | 114.00 | 119.40 |
| 85 | 4 | 6062 | G | N9-C1'-C2' | -7.71 | 103.52 | 112.00 |
| 49 | 2 | 1865 | C | C2-N1-C1' | 7.71 | 127.28 | 118.80 |
| 45 | 5 | 2020 | U | N3-C2-O2 | -7.70 | 116.81 | 122.20 |
| 45 | 5 | 3810 | C | N1-C2-O2 | 7.69 | 123.51 | 118.90 |
| 85 | 4 | 6078 | A | P-O3'-C3' | -7.66 | 110.50 | 119.70 |
| 45 | 5 | 2022 | C | N3-C2-O2 | -7.66 | 116.54 | 121.90 |
| 45 | 5 | 67 | C | N1-C2-O2 | 7.64 | 123.48 | 118.90 |
| 85 | 4 | 6187 | A | C4'-C3'-O3' | -7.62 | 93.41 | 109.40 |
| 85 | 4 | 6065 | A | C4-N9-C1' | 7.61 | 139.99 | 126.30 |
| 45 | 5 | 202 | C | N1-C2-O2 | 7.51 | 123.41 | 118.90 |
| 49 | 2 | 178 | C | C6-N1-C2 | -7.49 | 117.30 | 120.30 |
| 49 | 2 | 1063 | C | N3-C2-O2 | -7.49 | 116.66 | 121.90 |
| 45 | 5 | 1429 | C | N1-C2-O2 | 7.47 | 123.38 | 118.90 |
| 45 | 5 | 1827 | C | N1-C2-O2 | 7.46 | 123.38 | 118.90 |
| 85 | 4 | 6067 | G | N9-C1'-C2' | 7.44 | 123.68 | 114.00 |
| 49 | 2 | 1520 | G | N3-C4-N9 | 7.44 | 130.46 | 126.00 |
| 85 | 4 | 6188 | G | P-O5'-C5' | 7.44 | 132.80 | 120.90 |
| 49 | 2 | 1261 | C | C6-N1-C2 | -7.42 | 117.33 | 120.30 |
| 45 | 5 | 2464 | C | N1-C2-O2 | 7.42 | 123.35 | 118.90 |
| 45 | 5 | 18 | C | N1-C2-O2 | 7.38 | 123.33 | 118.90 |
| 45 | 5 | 2020 | U | N1-C2-O2 | 7.38 | 127.97 | 122.80 |
| 85 | 4 | 6151 | A | C4-N9-C1' | -7.37 | 113.03 | 126.30 |
| 85 | 4 | 6076 | U | N1-C1'-C2' | -7.36 | 103.90 | 112.00 |
| 45 | 5 | 3778 | U | N1-C2-O2 | 7.36 | 127.95 | 122.80 |
| 45 | 5 | 174 | C | N3-C2-O2 | -7.35 | 116.76 | 121.90 |
| 49 | 2 | 1118 | C | C2-N1-C1' | 7.34 | 126.87 | 118.80 |
| 49 | 2 | 1597 | C | N1-C2-O2 | 7.33 | 123.30 | 118.90 |
| 45 | 5 | 2022 | C | N1-C2-O2 | 7.31 | 123.29 | 118.90 |
| 85 | 4 | 6166 | C | C3'-C2'-C1' | 7.30 | 107.34 | 101.50 |
| 45 | 5 | 4266 | G | C4-N9-C1' | 7.29 | 135.97 | 126.50 |
| 85 | 4 | 6187 | A | C2'-C3'-O3' | 7.28 | 125.52 | 109.50 |
| 49 | 2 | 178 | C | C2-N1-C1' | 7.27 | 126.80 | 118.80 |
| 45 | 5 | 233 | U | C2-N1-C1' | 7.27 | 126.42 | 117.70 |
| 45 | 5 | 3657 | U | N1-C2-O2 | 7.26 | 127.88 | 122.80 |
| 49 | 2 | 429 | C | N1-C2-O2 | 7.24 | 123.24 | 118.90 |
| 85 | 4 | 6216 | U | C4'-C3'-O3' | 7.24 | 127.47 | 113.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 4930 | C | C2-N1-C1' | 7.21 | 126.74 | 118.80 |
| 49 | 2 | 1742 | C | N1-C2-O2 | 7.21 | 123.23 | 118.90 |
| 45 | 5 | 4232 | U | P-O3'-C3' | 7.21 | 128.35 | 119.70 |
| 49 | 2 | 1852 | C | C2-N1-C1' | 7.20 | 126.72 | 118.80 |
| 85 | 4 | 6151 | A | C5'-C4'-O4' | 7.19 | 117.72 | 109.10 |
| 49 | 2 | 1520 | G | N3-C4-C5 | -7.17 | 125.01 | 128.60 |
| 45 | 5 | 4261 | C | N1-C2-O2 | 7.17 | 123.20 | 118.90 |
| 49 | 2 | 1315 | U | N1-C2-O2 | 7.16 | 127.81 | 122.80 |
| 49 | 2 | 1442 | U | C2-N1-C1' | 7.15 | 126.28 | 117.70 |
| 45 | 5 | 220 | C | N3-C2-O2 | -7.15 | 116.90 | 121.90 |
| 45 | 5 | 2655 | C | C2-N1-C1' | 7.14 | 126.65 | 118.80 |
| 85 | 4 | 6177 | U | C4'-C3'-O3' | 7.12 | 127.25 | 113.00 |
| 49 | 2 | 1624 | U | N1-C2-O2 | 7.12 | 127.78 | 122.80 |
| 49 | 2 | 1595 | U | N1-C2-O2 | 7.11 | 127.78 | 122.80 |
| 49 | 2 | 179 | C | N1-C2-O2 | 7.10 | 123.16 | 118.90 |
| 45 | 5 | 18 | C | C2-N1-C1' | 7.09 | 126.60 | 118.80 |
| 45 | 5 | 2655 | C | C6-N1-C2 | -7.09 | 117.47 | 120.30 |
| 49 | 2 | 1063 | C | C2-N1-C1' | 7.09 | 126.60 | 118.80 |
| 45 | 5 | 985 | C | N1-C2-O2 | 7.08 | 123.14 | 118.90 |
| 49 | 2 | 1298 | G | N3-C4-C5 | -7.07 | 125.07 | 128.60 |
| 45 | 5 | 2695 | A | P-O3'-C3' | 7.05 | 128.16 | 119.70 |
| 49 | 2 | 585 | C | N1-C2-O2 | 7.05 | 123.13 | 118.90 |
| 45 | 5 | 4925 | U | OP2-P-O3' | 7.05 | 120.71 | 105.20 |
| 45 | 5 | 4177 | C | N1-C2-O2 | 7.04 | 123.13 | 118.90 |
| 45 | 5 | 2351 | C | N1-C2-O2 | 7.03 | 123.12 | 118.90 |
| 49 | 2 | 1750 | C | N3-C2-O2 | -7.02 | 116.98 | 121.90 |
| 49 | 2 | 1298 | G | N3-C4-N9 | 7.00 | 130.20 | 126.00 |
| 85 | 4 | 6187 | A | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 49 | 2 | 1597 | C | N3-C2-O2 | -7.00 | 117.00 | 121.90 |
| 45 | 5 | 4266 | G | N3-C4-C5 | -6.98 | 125.11 | 128.60 |
| 49 | 2 | 1118 | C | N1-C2-O2 | 6.98 | 123.09 | 118.90 |
| 45 | 5 | 3909 | C | N3-C2-O2 | -6.97 | 117.02 | 121.90 |
| 49 | 2 | 1315 | U | N3-C2-O2 | -6.97 | 117.32 | 122.20 |
| 49 | 2 | 688 | U | P-O3'-C3' | 6.94 | 128.03 | 119.70 |
| 85 | 4 | 6215 | C | C3'-C2'-C1' | 6.94 | 107.05 | 101.50 |
| 49 | 2 | 494 | C | C2-N1-C1' | 6.94 | 126.43 | 118.80 |
| 45 | 5 | 4925 | U | P-O3'-C3' | 6.93 | 128.02 | 119.70 |
| 45 | 5 | 3657 | U | N3-C2-O2 | -6.93 | 117.35 | 122.20 |
| 45 | 5 | 390 | C | N1-C2-O2 | 6.92 | 123.05 | 118.90 |
| 45 | 5 | 2820 | C | N1-C2-O2 | 6.92 | 123.05 | 118.90 |
| 45 | 5 | 4266 | G | N3-C4-N9 | 6.90 | 130.14 | 126.00 |
| 49 | 2 | 1123 | C | N1-C2-O2 | 6.89 | 123.04 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 1612 | G | C4-N9-C1' | 6.89 | 135.46 | 126.50 |
| 49 | 2 | 1298 | G | C4-N9-C1' | 6.89 | 135.46 | 126.50 |
| 45 | 5 | 3778 | U | N3-C2-O2 | -6.87 | 117.39 | 122.20 |
| 45 | 5 | 3778 | U | C2-N1-C1' | 6.84 | 125.91 | 117.70 |
| 49 | 2 | 1624 | U | N3-C2-O2 | -6.84 | 117.41 | 122.20 |
| 49 | 2 | 1063 | C | C6-N1-C2 | -6.84 | 117.56 | 120.30 |
| 45 | 5 | 1612 | G | N3-C4-N9 | 6.82 | 130.09 | 126.00 |
| 45 | 5 | 2373 | C | N1-C2-O2 | 6.82 | 122.99 | 118.90 |
| 85 | 4 | 6180 | U | C4'-C3'-O3' | -6.80 | 95.13 | 109.40 |
| 45 | 5 | 220 | C | C6-N1-C2 | -6.79 | 117.58 | 120.30 |
| 45 | 5 | 4627 | U | N1-C2-O2 | 6.79 | 127.55 | 122.80 |
| 49 | 2 | 193 | C | N3-C2-O2 | -6.78 | 117.16 | 121.90 |
| 49 | 2 | 1772 | C | N1-C2-O2 | 6.77 | 122.96 | 118.90 |
| 45 | 5 | 2089 | G | P-O3'-C3' | 6.77 | 127.82 | 119.70 |
| 45 | 5 | 4774 | C | N1-C2-O2 | 6.77 | 122.96 | 118.90 |
| 85 | 4 | 6181 | C | C2-N1-C1' | 6.76 | 126.23 | 118.80 |
| 49 | 2 | 1852 | C | C6-N1-C2 | -6.75 | 117.60 | 120.30 |
| 85 | 4 | 6151 | A | C8-N9-C1' | 6.75 | 139.86 | 127.70 |
| 49 | 2 | 494 | C | N3-C2-O2 | -6.75 | 117.17 | 121.90 |
| 49 | 2 | 1750 | C | C6-N1-C2 | -6.74 | 117.61 | 120.30 |
| 47 | 8 | 64 | U | N3-C2-O2 | -6.74 | 117.48 | 122.20 |
| 45 | 5 | 4747 | C | N1-C2-O2 | 6.73 | 122.94 | 118.90 |
| 85 | 4 | 6198 | A | C5'-C4'-C3' | 6.73 | 126.77 | 116.00 |
| 45 | 5 | 4759 | C | N1-C2-O2 | 6.72 | 122.93 | 118.90 |
| 49 | 2 | 1595 | U | N3-C2-O2 | -6.70 | 117.51 | 122.20 |
| 45 | 5 | 2046 | G | P-O3'-C3' | 6.70 | 127.73 | 119.70 |
| 47 | 8 | 64 | U | N1-C2-O2 | 6.69 | 127.48 | 122.80 |
| 49 | 2 | 340 | C | N1-C2-O2 | 6.68 | 122.91 | 118.90 |
| 49 | 2 | 532 | C | P-O3'-C3' | 6.68 | 127.71 | 119.70 |
| 85 | 4 | 6179 | U | C2-N1-C1' | -6.68 | 109.69 | 117.70 |
| 85 | 4 | 6187 | A | P-O3'-C3' | 6.68 | 127.71 | 119.70 |
| 45 | 5 | 4880 | C | C2-N1-C1' | 6.67 | 126.14 | 118.80 |
| 49 | 2 | 1139 | C | N1-C2-O2 | 6.66 | 122.89 | 118.90 |
| 49 | 2 | 1271 | C | N1-C2-O2 | 6.66 | 122.89 | 118.90 |
| 85 | 4 | 6065 | A | C1'-C2'-O2' | -6.65 | 90.64 | 110.60 |
| 85 | 4 | 6065 | A | C2'-C3'-O3' | -6.65 | 94.87 | 109.50 |
| 49 | 2 | 24 | C | N1-C2-O2 | 6.64 | 122.89 | 118.90 |
| 49 | 2 | 1315 | U | C2-N1-C1' | 6.64 | 125.67 | 117.70 |
| 45 | 5 | 1276 | C | C2-N1-C1' | 6.64 | 126.10 | 118.80 |
| 45 | 5 | 3851 | U | N1-C2-O2 | 6.64 | 127.45 | 122.80 |
| 45 | 5 | 517 | C | N1-C2-O2 | 6.63 | 122.88 | 118.90 |
| 45 | 5 | 1977 | C | N1-C2-O2 | 6.63 | 122.88 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 8 | 129 | C | N1-C2-O2 | 6.62 | 122.87 | 118.90 |
| 49 | 2 | 879 | C | N1-C2-O2 | 6.61 | 122.87 | 118.90 |
| 45 | 5 | 1484 | G | C4-N9-C1' | 6.61 | 135.09 | 126.50 |
| 45 | 5 | 112 | C | N3-C2-O2 | -6.60 | 117.28 | 121.90 |
| 45 | 5 | 3831 | U | N3-C2-O2 | -6.60 | 117.58 | 122.20 |
| 45 | 5 | 4958 | C | N3-C2-O2 | -6.58 | 117.29 | 121.90 |
| 49 | 2 | 1865 | C | N3-C2-O2 | -6.57 | 117.30 | 121.90 |
| 49 | 2 | 1057 | C | C2-N1-C1' | 6.56 | 126.02 | 118.80 |
| 45 | 5 | 50 | C | N1-C2-O2 | 6.54 | 122.82 | 118.90 |
| 45 | 5 | 220 | C | C2-N1-C1' | 6.53 | 125.99 | 118.80 |
| 45 | 5 | 112 | C | C2-N1-C1' | 6.53 | 125.98 | 118.80 |
| 47 | 8 | 119 | C | N3-C2-O2 | -6.53 | 117.33 | 121.90 |
| 45 | 5 | 473 | C | N3-C2-O2 | -6.52 | 117.33 | 121.90 |
| 46 | 7 | 102 | U | N1-C2-O2 | 6.52 | 127.36 | 122.80 |
| 45 | 5 | 4627 | U | N3-C2-O2 | -6.51 | 117.64 | 122.20 |
| 45 | 5 | 4948 | C | C2-N1-C1' | 6.50 | 125.95 | 118.80 |
| 49 | 2 | 1664 | A | P-O3'-C3' | 6.50 | 127.50 | 119.70 |
| 85 | 4 | 6213 | A | O5'-P-OP1 | -6.48 | 99.87 | 105.70 |
| 45 | 5 | 4177 | C | C2-N1-C1' | 6.48 | 125.92 | 118.80 |
| 45 | 5 | 2020 | U | C2-N1-C1' | 6.47 | 125.47 | 117.70 |
| 49 | 2 | 553 | U | P-O3'-C3' | 6.47 | 127.46 | 119.70 |
| 83 | 3 | 74 | C | C2-N1-C1' | 6.46 | 125.91 | 118.80 |
| 49 | 2 | 752 | G | P-O3'-C3' | 6.45 | 127.44 | 119.70 |
| 2 | B | 309 | LEU | CA-CB-CG | 6.44 | 130.11 | 115.30 |
| 49 | 2 | 1395 | C | P-O3'-C3' | 6.43 | 127.42 | 119.70 |
| 49 | 2 | 1750 | C | C2-N1-C1' | 6.43 | 125.87 | 118.80 |
| 85 | 4 | 6198 | A | C8-N9-C1' | -6.43 | 116.13 | 127.70 |
| 45 | 5 | 2819 | U | C2-N1-C1' | 6.42 | 125.41 | 117.70 |
| 45 | 5 | 4054 | C | P-O3'-C3' | 6.42 | 127.40 | 119.70 |
| 45 | 5 | 3657 | U | C2-N1-C1' | 6.42 | 125.40 | 117.70 |
| 45 | 5 | 1484 | G | N3-C4-C5 | -6.41 | 125.39 | 128.60 |
| 85 | 4 | 6065 | A | C1'-O4'-C4' | -6.40 | 104.78 | 109.90 |
| 85 | 4 | 6209 | A | O4'-C1'-N9 | 6.40 | 113.32 | 108.20 |
| 45 | 5 | 1612 | G | N3-C4-C5 | -6.39 | 125.40 | 128.60 |
| 85 | 4 | 6188 | G | OP1-P-OP2 | -6.38 | 110.02 | 119.60 |
| 45 | 5 | 1725 | U | N3-C2-O2 | -6.38 | 117.74 | 122.20 |
| 85 | 4 | 6210 | U | O4'-C1'-C2' | 6.38 | 113.34 | 107.60 |
| 45 | 5 | 481 | G | P-O3'-C3' | 6.37 | 127.35 | 119.70 |
| 85 | 4 | 6169 | U | N1-C1'-C2' | 6.37 | 122.28 | 114.00 |
| 45 | 5 | 4958 | C | C2-N1-C1' | 6.37 | 125.80 | 118.80 |
| 49 | 2 | 1017 | U | N1-C2-O2 | 6.37 | 127.26 | 122.80 |
| 49 | 2 | 1637 | A | P-O3'-C3' | 6.36 | 127.34 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 1481 | C | N1-C2-O2 | 6.36 | 122.72 | 118.90 |
| 85 | 4 | 6209 | A | C8-N9-C1' | 6.36 | 139.15 | 127.70 |
| 45 | 5 | 2528 | G | C4-N9-C1' | 6.36 | 134.77 | 126.50 |
| 49 | 2 | 1520 | G | C8-N9-C1' | -6.36 | 118.73 | 127.00 |
| 45 | 5 | 3831 | U | N1-C2-O2 | 6.35 | 127.25 | 122.80 |
| 85 | 4 | 6188 | G | C5'-C4'-C3' | -6.35 | 105.84 | 116.00 |
| 45 | 5 | 1072 | C | P-O3'-C3' | 6.33 | 127.29 | 119.70 |
| 49 | 2 | 1139 | C | C6-N1-C2 | -6.33 | 117.77 | 120.30 |
| 49 | 2 | 193 | C | N1-C2-O2 | 6.32 | 122.69 | 118.90 |
| 49 | 2 | 1518 | C | C2-N1-C1' | 6.31 | 125.74 | 118.80 |
| 49 | 2 | 118 | C | N1-C2-O2 | 6.31 | 122.68 | 118.90 |
| 85 | 4 | 6209 | A | C4-N9-C1' | -6.31 | 114.95 | 126.30 |
| 49 | 2 | 183 | G | C4-N9-C1' | 6.30 | 134.69 | 126.50 |
| 49 | 2 | 1303 | C | N1-C2-O2 | 6.30 | 122.68 | 118.90 |
| 45 | 5 | 2661 | U | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 49 | 2 | 14 | C | C2-N1-C1' | 6.30 | 125.73 | 118.80 |
| 45 | 5 | 704 | C | N1-C2-O2 | 6.29 | 122.67 | 118.90 |
| 45 | 5 | 282 | C | N3-C2-O2 | -6.29 | 117.50 | 121.90 |
| 45 | 5 | 1725 | U | N1-C2-O2 | 6.29 | 127.20 | 122.80 |
| 45 | 5 | 233 | U | N1-C2-O2 | 6.28 | 127.19 | 122.80 |
| 45 | 5 | 3909 | C | C2-N1-C1' | 6.28 | 125.70 | 118.80 |
| 45 | 5 | 1276 | C | N3-C2-O2 | -6.27 | 117.51 | 121.90 |
| 45 | 5 | 131 | C | N3-C2-O2 | -6.25 | 117.53 | 121.90 |
| 49 | 2 | 1453 | C | C2-N1-C1' | 6.25 | 125.67 | 118.80 |
| 45 | 5 | 1084 | C | N1-C2-O2 | 6.24 | 122.64 | 118.90 |
| 45 | 5 | 1812 | C | N1-C2-O2 | 6.24 | 122.64 | 118.90 |
| 45 | 5 | 4709 | U | N1-C2-O2 | 6.24 | 127.17 | 122.80 |
| 85 | 4 | 6065 | A | C4'-C3'-O3' | 6.23 | 125.47 | 113.00 |
| 45 | 5 | 473 | C | C2-N1-C1' | 6.23 | 125.66 | 118.80 |
| 45 | 5 | 4263 | C | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 85 | 4 | 6181 | C | C4'-C3'-O3' | 6.23 | 125.46 | 113.00 |
| 45 | 5 | 2560 | C | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 45 | 5 | 1481 | C | C2-N1-C1' | 6.22 | 125.64 | 118.80 |
| 45 | 5 | 4759 | C | C2-N1-C1' | 6.22 | 125.64 | 118.80 |
| 45 | 5 | 1484 | G | N3-C4-N9 | 6.21 | 129.73 | 126.00 |
| 45 | 5 | 1478 | C | N1-C2-O2 | 6.21 | 122.62 | 118.90 |
| 85 | 4 | 6183 | G | C4'-C3'-O3' | -6.21 | 96.36 | 109.40 |
| 45 | 5 | 202 | C | C2-N1-C1' | 6.21 | 125.63 | 118.80 |
| 45 | 5 | 4413 | C | C2-N1-C1' | 6.21 | 125.63 | 118.80 |
| 45 | 5 | 1781 | U | N1-C2-O2 | 6.20 | 127.14 | 122.80 |
| 49 | 2 | 494 | C | C6-N1-C2 | -6.19 | 117.83 | 120.30 |
| 45 | 5 | 3855 | C | N1-C2-O2 | 6.19 | 122.61 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 1893 | C | N1-C2-O2 | 6.18 | 122.61 | 118.90 |
| 85 | 4 | 6217 | C | C3'-C2'-C1' | 6.18 | 106.44 | 101.50 |
| 49 | 2 | 1596 | U | N1-C2-O2 | 6.18 | 127.12 | 122.80 |
| 45 | 5 | 3909 | C | C6-N1-C2 | -6.17 | 117.83 | 120.30 |
| 49 | 2 | 1596 | U | N3-C2-O2 | -6.16 | 117.89 | 122.20 |
| 45 | 5 | 704 | C | C2-N1-C1' | 6.16 | 125.57 | 118.80 |
| 45 | 5 | 2464 | C | N3-C2-O2 | -6.15 | 117.59 | 121.90 |
| 45 | 5 | 1344 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 49 | 2 | 632 | C | N3-C2-O2 | -6.15 | 117.60 | 121.90 |
| 85 | 4 | 6198 | A | C5'-C4'-O4' | 6.15 | 116.47 | 109.10 |
| 46 | 7 | 102 | U | N3-C2-O2 | -6.14 | 117.90 | 122.20 |
| 85 | 4 | 6151 | A | O4'-C4'-C3' | -6.13 | 97.87 | 104.00 |
| 45 | 5 | 2627 | C | C2-N1-C1' | 6.12 | 125.53 | 118.80 |
| 45 | 5 | 3810 | C | N3-C2-O2 | -6.11 | 117.62 | 121.90 |
| 45 | 5 | 1081 | C | N1-C2-O2 | 6.11 | 122.57 | 118.90 |
| 45 | 5 | 2351 | C | N3-C2-O2 | -6.10 | 117.63 | 121.90 |
| 45 | 5 | 2499 | C | C2-N1-C1' | 6.10 | 125.50 | 118.80 |
| 85 | 4 | 6077 | U | C4'-C3'-O3' | 6.09 | 125.19 | 113.00 |
| 45 | 5 | 1993 | C | N1-C2-O2 | 6.09 | 122.55 | 118.90 |
| 49 | 2 | 86 | C | N1-C2-O2 | 6.09 | 122.55 | 118.90 |
| 45 | 5 | 1807 | C | C2-N1-C1' | 6.08 | 125.49 | 118.80 |
| 45 | 5 | 390 | C | N3-C2-O2 | -6.07 | 117.65 | 121.90 |
| 45 | 5 | 4266 | G | C8-N9-C1' | -6.07 | 119.11 | 127.00 |
| 49 | 2 | 13 | C | C2-N1-C1' | 6.07 | 125.48 | 118.80 |
| 49 | 2 | 429 | C | N3-C2-O2 | -6.07 | 117.65 | 121.90 |
| 85 | 4 | 6198 | A | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 85 | 4 | 6077 | U | N3-C4-C5 | -6.06 | 110.97 | 114.60 |
| 49 | 2 | 1017 | U | N3-C2-O2 | -6.05 | 117.96 | 122.20 |
| 49 | 2 | 568 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 49 | 2 | 179 | C | N3-C2-O2 | -6.04 | 117.67 | 121.90 |
| 45 | 5 | 1467 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 49 | 2 | 188 | C | C2-N1-C1' | 6.03 | 125.43 | 118.80 |
| 49 | 2 | 1443 | C | N1-C2-O2 | 6.02 | 122.51 | 118.90 |
| 45 | 5 | 4958 | C | C6-N1-C2 | -6.01 | 117.89 | 120.30 |
| 49 | 2 | 1303 | C | C2-N1-C1' | 6.01 | 125.42 | 118.80 |
| 45 | 5 | 4413 | C | N1-C2-O2 | 6.01 | 122.50 | 118.90 |
| 45 | 5 | 2802 | C | C2-N1-C1' | 6.00 | 125.40 | 118.80 |
| 85 | 4 | 6107 | A | C2'-C3'-O3' | 6.00 | 123.29 | 113.70 |
| 45 | 5 | 1081 | C | N3-C2-O2 | -5.99 | 117.71 | 121.90 |
| 47 | 8 | 119 | C | C6-N1-C2 | -5.99 | 117.91 | 120.30 |
| 49 | 2 | 632 | C | C6-N1-C2 | -5.99 | 117.91 | 120.30 |
| 45 | 5 | 3851 | U | N3-C2-O2 | -5.99 | 118.01 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 985 | C | N3-C2-O2 | -5.98 | 117.71 | 121.90 |
| 85 | 4 | 6212 | U | P-O3'-C3' | 5.98 | 126.88 | 119.70 |
| 45 | 5 | 4303 | C | C2-N1-C1' | 5.98 | 125.38 | 118.80 |
| 49 | 2 | 1298 | G | C8-N9-C1' | -5.98 | 119.23 | 127.00 |
| 45 | 5 | 4476 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 45 | 5 | 4893 | A | C2-N3-C4 | 5.97 | 113.58 | 110.60 |
| 45 | 5 | 2499 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 45 | 5 | 4612 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 47 | 8 | 64 | U | C2-N1-C1' | 5.96 | 124.86 | 117.70 |
| 45 | 5 | 1276 | C | C6-N1-C2 | -5.96 | 117.92 | 120.30 |
| 49 | 2 | 24 | C | P-O3'-C3' | 5.95 | 126.84 | 119.70 |
| 49 | 2 | 183 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 45 | 5 | 112 | C | C6-N1-C2 | -5.94 | 117.92 | 120.30 |
| 45 | 5 | 1994 | C | C2-N1-C1' | 5.94 | 125.33 | 118.80 |
| 49 | 2 | 801 | U | N1-C2-O2 | 5.93 | 126.95 | 122.80 |
| 49 | 2 | 1660 | C | C2-N1-C1' | 5.93 | 125.33 | 118.80 |
| 45 | 5 | 2528 | G | N3-C4-C5 | -5.93 | 125.64 | 128.60 |
| 45 | 5 | 2614 | C | C2-N1-C1' | 5.93 | 125.32 | 118.80 |
| 45 | 5 | 4592 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 49 | 2 | 801 | U | N3-C2-O2 | -5.92 | 118.05 | 122.20 |
| 45 | 5 | 1429 | C | N3-C2-O2 | -5.92 | 117.76 | 121.90 |
| 45 | 5 | 2572 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 49 | 2 | 1057 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 49 | 2 | 1399 | C | N1-C2-O2 | 5.91 | 122.45 | 118.90 |
| 45 | 5 | 1612 | G | C8-N9-C1' | -5.91 | 119.32 | 127.00 |
| 45 | 5 | 3882 | C | C2-N1-C1' | 5.90 | 125.29 | 118.80 |
| 45 | 5 | 174 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 45 | 5 | 2627 | C | N1-C2-O2 | 5.90 | 122.44 | 118.90 |
| 49 | 2 | 356 | C | C2-N1-C1' | 5.90 | 125.29 | 118.80 |
| 45 | 5 | 4930 | C | C6-N1-C2 | -5.88 | 117.95 | 120.30 |
| 66 | RR | 31 | LEU | CA-CB-CG | 5.86 | 128.78 | 115.30 |
| 45 | 5 | 3892 | U | N3-C2-O2 | -5.86 | 118.10 | 122.20 |
| 45 | 5 | 4928 | C | C2-N1-C1' | 5.86 | 125.24 | 118.80 |
| 49 | 2 | 1489 | A | P-O3'-C3' | 5.86 | 126.73 | 119.70 |
| 45 | 5 | 4170 | A | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 45 | 5 | 517 | C | C2-N1-C1' | 5.85 | 125.23 | 118.80 |
| 45 | 5 | 48 | G | P-O3'-C3' | 5.84 | 126.71 | 119.70 |
| 45 | 5 | 100 | C | C2-N1-C1' | 5.84 | 125.22 | 118.80 |
| 83 | 3 | 74 | C | C6-N1-C2 | -5.84 | 117.96 | 120.30 |
| 45 | 5 | 3855 | C | N3-C2-O2 | -5.83 | 117.82 | 121.90 |
| 85 | 4 | 6182 | A | C4-N9-C1' | -5.82 | 115.82 | 126.30 |
| 45 | 5 | 1431 | C | N1-C2-O2 | 5.82 | 122.39 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 49 | 2 | 1139 | C | N3-C2-O2 | -5.82 | 117.83 | 121.90 |
| 46 | 7 | 95 | C | N1-C2-O2 | 5.82 | 122.39 | 118.90 |
| 45 | 5 | 473 | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |
| 45 | 5 | 1796 | U | N1-C2-O2 | 5.82 | 126.87 | 122.80 |
| 45 | 5 | 2528 | G | N3-C4-N9 | 5.81 | 129.49 | 126.00 |
| 45 | 5 | 202 | C | N3-C2-O2 | -5.80 | 117.84 | 121.90 |
| 45 | 5 | 1193 | C | C6-N1-C2 | -5.79 | 117.98 | 120.30 |
| 49 | 2 | 1852 | C | C5-C6-N1 | 5.79 | 123.90 | 121.00 |
| 45 | 5 | 4709 | U | N3-C2-O2 | -5.79 | 118.15 | 122.20 |
| 49 | 2 | 853 | C | C2-N1-C1' | 5.79 | 125.17 | 118.80 |
| 45 | 5 | 2072 | C | N1-C2-O2 | 5.79 | 122.37 | 118.90 |
| 45 | 5 | 3693 | U | N1-C2-O2 | 5.77 | 126.84 | 122.80 |
| 45 | 5 | 2266 | C | P-O3'-C3' | 5.76 | 126.62 | 119.70 |
| 45 | 5 | 1237 | C | C2-N1-C1' | 5.76 | 125.14 | 118.80 |
| 45 | 5 | 1210 | C | C2-N1-C1' | 5.76 | 125.13 | 118.80 |
| 45 | 5 | 282 | C | C2-N1-C1' | 5.75 | 125.13 | 118.80 |
| 85 | 4 | 6216 | U | N1-C1'-C2' | -5.75 | 105.67 | 112.00 |
| 45 | 5 | 67 | C | N3-C2-O2 | -5.75 | 117.88 | 121.90 |
| 45 | 5 | 2820 | C | N3-C2-O2 | -5.75 | 117.88 | 121.90 |
| 45 | 5 | 74 | G | C4-N9-C1' | 5.75 | 133.97 | 126.50 |
| 85 | 4 | 6178 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 45 | 5 | 1781 | U | N3-C2-O2 | -5.73 | 118.19 | 122.20 |
| 49 | 2 | 356 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 49 | 2 | 553 | U | OP1-P-O3' | 5.73 | 117.81 | 105.20 |
| 47 | 8 | 124 | U | P-O3'-C3' | 5.73 | 126.58 | 119.70 |
| 49 | 2 | 1311 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 49 | 2 | 1022 | U | C2-N1-C1' | 5.72 | 124.57 | 117.70 |
| 45 | 5 | 1827 | C | N3-C2-O2 | -5.72 | 117.89 | 121.90 |
| 49 | 2 | 632 | C | C2-N1-C1' | 5.72 | 125.09 | 118.80 |
| 2 | B | 17 | LEU | CA-CB-CG | 5.72 | 128.45 | 115.30 |
| 47 | 8 | 119 | C | C2-N1-C1' | 5.72 | 125.09 | 118.80 |
| 49 | 2 | 1063 | C | C5-C6-N1 | 5.71 | 123.86 | 121.00 |
| 45 | 5 | 1467 | C | N3-C2-O2 | -5.71 | 117.91 | 121.90 |
| 45 | 5 | 304 | C | N1-C2-O2 | 5.71 | 122.32 | 118.90 |
| 45 | 5 | 233 | U | N3-C2-O2 | -5.70 | 118.21 | 122.20 |
| 49 | 2 | 1742 | C | N3-C2-O2 | -5.70 | 117.91 | 121.90 |
| 49 | 2 | 1261 | C | C5-C6-N1 | 5.69 | 123.85 | 121.00 |
| 45 | 5 | 971 | U | C2-N1-C1' | 5.69 | 124.53 | 117.70 |
| 45 | 5 | 67 | C | C2-N1-C1' | 5.69 | 125.05 | 118.80 |
| 45 | 5 | 4177 | C | N3-C2-O2 | -5.69 | 117.92 | 121.90 |
| 45 | 5 | 18 | C | N3-C2-O2 | -5.68 | 117.92 | 121.90 |
| 45 | 5 | 18 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 4948 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 85 | 4 | 6179 | U | O4'-C1'-N1 | 5.68 | 112.75 | 108.20 |
| 85 | 4 | 6187 | A | C3'-C2'-O2' | 5.68 | 129.78 | 113.30 |
| 45 | 5 | 4261 | C | N3-C2-O2 | -5.67 | 117.93 | 121.90 |
| 45 | 5 | 220 | C | C5-C6-N1 | 5.67 | 123.84 | 121.00 |
| 49 | 2 | 1019 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 45 | 5 | 3835 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 49 | 2 | 1453 | C | N1-C2-O2 | 5.66 | 122.30 | 118.90 |
| 45 | 5 | 2572 | C | C2-N1-C1' | 5.66 | 125.02 | 118.80 |
| 45 | 5 | 4476 | C | C2-N1-C1' | 5.66 | 125.02 | 118.80 |
| 45 | 5 | 4747 | C | C2-N1-C1' | 5.65 | 125.02 | 118.80 |
| 45 | 5 | 115 | C | C2-N1-C1' | 5.65 | 125.01 | 118.80 |
| 45 | 5 | 1193 | C | C6-N1-C1' | -5.64 | 114.03 | 120.80 |
| 45 | 5 | 4525 | C | N1-C2-O2 | 5.64 | 122.28 | 118.90 |
| 45 | 5 | 4360 | U | N1-C2-O2 | 5.63 | 126.75 | 122.80 |
| 85 | 4 | 6059 | U | C2'-C3'-O3' | 5.63 | 122.71 | 113.70 |
| 45 | 5 | 1193 | C | N1-C2-O2 | 5.62 | 122.28 | 118.90 |
| 45 | 5 | 390 | C | C6-N1-C2 | -5.62 | 118.05 | 120.30 |
| 45 | 5 | 1827 | C | C2-N1-C1' | 5.62 | 124.98 | 118.80 |
| 49 | 2 | 1314 | U | C2-N1-C1' | 5.62 | 124.45 | 117.70 |
| 49 | 2 | 899 | U | N1-C2-O2 | 5.62 | 126.73 | 122.80 |
| 45 | 5 | 1727 | U | C2-N1-C1' | 5.61 | 124.43 | 117.70 |
| 45 | 5 | 126 | C | C2-N1-C1' | 5.61 | 124.97 | 118.80 |
| 49 | 2 | 1660 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 49 | 2 | 1253 | A | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 85 | 4 | 6215 | C | C2'-C3'-O3' | -5.60 | 97.19 | 109.50 |
| 49 | 2 | 801 | U | C2-N1-C1' | 5.59 | 124.41 | 117.70 |
| 49 | 2 | 178 | C | C5-C6-N1 | 5.59 | 123.80 | 121.00 |
| 49 | 2 | 585 | C | N3-C2-O2 | -5.59 | 117.99 | 121.90 |
| 49 | 2 | 621 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 45 | 5 | 4261 | C | C2-N1-C1' | 5.59 | 124.95 | 118.80 |
| 45 | 5 | 4560 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 45 | 5 | 1781 | U | C2-N1-C1' | 5.59 | 124.41 | 117.70 |
| 49 | 2 | 1595 | U | C2-N1-C1' | 5.58 | 124.40 | 117.70 |
| 45 | 5 | 4885 | U | N1-C2-O2 | 5.58 | 126.70 | 122.80 |
| 49 | 2 | 1123 | C | N3-C2-O2 | -5.58 | 118.00 | 121.90 |
| 45 | 5 | 3693 | U | N3-C2-O2 | -5.56 | 118.31 | 122.20 |
| 49 | 2 | 130 | G | N3-C4-N9 | 5.56 | 129.34 | 126.00 |
| 49 | 2 | 899 | U | N3-C2-O2 | -5.55 | 118.31 | 122.20 |
| 49 | 2 | 130 | G | N3-C4-C5 | -5.55 | 125.83 | 128.60 |
| 45 | 5 | 4885 | U | N3-C2-O2 | -5.55 | 118.32 | 122.20 |
| 45 | 5 | 1796 | U | N3-C2-O2 | -5.54 | 118.32 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 4052 | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 85 | 4 | 6187 | A | C4-N9-C1' | -5.54 | 116.32 | 126.30 |
| 45 | 5 | 2351 | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 49 | 2 | 183 | G | N3-C4-N9 | 5.54 | 129.32 | 126.00 |
| 45 | 5 | 4880 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 49 | 2 | 1753 | C | C2-N1-C1' | 5.53 | 124.88 | 118.80 |
| 85 | 4 | 6065 | A | C5'-C4'-C3' | 5.52 | 124.84 | 116.00 |
| 45 | 5 | 4929 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 45 | 5 | 4893 | A | C4-N9-C1' | 5.52 | 136.24 | 126.30 |
| 49 | 2 | 430 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 49 | 2 | 1118 | C | N3-C2-O2 | -5.52 | 118.04 | 121.90 |
| 85 | 4 | 6179 | U | C5'-C4'-C3' | 5.52 | 124.83 | 116.00 |
| 49 | 2 | 55 | U | C2-N1-C1' | 5.51 | 124.31 | 117.70 |
| 45 | 5 | 2008 | U | C2-N1-C1' | 5.51 | 124.31 | 117.70 |
| 45 | 5 | 1458 | C | N1-C2-O2 | 5.51 | 122.20 | 118.90 |
| 85 | 4 | 6182 | A | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 85 | 4 | 6150 | C | C4'-C3'-O3' | 5.50 | 124.01 | 113.00 |
| 45 | 5 | 1429 | C | C2-N1-C1' | 5.50 | 124.85 | 118.80 |
| 45 | 5 | 1478 | C | C2-N1-C1' | 5.49 | 124.84 | 118.80 |
| 45 | 5 | 2373 | C | N3-C2-O2 | -5.49 | 118.06 | 121.90 |
| 49 | 2 | 630 | U | C2-N1-C1' | 5.49 | 124.29 | 117.70 |
| 49 | 2 | 1395 | C | OP1-P-O3' | 5.49 | 117.27 | 105.20 |
| 49 | 2 | 823 | U | N3-C2-O2 | -5.48 | 118.36 | 122.20 |
| 45 | 5 | 1179 | U | C2-N1-C1' | 5.48 | 124.27 | 117.70 |
| 49 | 2 | 24 | C | C2-N1-C1' | 5.48 | 124.82 | 118.80 |
| 45 | 5 | 3870 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 45 | 5 | 4303 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 45 | 5 | 985 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 45 | 5 | 4148 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 45 | 5 | 130 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 45 | 5 | 180 | C | N1-C2-O2 | 5.46 | 122.17 | 118.90 |
| 45 | 5 | 196 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 45 | 5 | 1484 | G | C8-N9-C1' | -5.45 | 119.91 | 127.00 |
| 47 | 8 | 130 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 45 | 5 | 282 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 49 | 2 | 1271 | C | N3-C2-O2 | -5.45 | 118.09 | 121.90 |
| 49 | 2 | 1513 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 49 | 2 | 14 | C | C5-C6-N1 | 5.45 | 123.72 | 121.00 |
| 45 | 5 | 1237 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 45 | 5 | 1460 | C | N1-C2-O2 | 5.44 | 122.16 | 118.90 |
| 85 | 4 | 6166 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 49 | 2 | 24 | C | N3-C2-O2 | -5.44 | 118.09 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 49 | 2 | 1742 | C | C2-N1-C1' | 5.44 | 124.78 | 118.80 |
| 85 | 4 | 6182 | A | C8-N9-C1' | 5.44 | 137.48 | 127.70 |
| 57 | II | 122 | LEU | CA-CB-CG | 5.43 | 127.78 | 115.30 |
| 45 | 5 | 1215 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 45 | 5 | 1325 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 45 | 5 | 3835 | C | N3-C2-O2 | -5.42 | 118.11 | 121.90 |
| 49 | 2 | 182 | C | P-O3'-C3' | 5.42 | 126.20 | 119.70 |
| 45 | 5 | 4709 | U | C2-N1-C1' | 5.42 | 124.20 | 117.70 |
| 49 | 2 | 183 | G | C8-N9-C1' | -5.41 | 119.96 | 127.00 |
| 49 | 2 | 55 | U | N1-C2-O2 | 5.41 | 126.59 | 122.80 |
| 85 | 4 | 6216 | U | C2-N1-C1' | -5.41 | 111.21 | 117.70 |
| 45 | 5 | 654 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 45 | 5 | 3882 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 49 | 2 | 1518 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 45 | 5 | 2351 | C | C2-N1-C1' | 5.40 | 124.74 | 118.80 |
| 49 | 2 | 585 | C | C2-N1-C1' | 5.40 | 124.74 | 118.80 |
| 49 | 2 | 17 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 49 | 2 | 879 | C | N3-C2-O2 | -5.39 | 118.13 | 121.90 |
| 85 | 4 | 6064 | G | C4'-C3'-O3' | 5.39 | 123.78 | 113.00 |
| 1 | A | 29 | LEU | CA-CB-CG | 5.38 | 127.68 | 115.30 |
| 49 | 2 | 295 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 45 | 5 | 221 | C | C2-N1-C1' | 5.38 | 124.72 | 118.80 |
| 45 | 5 | 4398 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 49 | 2 | 130 | G | C4-N9-C1' | 5.38 | 133.49 | 126.50 |
| 45 | 5 | 2856 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 45 | 5 | 3810 | C | C6-N1-C1' | -5.37 | 114.35 | 120.80 |
| 49 | 2 | 1533 | A | C2-N3-C4 | 5.37 | 113.29 | 110.60 |
| 85 | 4 | 6199 | A | O4'-C1'-C2' | 5.36 | 112.43 | 107.60 |
| 85 | 4 | 6204 | A | OP1-P-O3' | 5.36 | 116.98 | 105.20 |
| 45 | 5 | 3829 | G | N3-C4-C5 | -5.35 | 125.92 | 128.60 |
| 85 | 4 | 6169 | U | C4'-C3'-O3' | 5.35 | 123.71 | 113.00 |
| 85 | 4 | 6187 | A | C8-N9-C1' | 5.35 | 137.33 | 127.70 |
| 45 | 5 | 934 | C | N1-C2-O2 | 5.35 | 122.11 | 118.90 |
| 49 | 2 | 1853 | C | N1-C2-O2 | 5.34 | 122.11 | 118.90 |
| 45 | 5 | 3762 | U | N1-C2-O2 | 5.34 | 126.54 | 122.80 |
| 49 | 2 | 340 | C | N3-C2-O2 | -5.34 | 118.16 | 121.90 |
| 45 | 5 | 4127 | A | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 45 | 5 | 4177 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 45 | 5 | 2528 | G | C8-N9-C1' | -5.33 | 120.07 | 127.00 |
| 45 | 5 | 2439 | G | C4-N9-C1' | 5.32 | 133.42 | 126.50 |
| 49 | 2 | 427 | U | C2-N1-C1' | 5.32 | 124.08 | 117.70 |
| 85 | 4 | 6197 | A | C4'-C3'-O3' | 5.32 | 123.64 | 113.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 67 | C | C6-N1-C2 | -5.32 | 118.17 | 120.30 |
| 45 | 5 | 5059 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 49 | 2 | 1117 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 45 | 5 | 1180 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 49 | 2 | 183 | G | N3-C4-C5 | -5.31 | 125.94 | 128.60 |
| 49 | 2 | 1865 | C | C6-N1-C2 | -5.31 | 118.18 | 120.30 |
| 45 | 5 | 3892 | U | N1-C2-O2 | 5.31 | 126.51 | 122.80 |
| 45 | 5 | 4942 | C | N1-C2-O2 | 5.31 | 122.08 | 118.90 |
| 45 | 5 | 4360 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 45 | 5 | 1977 | C | N3-C2-O2 | -5.30 | 118.19 | 121.90 |
| 45 | 5 | 2439 | G | N3-C4-C5 | -5.29 | 125.95 | 128.60 |
| 45 | 5 | 4774 | C | N3-C2-O2 | -5.29 | 118.19 | 121.90 |
| 49 | 2 | 142 | C | N1-C2-O2 | 5.29 | 122.08 | 118.90 |
| 49 | 2 | 676 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 85 | 4 | 6183 | G | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 45 | 5 | 4592 | C | N3-C2-O2 | -5.28 | 118.20 | 121.90 |
| 85 | 4 | 6210 | U | P-O3'-C3' | 5.28 | 126.04 | 119.70 |
| 45 | 5 | 4774 | C | C2-N1-C1' | 5.28 | 124.60 | 118.80 |
| 67 | SS | 96 | ILE | CG1-CB-CG2 | -5.28 | 99.79 | 111.40 |
| 45 | 5 | 1893 | C | C2-N1-C1' | 5.28 | 124.60 | 118.80 |
| 45 | 5 | 1211 | G | P-O3'-C3' | 5.27 | 126.03 | 119.70 |
| 45 | 5 | 4627 | U | C2-N1-C1' | 5.27 | 124.02 | 117.70 |
| 49 | 2 | 687 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 45 | 5 | 2502 | A | P-O3'-C3' | 5.27 | 126.02 | 119.70 |
| 45 | 5 | 4405 | G | C4-N9-C1' | 5.27 | 133.35 | 126.50 |
| 45 | 5 | 1429 | C | C6-N1-C2 | -5.26 | 118.19 | 120.30 |
| 45 | 5 | 4928 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 49 | 2 | 638 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 45 | 5 | 345 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 49 | 2 | 18 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 85 | 4 | 6198 | A | N9-C1'-C2' | 5.26 | 120.84 | 114.00 |
| 49 | 2 | 1750 | C | C5-C6-N1 | 5.25 | 123.63 | 121.00 |
| 45 | 5 | 4759 | C | N3-C2-O2 | -5.25 | 118.22 | 121.90 |
| 45 | 5 | 3855 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 45 | 5 | 1639 | U | C2-N1-C1' | 5.24 | 123.99 | 117.70 |
| 45 | 5 | 2464 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 45 | 5 | 2439 | G | N3-C4-N9 | 5.24 | 129.14 | 126.00 |
| 85 | 4 | 6167 | U | C4'-C3'-C2' | 5.23 | 107.83 | 102.60 |
| 37 | 1 | 49 | LEU | CA-CB-CG | 5.23 | 127.33 | 115.30 |
| 45 | 5 | 517 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 49 | 2 | 1017 | U | C2-N1-C1' | 5.23 | 123.98 | 117.70 |
| 85 | 4 | 6204 | A | OP2-P-O3' | 5.23 | 116.70 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 46 | 7 | 29 | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 49 | 2 | 179 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 49 | 2 | 879 | C | C2-N1-C1' | 5.22 | 124.54 | 118.80 |
| 45 | 5 | 2271 | C | N3-C2-O2 | -5.22 | 118.25 | 121.90 |
| 45 | 5 | 458 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 49 | 2 | 1865 | C | C6-N1-C1' | -5.21 | 114.55 | 120.80 |
| 45 | 5 | 4893 | A | N3-C4-N9 | 5.21 | 131.56 | 127.40 |
| 46 | 7 | 102 | U | C2-N1-C1' | 5.20 | 123.94 | 117.70 |
| 49 | 2 | 1636 | G | C4-N9-C1' | 5.20 | 133.26 | 126.50 |
| 85 | 4 | 6151 | A | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 49 | 2 | 805 | U | N3-C2-O2 | -5.20 | 118.56 | 122.20 |
| 49 | 2 | 496 | C | C2-N1-C1' | 5.19 | 124.51 | 118.80 |
| 45 | 5 | 4405 | G | N3-C4-N9 | 5.19 | 129.11 | 126.00 |
| 45 | 5 | 4930 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 45 | 5 | 3831 | U | C2-N1-C1' | 5.18 | 123.92 | 117.70 |
| 45 | 5 | 4969 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 45 | 5 | 1633 | G | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 45 | 5 | 4747 | C | N3-C2-O2 | -5.17 | 118.28 | 121.90 |
| 45 | 5 | 4775 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 49 | 2 | 340 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 45 | 5 | 4930 | C | C5-C6-N1 | 5.17 | 123.58 | 121.00 |
| 45 | 5 | 4958 | C | C5-C6-N1 | 5.17 | 123.58 | 121.00 |
| 45 | 5 | 202 | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 45 | 5 | 2655 | C | C5-C6-N1 | 5.16 | 123.58 | 121.00 |
| 45 | 5 | 4696 | C | N1-C2-O2 | 5.16 | 121.99 | 118.90 |
| 49 | 2 | 494 | C | C5-C6-N1 | 5.15 | 123.58 | 121.00 |
| 49 | 2 | 1261 | C | C6-N1-C1' | -5.14 | 114.63 | 120.80 |
| 85 | 4 | 6066 | G | P-O5'-C5' | 5.14 | 129.12 | 120.90 |
| 49 | 2 | 55 | U | N3-C2-O2 | -5.14 | 118.60 | 122.20 |
| 45 | 5 | 2819 | U | C6-N1-C2 | -5.14 | 117.92 | 121.00 |
| 45 | 5 | 50 | C | N3-C2-O2 | -5.13 | 118.31 | 121.90 |
| 45 | 5 | 2073 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 45 | 5 | 2470 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 49 | 2 | 14 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 49 | 2 | 459 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 45 | 5 | 2726 | G | N3-C4-C5 | -5.13 | 126.03 | 128.60 |
| 45 | 5 | 1478 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 45 | 5 | 4206 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 45 | 5 | 930 | G | P-O3'-C3' | 5.12 | 125.85 | 119.70 |
| 85 | 4 | 6178 | U | N3-C2-O2 | -5.12 | 118.61 | 122.20 |
| 49 | 2 | 293 | C | C2-N1-C1' | 5.12 | 124.43 | 118.80 |
| 45 | 5 | 112 | C | C5-C6-N1 | 5.12 | 123.56 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 85 | 4 | 6198 | A | O4'-C4'-C3' | 5.12 | 110.19 | 106.10 |
| 49 | 2 | 632 | C | C5-C6-N1 | 5.12 | 123.56 | 121.00 |
| 45 | 5 | 4158 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 45 | 5 | 3761 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 49 | 2 | 857 | U | N3-C2-O2 | -5.11 | 118.62 | 122.20 |
| 45 | 5 | 1594 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 49 | 2 | 1118 | C | C6-N1-C1' | -5.11 | 114.67 | 120.80 |
| 45 | 5 | 3767 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 45 | 5 | 74 | G | C8-N9-C1' | -5.10 | 120.37 | 127.00 |
| 45 | 5 | 1976 | G | C4-N9-C1' | 5.10 | 133.13 | 126.50 |
| 45 | 5 | 2532 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 49 | 2 | 1518 | C | N3-C2-O2 | -5.09 | 118.33 | 121.90 |
| 45 | 5 | 3851 | U | C2-N1-C1' | 5.09 | 123.81 | 117.70 |
| 45 | 5 | 4130 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 45 | 5 | 2817 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 49 | 2 | 1442 | U | C5-C6-N1 | 5.09 | 125.24 | 122.70 |
| 45 | 5 | 1084 | C | N3-C2-O2 | -5.09 | 118.34 | 121.90 |
| 45 | 5 | 126 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 45 | 5 | 4423 | U | C2-N1-C1' | 5.08 | 123.80 | 117.70 |
| 45 | 5 | 517 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 45 | 5 | 1179 | U | N1-C2-O2 | 5.07 | 126.35 | 122.80 |
| 45 | 5 | 3810 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 45 | 5 | 2540 | C | C5-C6-N1 | 5.07 | 123.53 | 121.00 |
| 45 | 5 | 2818 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 49 | 2 | 1757 | G | N3-C4-C5 | -5.07 | 126.07 | 128.60 |
| 45 | 5 | 304 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 85 | 4 | 6169 | U | C5'-C4'-C3' | 5.07 | 124.10 | 116.00 |
| 61 | MM | 42 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 45 | 5 | 3625 | G | P-O3'-C3' | 5.05 | 125.76 | 119.70 |
| 45 | 5 | 3690 | U | N3-C2-O2 | -5.05 | 118.66 | 122.20 |
| 49 | 2 | 1624 | U | C6-N1-C1' | -5.05 | 114.13 | 121.20 |
| 85 | 4 | 6196 | A | C2'-C3'-O3' | 5.05 | 121.77 | 113.70 |
| 45 | 5 | 3673 | C | N1-C2-O2 | 5.04 | 121.93 | 118.90 |
| 45 | 5 | 3762 | U | C2-N1-C1' | 5.04 | 123.75 | 117.70 |
| 49 | 2 | 1271 | C | C2-N1-C1' | 5.04 | 124.35 | 118.80 |
| 49 | 2 | 1123 | C | C2-N1-C1' | 5.04 | 124.35 | 118.80 |
| 45 | 5 | 1812 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 45 | 5 | 125 | C | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 49 | 2 | 1664 | A | OP1-P-O3' | 5.04 | 116.28 | 105.20 |
| 49 | 2 | 402 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 45 | 5 | 4896 | G | C4-N9-C1' | 5.02 | 133.03 | 126.50 |
| 49 | 2 | 151 | C | C2-N1-C1' | 5.02 | 124.32 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 5 | 4053 | A | C8-N9-C4 | -5.02 | 103.79 | 105.80 |
| 49 | 2 | 1738 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 49 | 2 | 568 | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 45 | 5 | 1727 | U | N1-C2-O2 | 5.01 | 126.31 | 122.80 |
| 45 | 5 | 4869 | U | C2-N1-C1' | 5.01 | 123.71 | 117.70 |
| 49 | 2 | 179 | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 45 | 5 | 704 | C | N3-C2-O2 | -5.00 | 118.40 | 121.90 |
| 45 | 5 | 3709 | U | C2-N1-C1' | 5.00 | 123.70 | 117.70 |
| 85 | 4 | 6187 | A | N9-C1'-C2' | 5.00 | 120.50 | 114.00 |
| 45 | 5 | 1210 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |
| 45 | 5 | 2072 | C | N3-C2-O2 | -5.00 | 118.40 | 121.90 |
| 45 | 5 | 2819 | U | C5-C6-N1 | 5.00 | 125.20 | 122.70 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 85 | 4 | 6210 | U | C1' |

All (20) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 85 | 4 | 6065 | A | Sidechain |
| 85 | 4 | 6066 | G | Sidechain |
| 85 | 4 | 6067 | G | Sidechain |
| 85 | 4 | 6077 | U | Sidechain |
| 85 | 4 | 6151 | A | Sidechain |
| 85 | 4 | 6177 | U | Sidechain |
| 85 | 4 | 6178 | U | Sidechain |
| 85 | 4 | 6179 | U | Sidechain |
| 85 | 4 | 6181 | C | Sidechain |
| 85 | 4 | 6197 | A | Sidechain |
| 85 | 4 | 6198 | A | Sidechain |
| 85 | 4 | 6199 | A | Sidechain |
| 85 | 4 | 6210 | U | Sidechain |
| 85 | 4 | 6216 | U | Sidechain |
| 84 | 9 | 240 | GLY | Peptide |
| 50 | BB | 12 | GLU | Peptide |
| 3 | C | 151 | PRO | Peptide |
| 65 | QQ | 19 | GLY | Peptide |
| 67 | SS | 89 | SER | Peptide |
| 73 | YY | 61 | GLN | 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 | |
|---|---|---|---|---|---|---|---|
| 1 | A | 237/257 (92%) | 223 (94%) | 14 (6%) | 0 | 100 | 100 |
| 2 | B | 392/403 (97%) | 381 (97%) | 11 (3%) | 0 | 100 | 100 |
| 3 | C | 358/392 (91%) | 341 (95%) | 17 (5%) | 0 | 100 | 100 |
| 4 | D | 291/297 (98%) | 281 (97%) | 10 (3%) | 0 | 100 | 100 |
| 5 | E | 208/291 (72%) | 198 (95%) | 10 (5%) | 0 | 100 | 100 |
| 6 | F | 223/249 (90%) | 214 (96%) | 9 (4%) | 0 | 100 | 100 |
| 7 | G | 229/242 (95%) | 218 (95%) | 11 (5%) | 0 | 100 | 100 |
| 8 | H | 188/192 (98%) | 176 (94%) | 12 (6%) | 0 | 100 | 100 |
| 9 | I | 201/214 (94%) | 192 (96%) | 9 (4%) | 0 | 100 | 100 |
| 10 | J | 168/178 (94%) | 165 (98%) | 3 (2%) | 0 | 100 | 100 |
| 11 | L | 208/211 (99%) | 198 (95%) | 10 (5%) | 0 | 100 | 100 |
| 12 | M | 133/198 (67%) | 128 (96%) | 5 (4%) | 0 | 100 | 100 |
| 13 | N | 201/204 (98%) | 189 (94%) | 12 (6%) | 0 | 100 | 100 |
| 14 | O | 194/198 (98%) | 186 (96%) | 8 (4%) | 0 | 100 | 100 |
| 15 | P | 151/187 (81%) | 147 (97%) | 4 (3%) | 0 | 100 | 100 |
| 16 | Q | 185/187 (99%) | 179 (97%) | 6 (3%) | 0 | 100 | 100 |
| 17 | R | 178/181 (98%) | 174 (98%) | 4 (2%) | 0 | 100 | 100 |
| 18 | S | 174/176 (99%) | 167 (96%) | 7 (4%) | 0 | 100 | 100 |
| 19 | T | 157/160 (98%) | 150 (96%) | 7 (4%) | 0 | 100 | 100 |
| 20 | U | 97/99 (98%) | 96 (99%) | 1 (1%) | 0 | 100 | 100 |
| 21 | V | 127/140 (91%) | 123 (97%) | 4 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 22 | W | 102/157 (65%) | 99 (97%) | 3 (3%) | 0 | 100 | 100 |
| 23 | X | 116/156 (74%) | 109 (94%) | 7 (6%) | 0 | 100 | 100 |
| 24 | Y | 132/145 (91%) | 129 (98%) | 3 (2%) | 0 | 100 | 100 |
| 25 | Z | 133/136 (98%) | 123 (92%) | 10 (8%) | 0 | 100 | 100 |
| 26 | a | 145/148 (98%) | 137 (94%) | 8 (6%) | 0 | 100 | 100 |
| 27 | b | 100/226 (44%) | 99 (99%) | 1 (1%) | 0 | 100 | 100 |
| 28 | c | 96/115 (84%) | 94 (98%) | 2 (2%) | 0 | 100 | 100 |
| 29 | d | 105/125 (84%) | 97 (92%) | 8 (8%) | 0 | 100 | 100 |
| 30 | e | 126/135 (93%) | 123 (98%) | 3 (2%) | 0 | 100 | 100 |
| 31 | f | 107/110 (97%) | 98 (92%) | 9 (8%) | 0 | 100 | 100 |
| 32 | g | 112/126 (89%) | 109 (97%) | 3 (3%) | 0 | 100 | 100 |
| 33 | h | 120/123 (98%) | 118 (98%) | 2 (2%) | 0 | 100 | 100 |
| 34 | i | 100/105 (95%) | 98 (98%) | 2 (2%) | 0 | 100 | 100 |
| 35 | j | 84/97 (87%) | 79 (94%) | 5 (6%) | 0 | 100 | 100 |
| 36 | k | 67/69 (97%) | 65 (97%) | 2 (3%) | 0 | 100 | 100 |
| 37 | l | 48/51 (94%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 38 | m | 50/52 (96%) | 47 (94%) | 3 (6%) | 0 | 100 | 100 |
| 39 | n | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 40 | o | 102/106 (96%) | 97 (95%) | 5 (5%) | 0 | 100 | 100 |
| 41 | p | 89/92 (97%) | 86 (97%) | 3 (3%) | 0 | 100 | 100 |
| 42 | r | 122/137 (89%) | 119 (98%) | 3 (2%) | 0 | 100 | 100 |
| 43 | s | 194/303 (64%) | 186 (96%) | 8 (4%) | 0 | 100 | 100 |
| 44 | t | 151/195 (77%) | 135 (89%) | 16 (11%) | 0 | 100 | 100 |
| 48 | K | 204/217 (94%) | 182 (89%) | 21 (10%) | 1 (0%) | 29 | 67 |
| 50 | BB | 215/217 (99%) | 202 (94%) | 13 (6%) | 0 | 100 | 100 |
| 51 | CC | 211/264 (80%) | 197 (93%) | 14 (7%) | 0 | 100 | 100 |
| 52 | DD | 219/221 (99%) | 216 (99%) | 3 (1%) | 0 | 100 | 100 |
| 53 | EE | 226/281 (80%) | 217 (96%) | 9 (4%) | 0 | 100 | 100 |
| 54 | FF | 260/262 (99%) | 244 (94%) | 16 (6%) | 0 | 100 | 100 |
| 55 | GG | 181/204 (89%) | 173 (96%) | 8 (4%) | 0 | 100 | 100 |
| 56 | HH | 235/249 (94%) | 227 (97%) | 8 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 57 | II | 181/194 (93%) | 173 (96%) | 8 (4%) | 0 | 100 | 100 |
| 58 | JJ | 204/206 (99%) | 190 (93%) | 14 (7%) | 0 | 100 | 100 |
| 59 | KK | 183/194 (94%) | 181 (99%) | 2 (1%) | 0 | 100 | 100 |
| 60 | LL | 94/149 (63%) | 90 (96%) | 4 (4%) | 0 | 100 | 100 |
| 61 | MM | 139/158 (88%) | 132 (95%) | 7 (5%) | 0 | 100 | 100 |
| 62 | NN | 115/132 (87%) | 107 (93%) | 8 (7%) | 0 | 100 | 100 |
| 63 | OO | 147/151 (97%) | 145 (99%) | 2 (1%) | 0 | 100 | 100 |
| 64 | PP | 134/151 (89%) | 126 (94%) | 8 (6%) | 0 | 100 | 100 |
| 65 | QQ | 113/145 (78%) | 102 (90%) | 10 (9%) | 1 (1%) | 17 | 56 |
| 66 | RR | 140/172 (81%) | 133 (95%) | 7 (5%) | 0 | 100 | 100 |
| 67 | SS | 130/135 (96%) | 119 (92%) | 11 (8%) | 0 | 100 | 100 |
| 68 | TT | 142/152 (93%) | 133 (94%) | 9 (6%) | 0 | 100 | 100 |
| 69 | UU | 139/145 (96%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 70 | VV | 98/119 (82%) | 96 (98%) | 2 (2%) | 0 | 100 | 100 |
| 71 | WW | 81/83 (98%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 72 | XX | 127/130 (98%) | 120 (94%) | 7 (6%) | 0 | 100 | 100 |
| 73 | YY | 139/143 (97%) | 131 (94%) | 7 (5%) | 1 (1%) | 22 | 61 |
| 74 | ZZ | 122/134 (91%) | 120 (98%) | 2 (2%) | 0 | 100 | 100 |
| 75 | aa | 73/125 (58%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 76 | bb | 99/101 (98%) | 92 (93%) | 7 (7%) | 0 | 100 | 100 |
| 77 | cc | 81/84 (96%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 78 | dd | 60/69 (87%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 79 | ee | 53/56 (95%) | 48 (91%) | 5 (9%) | 0 | 100 | 100 |
| 80 | ff | 55/133 (41%) | 49 (89%) | 6 (11%) | 0 | 100 | 100 |
| 81 | gg | 66/156 (42%) | 63 (96%) | 3 (4%) | 0 | 100 | 100 |
| 82 | hh | 310/317 (98%) | 292 (94%) | 18 (6%) | 0 | 100 | 100 |
| 84 | 9 | 854/856 (100%) | 801 (94%) | 53 (6%) | 0 | 100 | 100 |
| All | All | 12554/14095 (89%) | 11964 (95%) | 587 (5%) | 3 (0%) | 100 | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | K | 59 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 73 | YY | 62 | PRO |
| 65 | QQ | 19 | GLY |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 172/199 (86%) | 167 (97%) | 5 (3%) | 42 74 |
| 2 | B | 342/348 (98%) | 341 (100%) | 1 (0%) | 92 96 |
| 3 | C | 302/323 (94%) | 295 (98%) | 7 (2%) | 50 78 |
| 4 | D | 247/250 (99%) | 245 (99%) | 2 (1%) | 81 93 |
| 5 | E | 190/251 (76%) | 188 (99%) | 2 (1%) | 73 88 |
| 6 | F | 196/218 (90%) | 195 (100%) | 1 (0%) | 88 95 |
| 7 | G | 200/208 (96%) | 197 (98%) | 3 (2%) | 65 85 |
| 8 | H | 169/171 (99%) | 164 (97%) | 5 (3%) | 41 73 |
| 9 | I | 175/181 (97%) | 173 (99%) | 2 (1%) | 73 88 |
| 10 | J | 143/149 (96%) | 142 (99%) | 1 (1%) | 84 94 |
| 11 | L | 175/176 (99%) | 173 (99%) | 2 (1%) | 73 88 |
| 12 | M | 116/151 (77%) | 115 (99%) | 1 (1%) | 78 91 |
| 13 | N | 171/172 (99%) | 171 (100%) | 0 | 100 100 |
| 14 | O | 170/170 (100%) | 167 (98%) | 3 (2%) | 59 82 |
| 15 | P | 134/165 (81%) | 132 (98%) | 2 (2%) | 65 85 |
| 16 | Q | 164/164 (100%) | 162 (99%) | 2 (1%) | 71 88 |
| 17 | R | 159/160 (99%) | 157 (99%) | 2 (1%) | 69 87 |
| 18 | S | 157/157 (100%) | 157 (100%) | 0 | 100 100 |
| 19 | T | 139/140 (99%) | 137 (99%) | 2 (1%) | 67 86 |
| 20 | U | 89/89 (100%) | 89 (100%) | 0 | 100 100 |
| 21 | V | 100/107 (94%) | 98 (98%) | 2 (2%) | 55 80 |
| 22 | W | 86/126 (68%) | 86 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 23 | X | 106/134 (79%) | 106 (100%) | 0 | 100 | 100 |
| 24 | Y | 124/135 (92%) | 123 (99%) | 1 (1%) | 81 | 93 |
| 25 | Z | 117/118 (99%) | 117 (100%) | 0 | 100 | 100 |
| 26 | a | 119/120 (99%) | 117 (98%) | 2 (2%) | 60 | 83 |
| 27 | b | 84/172 (49%) | 82 (98%) | 2 (2%) | 49 | 77 |
| 28 | c | 84/98 (86%) | 84 (100%) | 0 | 100 | 100 |
| 29 | d | 98/110 (89%) | 96 (98%) | 2 (2%) | 55 | 80 |
| 30 | e | 114/121 (94%) | 114 (100%) | 0 | 100 | 100 |
| 31 | f | 88/89 (99%) | 85 (97%) | 3 (3%) | 37 | 70 |
| 32 | g | 98/106 (92%) | 98 (100%) | 0 | 100 | 100 |
| 33 | h | 109/110 (99%) | 109 (100%) | 0 | 100 | 100 |
| 34 | i | 86/89 (97%) | 85 (99%) | 1 (1%) | 71 | 88 |
| 35 | j | 73/80 (91%) | 72 (99%) | 1 (1%) | 67 | 86 |
| 36 | k | 64/64 (100%) | 64 (100%) | 0 | 100 | 100 |
| 37 | l | 47/48 (98%) | 46 (98%) | 1 (2%) | 53 | 79 |
| 38 | m | 48/48 (100%) | 47 (98%) | 1 (2%) | 53 | 79 |
| 39 | n | 24/24 (100%) | 24 (100%) | 0 | 100 | 100 |
| 40 | o | 92/94 (98%) | 89 (97%) | 3 (3%) | 38 | 71 |
| 41 | p | 74/75 (99%) | 74 (100%) | 0 | 100 | 100 |
| 42 | r | 108/121 (89%) | 107 (99%) | 1 (1%) | 78 | 91 |
| 43 | s | 164/258 (64%) | 163 (99%) | 1 (1%) | 86 | 94 |
| 44 | t | 126/163 (77%) | 126 (100%) | 0 | 100 | 100 |
| 48 | K | 190/196 (97%) | 188 (99%) | 2 (1%) | 73 | 88 |
| 50 | BB | 180/181 (99%) | 177 (98%) | 3 (2%) | 60 | 83 |
| 51 | CC | 194/231 (84%) | 190 (98%) | 4 (2%) | 53 | 79 |
| 52 | DD | 187/187 (100%) | 187 (100%) | 0 | 100 | 100 |
| 53 | EE | 190/232 (82%) | 184 (97%) | 6 (3%) | 39 | 71 |
| 54 | FF | 224/224 (100%) | 223 (100%) | 1 (0%) | 91 | 95 |
| 55 | GG | 158/170 (93%) | 156 (99%) | 2 (1%) | 69 | 87 |
| 56 | HH | 207/218 (95%) | 206 (100%) | 1 (0%) | 88 | 95 |
| 57 | II | 165/174 (95%) | 165 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 58 | JJ | 178/178 (100%) | 177 (99%) | 1 (1%) | 86 94 |
| 59 | KK | 161/168 (96%) | 158 (98%) | 3 (2%) | 57 81 |
| 60 | LL | 87/125 (70%) | 87 (100%) | 0 | 100 100 |
| 61 | MM | 130/142 (92%) | 127 (98%) | 3 (2%) | 50 78 |
| 62 | NN | 99/108 (92%) | 98 (99%) | 1 (1%) | 76 90 |
| 63 | OO | 130/131 (99%) | 128 (98%) | 2 (2%) | 65 85 |
| 64 | PP | 106/119 (89%) | 106 (100%) | 0 | 100 100 |
| 65 | QQ | 105/130 (81%) | 105 (100%) | 0 | 100 100 |
| 66 | RR | 117/140 (84%) | 117 (100%) | 0 | 100 100 |
| 67 | SS | 119/121 (98%) | 118 (99%) | 1 (1%) | 81 93 |
| 68 | TT | 125/132 (95%) | 123 (98%) | 2 (2%) | 62 84 |
| 69 | UU | 111/116 (96%) | 110 (99%) | 1 (1%) | 78 91 |
| 70 | VV | 92/107 (86%) | 91 (99%) | 1 (1%) | 73 88 |
| 71 | WW | 67/67 (100%) | 65 (97%) | 2 (3%) | 41 73 |
| 72 | XX | 112/113 (99%) | 111 (99%) | 1 (1%) | 78 91 |
| 73 | YY | 113/114 (99%) | 113 (100%) | 0 | 100 100 |
| 74 | ZZ | 107/115 (93%) | 105 (98%) | 2 (2%) | 57 81 |
| 75 | aa | 66/103 (64%) | 66 (100%) | 0 | 100 100 |
| 76 | bb | 88/88 (100%) | 88 (100%) | 0 | 100 100 |
| 77 | cc | 75/76 (99%) | 75 (100%) | 0 | 100 100 |
| 78 | dd | 55/62 (89%) | 55 (100%) | 0 | 100 100 |
| 79 | ee | 48/49 (98%) | 48 (100%) | 0 | 100 100 |
| 80 | ff | 47/106 (44%) | 45 (96%) | 2 (4%) | 29 64 |
| 81 | gg | 61/140 (44%) | 60 (98%) | 1 (2%) | 62 84 |
| 82 | hh | 272/275 (99%) | 270 (99%) | 2 (1%) | 84 94 |
| 84 | 9 | 728/728 (100%) | 723 (99%) | 5 (1%) | 84 94 |
| All | All | 10937/12018 (91%) | 10824 (99%) | 113 (1%) | 77 90 |

All (113) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 64 | ARG |
| 1 | A | 128 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 140 | ASN |
| 1 | A | 194 | ASN |
| 1 | A | 242 | ARG |
| 2 | B | 10 | ARG |
| 3 | C | 38 | ASN |
| 3 | C | 95 | MET |
| 3 | C | 100 | ARG |
| 3 | C | 188 | ARG |
| 3 | C | 222 | ARG |
| 3 | C | 281 | MET |
| 3 | C | 312 | ARG |
| 4 | D | 111 | ASN |
| 4 | D | 268 | ARG |
| 5 | E | 58 | ARG |
| 5 | E | 117 | ARG |
| 6 | F | 205 | ASN |
| 7 | G | 242 | ARG |
| 7 | G | 282 | ARG |
| 7 | G | 293 | ASN |
| 8 | H | 1 | MET |
| 8 | H | 15 | ASN |
| 8 | H | 42 | ASN |
| 8 | H | 102 | ASN |
| 8 | H | 116 | ASN |
| 9 | I | 3 | ARG |
| 9 | I | 100 | ASN |
| 10 | J | 16 | ARG |
| 11 | L | 159 | ASN |
| 11 | L | 162 | LYS |
| 12 | M | 119 | ARG |
| 14 | O | 85 | ARG |
| 14 | O | 117 | ARG |
| 14 | O | 176 | ARG |
| 15 | P | 127 | ARG |
| 15 | P | 128 | ARG |
| 16 | Q | 37 | ARG |
| 16 | Q | 97 | LYS |
| 17 | R | 36 | ASN |
| 17 | R | 133 | LYS |
| 19 | T | 136 | ARG |
| 19 | T | 146 | LYS |
| 21 | V | 15 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | V | 48 | ARG |
| 24 | Y | 2 | LYS |
| 26 | a | 4 | ARG |
| 26 | a | 44 | ASN |
| 27 | b | 60 | ASN |
| 27 | b | 72 | ILE |
| 29 | d | 18 | ASN |
| 29 | d | 31 | LYS |
| 31 | f | 16 | ARG |
| 31 | f | 76 | ARG |
| 31 | f | 80 | ASN |
| 34 | i | 29 | ARG |
| 35 | j | 20 | ARG |
| 37 | l | 21 | ARG |
| 38 | m | 96 | ARG |
| 40 | o | 9 | ARG |
| 40 | o | 61 | LYS |
| 40 | o | 82 | MET |
| 42 | r | 35 | ARG |
| 43 | s | 61 | MET |
| 48 | K | 156 | LYS |
| 48 | K | 159 | MET |
| 50 | BB | 29 | ASN |
| 50 | BB | 41 | ARG |
| 50 | BB | 50 | ASN |
| 51 | CC | 40 | ASN |
| 51 | CC | 147 | ASN |
| 51 | CC | 162 | ARG |
| 51 | CC | 213 | ARG |
| 53 | EE | 57 | ASN |
| 53 | EE | 64 | ARG |
| 53 | EE | 76 | ARG |
| 53 | EE | 94 | ARG |
| 53 | EE | 106 | ARG |
| 53 | EE | 227 | LYS |
| 54 | FF | 232 | ASN |
| 55 | GG | 81 | ARG |
| 55 | GG | 135 | ARG |
| 56 | HH | 63 | MET |
| 58 | JJ | 99 | ASN |
| 59 | KK | 69 | ARG |
| 59 | KK | 70 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 59 | KK | 79 | ARG |
| 61 | MM | 20 | LYS |
| 61 | MM | 42 | LEU |
| 61 | MM | 69 | ARG |
| 62 | NN | 33 | ARG |
| 63 | OO | 27 | LYS |
| 63 | OO | 127 | ARG |
| 67 | SS | 127 | ASN |
| 68 | TT | 8 | LYS |
| 68 | TT | 101 | ASN |
| 69 | UU | 62 | ARG |
| 70 | VV | 47 | ASN |
| 71 | WW | 21 | ASN |
| 71 | WW | 82 | ASN |
| 72 | XX | 91 | ASN |
| 74 | ZZ | 99 | LYS |
| 74 | ZZ | 110 | ARG |
| 80 | ff | 99 | LYS |
| 80 | ff | 104 | ARG |
| 81 | gg | 138 | ARG |
| 82 | hh | 159 | ASN |
| 82 | hh | 178 | ASN |
| 84 | 9 | 93 | LYS |
| 84 | 9 | 144 | ARG |
| 84 | 9 | 158 | ASN |
| 84 | 9 | 701 | ARG |
| 84 | 9 | 827 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 22 | HIS |
| 1 | A | 140 | ASN |
| 1 | A | 194 | ASN |
| 2 | B | 42 | HIS |
| 2 | B | 315 | ASN |
| 3 | C | 38 | ASN |
| 3 | C | 203 | GLN |
| 3 | C | 223 | ASN |
| 4 | D | 202 | GLN |
| 5 | E | 193 | HIS |
| 5 | E | 253 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | E | 287 | HIS |
| 6 | F | 109 | GLN |
| 6 | F | 205 | ASN |
| 7 | G | 293 | ASN |
| 8 | H | 42 | ASN |
| 8 | H | 102 | ASN |
| 8 | H | 116 | ASN |
| 8 | H | 163 | GLN |
| 9 | I | 95 | HIS |
| 9 | I | 100 | ASN |
| 10 | J | 104 | ASN |
| 10 | J | 155 | HIS |
| 11 | L | 104 | ASN |
| 11 | L | 159 | ASN |
| 14 | O | 184 | ASN |
| 15 | P | 34 | GLN |
| 15 | P | 64 | ASN |
| 15 | P | 97 | ASN |
| 15 | P | 120 | ASN |
| 17 | R | 36 | ASN |
| 17 | R | 58 | HIS |
| 19 | T | 3 | ASN |
| 19 | T | 58 | HIS |
| 21 | V | 77 | HIS |
| 21 | V | 84 | GLN |
| 23 | X | 111 | GLN |
| 25 | Z | 79 | HIS |
| 28 | c | 51 | ASN |
| 29 | d | 18 | ASN |
| 31 | f | 24 | HIS |
| 31 | f | 80 | ASN |
| 32 | g | 114 | GLN |
| 42 | r | 6 | GLN |
| 42 | r | 121 | GLN |
| 43 | s | 68 | HIS |
| 44 | t | 100 | HIS |
| 44 | t | 137 | GLN |
| 48 | K | 143 | ASN |
| 48 | K | 182 | ASN |
| 50 | BB | 29 | ASN |
| 50 | BB | 50 | ASN |
| 50 | BB | 81 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | BB | 84 | GLN |
| 50 | BB | 141 | ASN |
| 51 | CC | 40 | ASN |
| 51 | CC | 147 | ASN |
| 51 | CC | 232 | HIS |
| 52 | DD | 115 | GLN |
| 52 | DD | 267 | GLN |
| 53 | EE | 57 | ASN |
| 54 | FF | 142 | HIS |
| 54 | FF | 232 | ASN |
| 56 | HH | 13 | GLN |
| 56 | HH | 65 | GLN |
| 57 | II | 91 | HIS |
| 57 | II | 186 | ASN |
| 57 | II | 193 | GLN |
| 58 | JJ | 99 | ASN |
| 58 | JJ | 165 | GLN |
| 58 | JJ | 168 | GLN |
| 60 | LL | 7 | ASN |
| 60 | LL | 61 | GLN |
| 61 | MM | 100 | ASN |
| 63 | OO | 101 | HIS |
| 63 | OO | 105 | ASN |
| 64 | PP | 94 | HIS |
| 66 | RR | 48 | GLN |
| 66 | RR | 86 | GLN |
| 68 | TT | 76 | GLN |
| 68 | TT | 101 | ASN |
| 68 | TT | 120 | HIS |
| 68 | TT | 135 | HIS |
| 70 | VV | 47 | ASN |
| 70 | VV | 81 | GLN |
| 71 | WW | 21 | ASN |
| 71 | WW | 35 | ASN |
| 71 | WW | 82 | ASN |
| 72 | XX | 91 | ASN |
| 72 | XX | 113 | HIS |
| 73 | YY | 20 | GLN |
| 74 | ZZ | 19 | GLN |
| 75 | aa | 46 | ASN |
| 80 | ff | 117 | ASN |
| 82 | hh | 133 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 82 | hh | 159 | ASN |
| 82 | hh | 178 | ASN |
| 84 | 9 | 21 | ASN |
| 84 | 9 | 30 | HIS |
| 84 | 9 | 64 | GLN |
| 84 | 9 | 101 | ASN |
| 84 | 9 | 158 | ASN |
| 84 | 9 | 291 | GLN |
| 84 | 9 | 306 | ASN |
| 84 | 9 | 493 | ASN |
| 84 | 9 | 670 | GLN |
| 84 | 9 | 696 | ASN |
| 84 | 9 | 811 | GLN |
| 84 | 9 | 827 | ASN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 45 | 5 | 3558/3594 (98%) | 900 (25%) | 29 (0%) |
| 46 | 7 | 118/119 (99%) | 16 (13%) | 0 |
| 47 | 8 | 149/151 (98%) | 37 (24%) | 1 (0%) |
| 49 | 2 | 1676/1697 (98%) | 408 (24%) | 14 (0%) |
| 83 | 3 | 86/87 (98%) | 25 (29%) | 0 |
| 85 | 4 | 188/190 (98%) | 123 (65%) | 48 (25%) |
| All | All | 5775/5838 (98%) | 1509 (26%) | 92 (1%) |

All (1509) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 5 | A |
| 45 | 5 | 7 | C |
| 45 | 5 | 11 | G |
| 45 | 5 | 12 | A |
| 45 | 5 | 14 | C |
| 45 | 5 | 21 | G |
| 45 | 5 | 25 | A |
| 45 | 5 | 36 | U |
| 45 | 5 | 39 | A |
| 45 | 5 | 42 | A |
| 45 | 5 | 48 | G |
| 45 | 5 | 49 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 56 | A |
| 45 | 5 | 58 | G |
| 45 | 5 | 59 | A |
| 45 | 5 | 64 | A |
| 45 | 5 | 65 | A |
| 45 | 5 | 67 | C |
| 45 | 5 | 70 | A |
| 45 | 5 | 72 | C |
| 45 | 5 | 73 | A |
| 45 | 5 | 74 | G |
| 45 | 5 | 75 | G |
| 45 | 5 | 84 | A |
| 45 | 5 | 85 | G |
| 45 | 5 | 91 | G |
| 45 | 5 | 92 | C |
| 45 | 5 | 93 | G |
| 45 | 5 | 98 | A |
| 45 | 5 | 105 | A |
| 45 | 5 | 109 | G |
| 45 | 5 | 110 | C |
| 45 | 5 | 116 | G |
| 45 | 5 | 117 | C |
| 45 | 5 | 118 | C |
| 45 | 5 | 119 | G |
| 45 | 5 | 120 | A |
| 45 | 5 | 122 | U |
| 45 | 5 | 123 | C |
| 45 | 5 | 126 | C |
| 45 | 5 | 131 | C |
| 45 | 5 | 132 | G |
| 45 | 5 | 134 | G |
| 45 | 5 | 135 | G |
| 45 | 5 | 136 | C |
| 45 | 5 | 140 | G |
| 45 | 5 | 142 | G |
| 45 | 5 | 143 | C |
| 45 | 5 | 144 | G |
| 45 | 5 | 157 | U |
| 45 | 5 | 158 | A |
| 45 | 5 | 159 | C |
| 45 | 5 | 169 | A |
| 45 | 5 | 172 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 173 | C |
| 45 | 5 | 174 | C |
| 45 | 5 | 193 | G |
| 45 | 5 | 194 | C |
| 45 | 5 | 197 | A |
| 45 | 5 | 200 | U |
| 45 | 5 | 201 | C |
| 45 | 5 | 209 | U |
| 45 | 5 | 216 | C |
| 45 | 5 | 217 | C |
| 45 | 5 | 218 | A |
| 45 | 5 | 220 | C |
| 45 | 5 | 224 | U |
| 45 | 5 | 225 | G |
| 45 | 5 | 232 | G |
| 45 | 5 | 233 | U |
| 45 | 5 | 234 | G |
| 45 | 5 | 244 | G |
| 45 | 5 | 256 | G |
| 45 | 5 | 265 | C |
| 45 | 5 | 266 | C |
| 45 | 5 | 274 | C |
| 45 | 5 | 276 | C |
| 45 | 5 | 278 | G |
| 45 | 5 | 279 | A |
| 45 | 5 | 280 | G |
| 45 | 5 | 295 | A |
| 45 | 5 | 297 | U |
| 45 | 5 | 306 | A |
| 45 | 5 | 308 | G |
| 45 | 5 | 309 | C |
| 45 | 5 | 315 | G |
| 45 | 5 | 316 | U |
| 45 | 5 | 321 | U |
| 45 | 5 | 326 | C |
| 45 | 5 | 334 | A |
| 45 | 5 | 336 | A |
| 45 | 5 | 340 | C |
| 45 | 5 | 344 | A |
| 45 | 5 | 345 | C |
| 45 | 5 | 349 | A |
| 45 | 5 | 350 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 355 | A |
| 45 | 5 | 357 | U |
| 45 | 5 | 360 | A |
| 45 | 5 | 361 | C |
| 45 | 5 | 363 | A |
| 45 | 5 | 364 | G |
| 45 | 5 | 365 | U |
| 45 | 5 | 381 | U |
| 45 | 5 | 386 | A |
| 45 | 5 | 387 | G |
| 45 | 5 | 410 | A |
| 45 | 5 | 412 | G |
| 45 | 5 | 413 | G |
| 45 | 5 | 415 | G |
| 45 | 5 | 418 | A |
| 45 | 5 | 431 | G |
| 45 | 5 | 432 | U |
| 45 | 5 | 433 | A |
| 45 | 5 | 440 | U |
| 45 | 5 | 446 | C |
| 45 | 5 | 448 | G |
| 45 | 5 | 449 | C |
| 45 | 5 | 450 | G |
| 45 | 5 | 452 | A |
| 45 | 5 | 453 | G |
| 45 | 5 | 454 | U |
| 45 | 5 | 455 | C |
| 45 | 5 | 463 | A |
| 45 | 5 | 464 | G |
| 45 | 5 | 467 | U |
| 45 | 5 | 468 | U |
| 45 | 5 | 481 | G |
| 45 | 5 | 482 | G |
| 45 | 5 | 483 | G |
| 45 | 5 | 485 | C |
| 45 | 5 | 492 | U |
| 45 | 5 | 493 | G |
| 45 | 5 | 499 | G |
| 45 | 5 | 505 | G |
| 45 | 5 | 510 | U |
| 45 | 5 | 518 | G |
| 45 | 5 | 643 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 666 | G |
| 45 | 5 | 668 | C |
| 45 | 5 | 677 | G |
| 45 | 5 | 685 | C |
| 45 | 5 | 686 | A |
| 45 | 5 | 691 | C |
| 45 | 5 | 696 | C |
| 45 | 5 | 697 | G |
| 45 | 5 | 704 | C |
| 45 | 5 | 729 | G |
| 45 | 5 | 731 | G |
| 45 | 5 | 733 | A |
| 45 | 5 | 743 | G |
| 45 | 5 | 749 | G |
| 45 | 5 | 750 | U |
| 45 | 5 | 751 | G |
| 45 | 5 | 758 | G |
| 45 | 5 | 760 | G |
| 45 | 5 | 905 | C |
| 45 | 5 | 907 | C |
| 45 | 5 | 913 | U |
| 45 | 5 | 914 | U |
| 45 | 5 | 915 | A |
| 45 | 5 | 917 | A |
| 45 | 5 | 918 | G |
| 45 | 5 | 924 | C |
| 45 | 5 | 925 | C |
| 45 | 5 | 926 | G |
| 45 | 5 | 927 | G |
| 45 | 5 | 928 | C |
| 45 | 5 | 931 | C |
| 45 | 5 | 932 | A |
| 45 | 5 | 933 | G |
| 45 | 5 | 934 | C |
| 45 | 5 | 935 | A |
| 45 | 5 | 935(A) | G |
| 45 | 5 | 936 | C |
| 45 | 5 | 941 | C |
| 45 | 5 | 943 | A |
| 45 | 5 | 944 | A |
| 45 | 5 | 945 | U |
| 45 | 5 | 946 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 958 | G |
| 45 | 5 | 959 | G |
| 45 | 5 | 960 | A |
| 45 | 5 | 962 | C |
| 45 | 5 | 963 | G |
| 45 | 5 | 964 | A |
| 45 | 5 | 966 | A |
| 45 | 5 | 967 | C |
| 45 | 5 | 968 | C |
| 45 | 5 | 969 | C |
| 45 | 5 | 970 | G |
| 45 | 5 | 979 | C |
| 45 | 5 | 983 | C |
| 45 | 5 | 990 | C |
| 45 | 5 | 1067 | G |
| 45 | 5 | 1071 | C |
| 45 | 5 | 1072 | C |
| 45 | 5 | 1073 | G |
| 45 | 5 | 1081 | C |
| 45 | 5 | 1084 | C |
| 45 | 5 | 1093 | C |
| 45 | 5 | 1179 | U |
| 45 | 5 | 1180 | C |
| 45 | 5 | 1193 | C |
| 45 | 5 | 1194 | G |
| 45 | 5 | 1195 | G |
| 45 | 5 | 1204 | C |
| 45 | 5 | 1211 | G |
| 45 | 5 | 1212 | G |
| 45 | 5 | 1214 | C |
| 45 | 5 | 1215 | C |
| 45 | 5 | 1216 | C |
| 45 | 5 | 1234 | G |
| 45 | 5 | 1235 | G |
| 45 | 5 | 1236 | C |
| 45 | 5 | 1238 | A |
| 45 | 5 | 1245 | C |
| 45 | 5 | 1246 | G |
| 45 | 5 | 1249 | C |
| 45 | 5 | 1272 | C |
| 45 | 5 | 1273 | G |
| 45 | 5 | 1275 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 1276 | C |
| 45 | 5 | 1284 | G |
| 45 | 5 | 1287 | G |
| 45 | 5 | 1288 | G |
| 45 | 5 | 1289 | C |
| 45 | 5 | 1291 | G |
| 45 | 5 | 1292 | C |
| 45 | 5 | 1296 | G |
| 45 | 5 | 1301 | C |
| 45 | 5 | 1314 | C |
| 45 | 5 | 1316 | G |
| 45 | 5 | 1322 | A |
| 45 | 5 | 1325 | C |
| 45 | 5 | 1326 | A |
| 45 | 5 | 1338 | G |
| 45 | 5 | 1354 | A |
| 45 | 5 | 1358 | G |
| 45 | 5 | 1359 | G |
| 45 | 5 | 1360 | G |
| 45 | 5 | 1370 | G |
| 45 | 5 | 1371 | A |
| 45 | 5 | 1377 | G |
| 45 | 5 | 1379 | C |
| 45 | 5 | 1380 | G |
| 45 | 5 | 1381 | U |
| 45 | 5 | 1382 | G |
| 45 | 5 | 1387 | A |
| 45 | 5 | 1390 | G |
| 45 | 5 | 1394 | G |
| 45 | 5 | 1397 | A |
| 45 | 5 | 1398 | A |
| 45 | 5 | 1411(C) | C |
| 45 | 5 | 1412 | G |
| 45 | 5 | 1415 | G |
| 45 | 5 | 1420 | A |
| 45 | 5 | 1432 | G |
| 45 | 5 | 1438 | U |
| 45 | 5 | 1443 | A |
| 45 | 5 | 1445 | U |
| 45 | 5 | 1446 | C |
| 45 | 5 | 1456 | C |
| 45 | 5 | 1457 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 1465 | G |
| 45 | 5 | 1475 | G |
| 45 | 5 | 1478 | C |
| 45 | 5 | 1480 | C |
| 45 | 5 | 1481 | C |
| 45 | 5 | 1482 | G |
| 45 | 5 | 1483 | C |
| 45 | 5 | 1484 | G |
| 45 | 5 | 1497 | A |
| 45 | 5 | 1498 | G |
| 45 | 5 | 1499 | C |
| 45 | 5 | 1501 | C |
| 45 | 5 | 1503 | A |
| 45 | 5 | 1518 | A |
| 45 | 5 | 1519 | C |
| 45 | 5 | 1523 | A |
| 45 | 5 | 1534 | A |
| 45 | 5 | 1547 | A |
| 45 | 5 | 1566 | C |
| 45 | 5 | 1574 | G |
| 45 | 5 | 1575 | A |
| 45 | 5 | 1577 | G |
| 45 | 5 | 1578 | U |
| 45 | 5 | 1586 | G |
| 45 | 5 | 1591 | U |
| 45 | 5 | 1596 | U |
| 45 | 5 | 1598 | C |
| 45 | 5 | 1600 | A |
| 45 | 5 | 1602 | U |
| 45 | 5 | 1607 | C |
| 45 | 5 | 1611 | C |
| 45 | 5 | 1612 | G |
| 45 | 5 | 1613 | A |
| 45 | 5 | 1624 | G |
| 45 | 5 | 1625 | G |
| 45 | 5 | 1631 | A |
| 45 | 5 | 1633 | G |
| 45 | 5 | 1634 | A |
| 45 | 5 | 1638 | A |
| 45 | 5 | 1639 | U |
| 45 | 5 | 1641 | G |
| 45 | 5 | 1649 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 1650 | A |
| 45 | 5 | 1651 | G |
| 45 | 5 | 1654 | G |
| 45 | 5 | 1655 | C |
| 45 | 5 | 1660 | U |
| 45 | 5 | 1661 | C |
| 45 | 5 | 1671 | U |
| 45 | 5 | 1676 | C |
| 45 | 5 | 1679 | A |
| 45 | 5 | 1680 | G |
| 45 | 5 | 1691 | G |
| 45 | 5 | 1724 | G |
| 45 | 5 | 1725 | U |
| 45 | 5 | 1729 | A |
| 45 | 5 | 1731 | C |
| 45 | 5 | 1733 | G |
| 45 | 5 | 1734 | G |
| 45 | 5 | 1741 | G |
| 45 | 5 | 1742 | A |
| 45 | 5 | 1753 | G |
| 45 | 5 | 1755 | C |
| 45 | 5 | 1756 | U |
| 45 | 5 | 1757 | U |
| 45 | 5 | 1758 | G |
| 45 | 5 | 1760 | G |
| 45 | 5 | 1761 | G |
| 45 | 5 | 1764 | G |
| 45 | 5 | 1766 | A |
| 45 | 5 | 1768 | C |
| 45 | 5 | 1769 | G |
| 45 | 5 | 1772 | C |
| 45 | 5 | 1776 | A |
| 45 | 5 | 1781 | U |
| 45 | 5 | 1787 | A |
| 45 | 5 | 1790 | U |
| 45 | 5 | 1803 | G |
| 45 | 5 | 1804 | A |
| 45 | 5 | 1805 | A |
| 45 | 5 | 1812 | C |
| 45 | 5 | 1815 | G |
| 45 | 5 | 1818 | G |
| 45 | 5 | 1819 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 1821 | G |
| 45 | 5 | 1822 | U |
| 45 | 5 | 1827 | C |
| 45 | 5 | 1828 | C |
| 45 | 5 | 1830 | G |
| 45 | 5 | 1833 | G |
| 45 | 5 | 1836 | G |
| 45 | 5 | 1837 | A |
| 45 | 5 | 1842 | G |
| 45 | 5 | 1854 | G |
| 45 | 5 | 1855 | G |
| 45 | 5 | 1878 | G |
| 45 | 5 | 1881 | C |
| 45 | 5 | 1882 | U |
| 45 | 5 | 1891 | A |
| 45 | 5 | 1893 | C |
| 45 | 5 | 1897 | A |
| 45 | 5 | 1910 | G |
| 45 | 5 | 1912 | G |
| 45 | 5 | 1915 | C |
| 45 | 5 | 1916 | G |
| 45 | 5 | 1918 | U |
| 45 | 5 | 1920 | C |
| 45 | 5 | 1921 | C |
| 45 | 5 | 1922 | G |
| 45 | 5 | 1925 | G |
| 45 | 5 | 1928 | C |
| 45 | 5 | 1929 | A |
| 45 | 5 | 1931 | C |
| 45 | 5 | 1933 | G |
| 45 | 5 | 1936 | C |
| 45 | 5 | 1945 | G |
| 45 | 5 | 1947 | U |
| 45 | 5 | 1951 | G |
| 45 | 5 | 1956 | A |
| 45 | 5 | 1960 | A |
| 45 | 5 | 1961 | G |
| 45 | 5 | 1962 | A |
| 45 | 5 | 1964 | A |
| 45 | 5 | 1969 | G |
| 45 | 5 | 1971 | U |
| 45 | 5 | 1972 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 1975 | G |
| 45 | 5 | 1982 | G |
| 45 | 5 | 1984 | A |
| 45 | 5 | 1985 | G |
| 45 | 5 | 1991 | A |
| 45 | 5 | 1992 | U |
| 45 | 5 | 1996 | C |
| 45 | 5 | 1997 | U |
| 45 | 5 | 1998 | A |
| 45 | 5 | 2001 | G |
| 45 | 5 | 2002 | A |
| 45 | 5 | 2003 | G |
| 45 | 5 | 2004 | U |
| 45 | 5 | 2011 | C |
| 45 | 5 | 2018 | C |
| 45 | 5 | 2025 | A |
| 45 | 5 | 2026 | A |
| 45 | 5 | 2031 | C |
| 45 | 5 | 2033 | A |
| 45 | 5 | 2034 | G |
| 45 | 5 | 2041 | A |
| 45 | 5 | 2042 | A |
| 45 | 5 | 2044 | U |
| 45 | 5 | 2045 | G |
| 45 | 5 | 2047 | A |
| 45 | 5 | 2048 | U |
| 45 | 5 | 2055 | G |
| 45 | 5 | 2056 | G |
| 45 | 5 | 2062 | C |
| 45 | 5 | 2069 | A |
| 45 | 5 | 2070 | U |
| 45 | 5 | 2073 | C |
| 45 | 5 | 2084 | U |
| 45 | 5 | 2085 | G |
| 45 | 5 | 2088 | A |
| 45 | 5 | 2090 | U |
| 45 | 5 | 2093 | G |
| 45 | 5 | 2094 | C |
| 45 | 5 | 2097 | A |
| 45 | 5 | 2099 | C |
| 45 | 5 | 2100 | G |
| 45 | 5 | 2102 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 2104 | A |
| 45 | 5 | 2105 | A |
| 45 | 5 | 2107 | A |
| 45 | 5 | 2108 | G |
| 45 | 5 | 2259 | G |
| 45 | 5 | 2260 | C |
| 45 | 5 | 2267 | U |
| 45 | 5 | 2268 | A |
| 45 | 5 | 2289 | C |
| 45 | 5 | 2300 | A |
| 45 | 5 | 2301 | G |
| 45 | 5 | 2306 | G |
| 45 | 5 | 2313 | A |
| 45 | 5 | 2314 | G |
| 45 | 5 | 2316 | G |
| 45 | 5 | 2318 | G |
| 45 | 5 | 2325 | C |
| 45 | 5 | 2331 | G |
| 45 | 5 | 2333 | G |
| 45 | 5 | 2348 | G |
| 45 | 5 | 2351 | C |
| 45 | 5 | 2360 | A |
| 45 | 5 | 2369 | U |
| 45 | 5 | 2382 | A |
| 45 | 5 | 2395 | A |
| 45 | 5 | 2402 | G |
| 45 | 5 | 2410 | C |
| 45 | 5 | 2416 | G |
| 45 | 5 | 2422 | C |
| 45 | 5 | 2424 | G |
| 45 | 5 | 2425 | U |
| 45 | 5 | 2428 | A |
| 45 | 5 | 2432 | U |
| 45 | 5 | 2433 | G |
| 45 | 5 | 2442 | G |
| 45 | 5 | 2467 | U |
| 45 | 5 | 2469 | C |
| 45 | 5 | 2475 | G |
| 45 | 5 | 2483 | G |
| 45 | 5 | 2485 | U |
| 45 | 5 | 2486 | G |
| 45 | 5 | 2488 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 2489 | C |
| 45 | 5 | 2490 | U |
| 45 | 5 | 2491 | C |
| 45 | 5 | 2492 | C |
| 45 | 5 | 2493 | G |
| 45 | 5 | 2494 | U |
| 45 | 5 | 2503 | G |
| 45 | 5 | 2504 | C |
| 45 | 5 | 2505 | C |
| 45 | 5 | 2506 | G |
| 45 | 5 | 2513 | A |
| 45 | 5 | 2516 | G |
| 45 | 5 | 2517 | A |
| 45 | 5 | 2520 | C |
| 45 | 5 | 2529 | A |
| 45 | 5 | 2530 | U |
| 45 | 5 | 2537 | A |
| 45 | 5 | 2544 | G |
| 45 | 5 | 2546 | G |
| 45 | 5 | 2547 | G |
| 45 | 5 | 2551 | A |
| 45 | 5 | 2552 | G |
| 45 | 5 | 2553 | A |
| 45 | 5 | 2560 | C |
| 45 | 5 | 2569 | G |
| 45 | 5 | 2572 | C |
| 45 | 5 | 2575 | U |
| 45 | 5 | 2576 | G |
| 45 | 5 | 2582 | A |
| 45 | 5 | 2583 | C |
| 45 | 5 | 2589 | C |
| 45 | 5 | 2600 | A |
| 45 | 5 | 2602 | G |
| 45 | 5 | 2623 | A |
| 45 | 5 | 2628 | U |
| 45 | 5 | 2632 | U |
| 45 | 5 | 2638 | G |
| 45 | 5 | 2647 | A |
| 45 | 5 | 2654 | C |
| 45 | 5 | 2657 | G |
| 45 | 5 | 2658 | G |
| 45 | 5 | 2660 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 2661 | U |
| 45 | 5 | 2662 | G |
| 45 | 5 | 2669 | C |
| 45 | 5 | 2675 | G |
| 45 | 5 | 2681 | G |
| 45 | 5 | 2683 | C |
| 45 | 5 | 2687 | U |
| 45 | 5 | 2694 | G |
| 45 | 5 | 2695 | A |
| 45 | 5 | 2696 | A |
| 45 | 5 | 2700 | G |
| 45 | 5 | 2708 | U |
| 45 | 5 | 2709 | C |
| 45 | 5 | 2710 | C |
| 45 | 5 | 2711 | G |
| 45 | 5 | 2712 | G |
| 45 | 5 | 2714 | G |
| 45 | 5 | 2719 | C |
| 45 | 5 | 2726 | G |
| 45 | 5 | 2740 | U |
| 45 | 5 | 2743 | A |
| 45 | 5 | 2752 | G |
| 45 | 5 | 2753 | G |
| 45 | 5 | 2754 | G |
| 45 | 5 | 2756 | G |
| 45 | 5 | 2758 | G |
| 45 | 5 | 2761 | U |
| 45 | 5 | 2764 | A |
| 45 | 5 | 2768 | C |
| 45 | 5 | 2769 | U |
| 45 | 5 | 2772 | C |
| 45 | 5 | 2787 | A |
| 45 | 5 | 2788 | U |
| 45 | 5 | 2789 | A |
| 45 | 5 | 2790 | U |
| 45 | 5 | 2794 | C |
| 45 | 5 | 2795 | A |
| 45 | 5 | 2796 | G |
| 45 | 5 | 2798 | A |
| 45 | 5 | 2799 | G |
| 45 | 5 | 2807 | A |
| 45 | 5 | 2811 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 2814 | C |
| 45 | 5 | 2825 | A |
| 45 | 5 | 2826 | U |
| 45 | 5 | 2827 | G |
| 45 | 5 | 2828 | U |
| 45 | 5 | 2833 | A |
| 45 | 5 | 2835 | A |
| 45 | 5 | 2837 | U |
| 45 | 5 | 2839 | U |
| 45 | 5 | 2842 | G |
| 45 | 5 | 2849 | A |
| 45 | 5 | 2853 | C |
| 45 | 5 | 2855 | G |
| 45 | 5 | 2857 | A |
| 45 | 5 | 2874 | U |
| 45 | 5 | 2875 | C |
| 45 | 5 | 2876 | G |
| 45 | 5 | 2880 | U |
| 45 | 5 | 2883 | G |
| 45 | 5 | 2884 | G |
| 45 | 5 | 2888 | G |
| 45 | 5 | 2897 | G |
| 45 | 5 | 2898 | G |
| 45 | 5 | 3598 | C |
| 45 | 5 | 3599 | A |
| 45 | 5 | 3603 | G |
| 45 | 5 | 3604 | A |
| 45 | 5 | 3616 | U |
| 45 | 5 | 3618 | C |
| 45 | 5 | 3619 | G |
| 45 | 5 | 3620 | G |
| 45 | 5 | 3621 | A |
| 45 | 5 | 3625 | G |
| 45 | 5 | 3626 | G |
| 45 | 5 | 3635 | A |
| 45 | 5 | 3639 | U |
| 45 | 5 | 3643 | A |
| 45 | 5 | 3646 | A |
| 45 | 5 | 3647 | A |
| 45 | 5 | 3657 | U |
| 45 | 5 | 3662 | A |
| 45 | 5 | 3664 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 3673 | C |
| 45 | 5 | 3678 | G |
| 45 | 5 | 3680 | U |
| 45 | 5 | 3688 | U |
| 45 | 5 | 3692 | A |
| 45 | 5 | 3698 | G |
| 45 | 5 | 3711 | A |
| 45 | 5 | 3727 | A |
| 45 | 5 | 3729 | U |
| 45 | 5 | 3747 | A |
| 45 | 5 | 3748 | A |
| 45 | 5 | 3753 | G |
| 45 | 5 | 3759 | A |
| 45 | 5 | 3760 | A |
| 45 | 5 | 3763 | A |
| 45 | 5 | 3772 | U |
| 45 | 5 | 3773 | U |
| 45 | 5 | 3775 | A |
| 45 | 5 | 3776 | G |
| 45 | 5 | 3777 | G |
| 45 | 5 | 3778 | U |
| 45 | 5 | 3783 | A |
| 45 | 5 | 3784 | A |
| 45 | 5 | 3785 | A |
| 45 | 5 | 3790 | U |
| 45 | 5 | 3791 | C |
| 45 | 5 | 3793 | U |
| 45 | 5 | 3795 | A |
| 45 | 5 | 3798 | U |
| 45 | 5 | 3802 | U |
| 45 | 5 | 3808 | C |
| 45 | 5 | 3810 | C |
| 45 | 5 | 3812 | C |
| 45 | 5 | 3814 | U |
| 45 | 5 | 3817 | A |
| 45 | 5 | 3818 | U |
| 45 | 5 | 3819 | G |
| 45 | 5 | 3825 | A |
| 45 | 5 | 3828 | A |
| 45 | 5 | 3829 | G |
| 45 | 5 | 3830 | A |
| 45 | 5 | 3839 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 3840 | U |
| 45 | 5 | 3843 | C |
| 45 | 5 | 3851 | U |
| 45 | 5 | 3852 | A |
| 45 | 5 | 3868 | G |
| 45 | 5 | 3869 | C |
| 45 | 5 | 3876 | A |
| 45 | 5 | 3877 | A |
| 45 | 5 | 3878 | C |
| 45 | 5 | 3879 | G |
| 45 | 5 | 3880 | G |
| 45 | 5 | 3889 | G |
| 45 | 5 | 3890 | A |
| 45 | 5 | 3897 | G |
| 45 | 5 | 3898 | G |
| 45 | 5 | 3901 | A |
| 45 | 5 | 3905 | A |
| 45 | 5 | 3906 | A |
| 45 | 5 | 3907 | G |
| 45 | 5 | 3914 | U |
| 45 | 5 | 3915 | U |
| 45 | 5 | 3917 | A |
| 45 | 5 | 3924 | C |
| 45 | 5 | 3926 | C |
| 45 | 5 | 3927 | U |
| 45 | 5 | 3938 | G |
| 45 | 5 | 3939 | G |
| 45 | 5 | 3956 | G |
| 45 | 5 | 3957 | U |
| 45 | 5 | 3958 | G |
| 45 | 5 | 3964 | U |
| 45 | 5 | 3965 | A |
| 45 | 5 | 3966 | A |
| 45 | 5 | 3968 | U |
| 45 | 5 | 3970 | G |
| 45 | 5 | 3972 | A |
| 45 | 5 | 3973 | G |
| 45 | 5 | 3975 | C |
| 45 | 5 | 4036 | G |
| 45 | 5 | 4040 | C |
| 45 | 5 | 4041 | C |
| 45 | 5 | 4045 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 4048 | A |
| 45 | 5 | 4049 | U |
| 45 | 5 | 4050 | A |
| 45 | 5 | 4052 | C |
| 45 | 5 | 4053 | A |
| 45 | 5 | 4055 | U |
| 45 | 5 | 4063 | U |
| 45 | 5 | 4064 | C |
| 45 | 5 | 4065 | G |
| 45 | 5 | 4072 | C |
| 45 | 5 | 4073 | A |
| 45 | 5 | 4074 | C |
| 45 | 5 | 4075 | U |
| 45 | 5 | 4076 | G |
| 45 | 5 | 4085 | A |
| 45 | 5 | 4086 | G |
| 45 | 5 | 4116 | C |
| 45 | 5 | 4119 | C |
| 45 | 5 | 4120 | U |
| 45 | 5 | 4125 | C |
| 45 | 5 | 4127 | A |
| 45 | 5 | 4131 | G |
| 45 | 5 | 4148 | C |
| 45 | 5 | 4157 | A |
| 45 | 5 | 4158 | C |
| 45 | 5 | 4162 | C |
| 45 | 5 | 4163 | U |
| 45 | 5 | 4164 | C |
| 45 | 5 | 4170 | A |
| 45 | 5 | 4171 | C |
| 45 | 5 | 4183 | G |
| 45 | 5 | 4184 | G |
| 45 | 5 | 4191 | G |
| 45 | 5 | 4194 | U |
| 45 | 5 | 4197 | G |
| 45 | 5 | 4203 | A |
| 45 | 5 | 4205 | A |
| 45 | 5 | 4213 | A |
| 45 | 5 | 4225 | G |
| 45 | 5 | 4229 | U |
| 45 | 5 | 4233 | A |
| 45 | 5 | 4234 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 4235 | G |
| 45 | 5 | 4249 | G |
| 45 | 5 | 4251 | A |
| 45 | 5 | 4253 | A |
| 45 | 5 | 4254 | G |
| 45 | 5 | 4260 | U |
| 45 | 5 | 4263 | C |
| 45 | 5 | 4265 | U |
| 45 | 5 | 4266 | G |
| 45 | 5 | 4268 | A |
| 45 | 5 | 4271 | A |
| 45 | 5 | 4273 | A |
| 45 | 5 | 4281 | A |
| 45 | 5 | 4282 | A |
| 45 | 5 | 4290 | U |
| 45 | 5 | 4291 | G |
| 45 | 5 | 4293 | U |
| 45 | 5 | 4297 | G |
| 45 | 5 | 4302 | U |
| 45 | 5 | 4304 | A |
| 45 | 5 | 4305 | G |
| 45 | 5 | 4313 | A |
| 45 | 5 | 4315 | A |
| 45 | 5 | 4317 | A |
| 45 | 5 | 4326 | G |
| 45 | 5 | 4330 | G |
| 45 | 5 | 4332 | C |
| 45 | 5 | 4335 | C |
| 45 | 5 | 4336 | A |
| 45 | 5 | 4339 | A |
| 45 | 5 | 4349 | C |
| 45 | 5 | 4350 | C |
| 45 | 5 | 4354 | U |
| 45 | 5 | 4355 | G |
| 45 | 5 | 4360 | U |
| 45 | 5 | 4373 | G |
| 45 | 5 | 4375 | C |
| 45 | 5 | 4376 | A |
| 45 | 5 | 4377 | G |
| 45 | 5 | 4378 | A |
| 45 | 5 | 4381 | A |
| 45 | 5 | 4387 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 4393 | G |
| 45 | 5 | 4394 | A |
| 45 | 5 | 4395 | U |
| 45 | 5 | 4398 | C |
| 45 | 5 | 4401 | G |
| 45 | 5 | 4419 | U |
| 45 | 5 | 4421 | C |
| 45 | 5 | 4422 | A |
| 45 | 5 | 4424 | A |
| 45 | 5 | 4426 | C |
| 45 | 5 | 4430 | G |
| 45 | 5 | 4436 | U |
| 45 | 5 | 4437 | U |
| 45 | 5 | 4448 | G |
| 45 | 5 | 4449 | A |
| 45 | 5 | 4452 | U |
| 45 | 5 | 4464 | A |
| 45 | 5 | 4466 | C |
| 45 | 5 | 4477 | A |
| 45 | 5 | 4478 | G |
| 45 | 5 | 4482 | U |
| 45 | 5 | 4483 | C |
| 45 | 5 | 4493 | U |
| 45 | 5 | 4500 | U |
| 45 | 5 | 4511 | A |
| 45 | 5 | 4512 | U |
| 45 | 5 | 4513 | A |
| 45 | 5 | 4518 | A |
| 45 | 5 | 4525 | C |
| 45 | 5 | 4527 | G |
| 45 | 5 | 4542 | U |
| 45 | 5 | 4548 | A |
| 45 | 5 | 4560 | C |
| 45 | 5 | 4569 | U |
| 45 | 5 | 4573 | G |
| 45 | 5 | 4574 | U |
| 45 | 5 | 4575 | G |
| 45 | 5 | 4577 | U |
| 45 | 5 | 4581 | G |
| 45 | 5 | 4585 | U |
| 45 | 5 | 4590 | A |
| 45 | 5 | 4592 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 4599 | A |
| 45 | 5 | 4616 | A |
| 45 | 5 | 4617 | G |
| 45 | 5 | 4636 | U |
| 45 | 5 | 4637 | G |
| 45 | 5 | 4652 | G |
| 45 | 5 | 4657 | U |
| 45 | 5 | 4658 | G |
| 45 | 5 | 4667 | C |
| 45 | 5 | 4670 | C |
| 45 | 5 | 4672 | A |
| 45 | 5 | 4677 | U |
| 45 | 5 | 4678 | G |
| 45 | 5 | 4687 | A |
| 45 | 5 | 4691 | A |
| 45 | 5 | 4694 | G |
| 45 | 5 | 4698 | C |
| 45 | 5 | 4700 | A |
| 45 | 5 | 4709 | U |
| 45 | 5 | 4719 | G |
| 45 | 5 | 4720 | C |
| 45 | 5 | 4721 | G |
| 45 | 5 | 4728 | U |
| 45 | 5 | 4736 | C |
| 45 | 5 | 4738 | C |
| 45 | 5 | 4739 | C |
| 45 | 5 | 4745 | G |
| 45 | 5 | 4754 | G |
| 45 | 5 | 4756 | C |
| 45 | 5 | 4757 | C |
| 45 | 5 | 4759 | C |
| 45 | 5 | 4765 | G |
| 45 | 5 | 4769 | G |
| 45 | 5 | 4771 | C |
| 45 | 5 | 4773 | C |
| 45 | 5 | 4775 | C |
| 45 | 5 | 4863 | G |
| 45 | 5 | 4865 | C |
| 45 | 5 | 4867 | G |
| 45 | 5 | 4870 | G |
| 45 | 5 | 4871 | C |
| 45 | 5 | 4872 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 4875 | G |
| 45 | 5 | 4876 | A |
| 45 | 5 | 4877 | G |
| 45 | 5 | 4882 | U |
| 45 | 5 | 4883 | C |
| 45 | 5 | 4885 | U |
| 45 | 5 | 4891 | G |
| 45 | 5 | 4895 | C |
| 45 | 5 | 4896 | G |
| 45 | 5 | 4910 | A |
| 45 | 5 | 4911 | A |
| 45 | 5 | 4912 | G |
| 45 | 5 | 4914 | G |
| 45 | 5 | 4915 | G |
| 45 | 5 | 4921 | C |
| 45 | 5 | 4924 | C |
| 45 | 5 | 4926 | C |
| 45 | 5 | 4931 | G |
| 45 | 5 | 4937 | C |
| 45 | 5 | 4943 | A |
| 45 | 5 | 4944 | C |
| 45 | 5 | 4947 | U |
| 45 | 5 | 4948 | C |
| 45 | 5 | 4949 | G |
| 45 | 5 | 4951 | G |
| 45 | 5 | 4955 | A |
| 45 | 5 | 4956 | A |
| 45 | 5 | 4958 | C |
| 45 | 5 | 4965 | U |
| 45 | 5 | 4966 | A |
| 45 | 5 | 4975 | G |
| 45 | 5 | 4976 | U |
| 45 | 5 | 4988 | U |
| 45 | 5 | 4989 | U |
| 45 | 5 | 4990 | C |
| 45 | 5 | 4999 | G |
| 45 | 5 | 5005 | G |
| 45 | 5 | 5006 | U |
| 45 | 5 | 5014 | A |
| 45 | 5 | 5017 | G |
| 45 | 5 | 5040 | U |
| 45 | 5 | 5041 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 5049 | G |
| 45 | 5 | 5050 | C |
| 45 | 5 | 5054 | C |
| 45 | 5 | 5061 | A |
| 45 | 5 | 5062 | G |
| 45 | 5 | 5066 | U |
| 46 | 7 | 7 | G |
| 46 | 7 | 33 | U |
| 46 | 7 | 41 | G |
| 46 | 7 | 50 | A |
| 46 | 7 | 53 | U |
| 46 | 7 | 54 | A |
| 46 | 7 | 63 | C |
| 46 | 7 | 64 | G |
| 46 | 7 | 74 | A |
| 46 | 7 | 76 | U |
| 46 | 7 | 84 | U |
| 46 | 7 | 85 | G |
| 46 | 7 | 97 | G |
| 46 | 7 | 100 | A |
| 46 | 7 | 110 | G |
| 46 | 7 | 117 | G |
| 47 | 8 | 2 | G |
| 47 | 8 | 3 | A |
| 47 | 8 | 14 | U |
| 47 | 8 | 16 | G |
| 47 | 8 | 23 | C |
| 47 | 8 | 34 | U |
| 47 | 8 | 35 | C |
| 47 | 8 | 38 | U |
| 47 | 8 | 46 | G |
| 47 | 8 | 51 | U |
| 47 | 8 | 52 | A |
| 47 | 8 | 59 | A |
| 47 | 8 | 62 | A |
| 47 | 8 | 63 | U |
| 47 | 8 | 71 | A |
| 47 | 8 | 72 | A |
| 47 | 8 | 78 | G |
| 47 | 8 | 86 | U |
| 47 | 8 | 87 | G |
| 47 | 8 | 88 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | 8 | 90 | C |
| 47 | 8 | 94 | G |
| 47 | 8 | 95 | A |
| 47 | 8 | 103 | A |
| 47 | 8 | 105 | C |
| 47 | 8 | 110 | U |
| 47 | 8 | 111 | U |
| 47 | 8 | 114 | G |
| 47 | 8 | 123 | U |
| 47 | 8 | 125 | C |
| 47 | 8 | 126 | C |
| 47 | 8 | 127 | U |
| 47 | 8 | 135 | C |
| 47 | 8 | 137 | A |
| 47 | 8 | 147 | G |
| 47 | 8 | 150 | C |
| 47 | 8 | 151 | G |
| 49 | 2 | 2 | A |
| 49 | 2 | 3 | C |
| 49 | 2 | 4 | C |
| 49 | 2 | 9 | U |
| 49 | 2 | 14 | C |
| 49 | 2 | 20 | G |
| 49 | 2 | 25 | A |
| 49 | 2 | 26 | U |
| 49 | 2 | 37 | C |
| 49 | 2 | 41 | G |
| 49 | 2 | 42 | A |
| 49 | 2 | 45 | A |
| 49 | 2 | 46 | A |
| 49 | 2 | 47 | G |
| 49 | 2 | 55 | U |
| 49 | 2 | 56 | G |
| 49 | 2 | 62 | G |
| 49 | 2 | 64 | A |
| 49 | 2 | 67 | C |
| 49 | 2 | 68 | A |
| 49 | 2 | 69 | C |
| 49 | 2 | 71 | G |
| 49 | 2 | 74 | G |
| 49 | 2 | 75 | G |
| 49 | 2 | 76 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 2 | 78 | C |
| 49 | 2 | 93 | U |
| 49 | 2 | 103 | A |
| 49 | 2 | 107 | A |
| 49 | 2 | 110 | U |
| 49 | 2 | 111 | A |
| 49 | 2 | 113 | G |
| 49 | 2 | 114 | G |
| 49 | 2 | 115 | U |
| 49 | 2 | 123 | G |
| 49 | 2 | 126 | G |
| 49 | 2 | 127 | C |
| 49 | 2 | 130 | G |
| 49 | 2 | 143 | U |
| 49 | 2 | 147 | A |
| 49 | 2 | 154 | U |
| 49 | 2 | 155 | G |
| 49 | 2 | 160 | U |
| 49 | 2 | 161 | U |
| 49 | 2 | 163 | U |
| 49 | 2 | 168 | C |
| 49 | 2 | 169 | U |
| 49 | 2 | 183 | G |
| 49 | 2 | 184 | G |
| 49 | 2 | 187 | G |
| 49 | 2 | 188 | C |
| 49 | 2 | 189 | U |
| 49 | 2 | 190 | G |
| 49 | 2 | 191 | A |
| 49 | 2 | 192 | C |
| 49 | 2 | 215 | G |
| 49 | 2 | 292 | A |
| 49 | 2 | 293 | C |
| 49 | 2 | 294 | U |
| 49 | 2 | 302 | A |
| 49 | 2 | 306 | C |
| 49 | 2 | 307 | G |
| 49 | 2 | 308 | G |
| 49 | 2 | 309 | G |
| 49 | 2 | 312 | G |
| 49 | 2 | 313 | A |
| 49 | 2 | 314 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 2 | 315 | C |
| 49 | 2 | 317 | C |
| 49 | 2 | 318 | A |
| 49 | 2 | 319 | C |
| 49 | 2 | 332 | G |
| 49 | 2 | 347 | G |
| 49 | 2 | 351 | G |
| 49 | 2 | 356 | C |
| 49 | 2 | 357 | C |
| 49 | 2 | 361 | U |
| 49 | 2 | 362 | C |
| 49 | 2 | 364 | A |
| 49 | 2 | 367 | U |
| 49 | 2 | 368 | U |
| 49 | 2 | 370 | G |
| 49 | 2 | 371 | A |
| 49 | 2 | 383 | G |
| 49 | 2 | 384 | U |
| 49 | 2 | 385 | G |
| 49 | 2 | 386 | C |
| 49 | 2 | 390 | C |
| 49 | 2 | 398 | A |
| 49 | 2 | 399 | C |
| 49 | 2 | 400 | C |
| 49 | 2 | 407 | G |
| 49 | 2 | 408 | A |
| 49 | 2 | 409 | C |
| 49 | 2 | 417 | C |
| 49 | 2 | 418 | A |
| 49 | 2 | 426 | A |
| 49 | 2 | 429 | C |
| 49 | 2 | 434 | G |
| 49 | 2 | 448 | A |
| 49 | 2 | 449 | A |
| 49 | 2 | 450 | C |
| 49 | 2 | 452 | G |
| 49 | 2 | 465 | A |
| 49 | 2 | 466 | G |
| 49 | 2 | 471 | G |
| 49 | 2 | 472 | C |
| 49 | 2 | 473 | A |
| 49 | 2 | 474 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 2 | 476 | A |
| 49 | 2 | 487 | U |
| 49 | 2 | 492 | C |
| 49 | 2 | 493 | A |
| 49 | 2 | 500 | A |
| 49 | 2 | 502 | C |
| 49 | 2 | 509 | G |
| 49 | 2 | 516 | A |
| 49 | 2 | 525 | A |
| 49 | 2 | 530 | U |
| 49 | 2 | 531 | A |
| 49 | 2 | 532 | C |
| 49 | 2 | 533 | A |
| 49 | 2 | 542 | U |
| 49 | 2 | 547 | G |
| 49 | 2 | 548 | C |
| 49 | 2 | 549 | C |
| 49 | 2 | 550 | C |
| 49 | 2 | 552 | G |
| 49 | 2 | 554 | A |
| 49 | 2 | 555 | A |
| 49 | 2 | 556 | U |
| 49 | 2 | 559 | G |
| 49 | 2 | 560 | A |
| 49 | 2 | 562 | U |
| 49 | 2 | 569 | A |
| 49 | 2 | 576 | A |
| 49 | 2 | 583 | A |
| 49 | 2 | 588 | G |
| 49 | 2 | 589 | G |
| 49 | 2 | 590 | A |
| 49 | 2 | 591 | U |
| 49 | 2 | 594 | A |
| 49 | 2 | 595 | U |
| 49 | 2 | 597 | G |
| 49 | 2 | 600 | G |
| 49 | 2 | 603 | C |
| 49 | 2 | 604 | A |
| 49 | 2 | 606 | G |
| 49 | 2 | 608 | C |
| 49 | 2 | 614 | C |
| 49 | 2 | 617 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 2 | 621 | C |
| 49 | 2 | 627 | U |
| 49 | 2 | 628 | A |
| 49 | 2 | 629 | A |
| 49 | 2 | 642 | U |
| 49 | 2 | 643 | A |
| 49 | 2 | 655 | A |
| 49 | 2 | 656 | G |
| 49 | 2 | 657 | U |
| 49 | 2 | 658 | U |
| 49 | 2 | 661 | U |
| 49 | 2 | 662 | G |
| 49 | 2 | 664 | A |
| 49 | 2 | 668 | A |
| 49 | 2 | 671 | A |
| 49 | 2 | 672 | A |
| 49 | 2 | 673 | G |
| 49 | 2 | 684 | G |
| 49 | 2 | 688 | U |
| 49 | 2 | 689 | U |
| 49 | 2 | 696 | G |
| 49 | 2 | 752 | G |
| 49 | 2 | 753 | C |
| 49 | 2 | 754 | G |
| 49 | 2 | 811 | A |
| 49 | 2 | 821 | G |
| 49 | 2 | 822 | U |
| 49 | 2 | 824 | C |
| 49 | 2 | 827 | A |
| 49 | 2 | 830 | A |
| 49 | 2 | 847 | A |
| 49 | 2 | 852 | G |
| 49 | 2 | 853 | C |
| 49 | 2 | 870 | A |
| 49 | 2 | 871 | U |
| 49 | 2 | 872 | A |
| 49 | 2 | 873 | G |
| 49 | 2 | 875 | A |
| 49 | 2 | 879 | C |
| 49 | 2 | 882 | U |
| 49 | 2 | 886 | A |
| 49 | 2 | 888 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 2 | 890 | U |
| 49 | 2 | 891 | G |
| 49 | 2 | 893 | U |
| 49 | 2 | 894 | G |
| 49 | 2 | 897 | U |
| 49 | 2 | 898 | U |
| 49 | 2 | 913 | A |
| 49 | 2 | 914 | U |
| 49 | 2 | 919 | A |
| 49 | 2 | 920 | A |
| 49 | 2 | 933 | G |
| 49 | 2 | 952 | G |
| 49 | 2 | 955 | A |
| 49 | 2 | 969 | U |
| 49 | 2 | 970 | G |
| 49 | 2 | 971 | G |
| 49 | 2 | 985 | G |
| 49 | 2 | 990 | A |
| 49 | 2 | 991 | G |
| 49 | 2 | 992 | A |
| 49 | 2 | 999 | G |
| 49 | 2 | 1002 | U |
| 49 | 2 | 1017 | U |
| 49 | 2 | 1023 | A |
| 49 | 2 | 1026 | C |
| 49 | 2 | 1034 | A |
| 49 | 2 | 1045 | U |
| 49 | 2 | 1055 | A |
| 49 | 2 | 1061 | U |
| 49 | 2 | 1073 | U |
| 49 | 2 | 1082 | A |
| 49 | 2 | 1083 | A |
| 49 | 2 | 1085 | C |
| 49 | 2 | 1086 | G |
| 49 | 2 | 1088 | U |
| 49 | 2 | 1114 | U |
| 49 | 2 | 1115 | U |
| 49 | 2 | 1116 | C |
| 49 | 2 | 1117 | C |
| 49 | 2 | 1123 | C |
| 49 | 2 | 1133 | A |
| 49 | 2 | 1138 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 2 | 1139 | C |
| 49 | 2 | 1148 | A |
| 49 | 2 | 1149 | A |
| 49 | 2 | 1150 | A |
| 49 | 2 | 1153 | C |
| 49 | 2 | 1154 | U |
| 49 | 2 | 1155 | U |
| 49 | 2 | 1157 | G |
| 49 | 2 | 1161 | U |
| 49 | 2 | 1165 | G |
| 49 | 2 | 1166 | G |
| 49 | 2 | 1170 | A |
| 49 | 2 | 1194 | A |
| 49 | 2 | 1195 | A |
| 49 | 2 | 1204 | A |
| 49 | 2 | 1207 | G |
| 49 | 2 | 1208 | A |
| 49 | 2 | 1215 | C |
| 49 | 2 | 1216 | C |
| 49 | 2 | 1217 | A |
| 49 | 2 | 1227 | G |
| 49 | 2 | 1228 | A |
| 49 | 2 | 1236 | G |
| 49 | 2 | 1242 | U |
| 49 | 2 | 1250 | A |
| 49 | 2 | 1251 | A |
| 49 | 2 | 1253 | A |
| 49 | 2 | 1254 | C |
| 49 | 2 | 1256 | G |
| 49 | 2 | 1257 | G |
| 49 | 2 | 1259 | A |
| 49 | 2 | 1261 | C |
| 49 | 2 | 1264 | C |
| 49 | 2 | 1269 | G |
| 49 | 2 | 1273 | C |
| 49 | 2 | 1274 | G |
| 49 | 2 | 1275 | G |
| 49 | 2 | 1284 | A |
| 49 | 2 | 1285 | G |
| 49 | 2 | 1286 | G |
| 49 | 2 | 1293 | A |
| 49 | 2 | 1294 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 2 | 1298 | G |
| 49 | 2 | 1299 | A |
| 49 | 2 | 1301 | A |
| 49 | 2 | 1302 | G |
| 49 | 2 | 1303 | C |
| 49 | 2 | 1306 | U |
| 49 | 2 | 1307 | U |
| 49 | 2 | 1308 | U |
| 49 | 2 | 1309 | C |
| 49 | 2 | 1314 | U |
| 49 | 2 | 1327 | G |
| 49 | 2 | 1333 | U |
| 49 | 2 | 1341 | C |
| 49 | 2 | 1342 | U |
| 49 | 2 | 1354 | G |
| 49 | 2 | 1356 | G |
| 49 | 2 | 1358 | U |
| 49 | 2 | 1364 | U |
| 49 | 2 | 1365 | G |
| 49 | 2 | 1371 | U |
| 49 | 2 | 1372 | U |
| 49 | 2 | 1374 | C |
| 49 | 2 | 1377 | U |
| 49 | 2 | 1378 | A |
| 49 | 2 | 1390 | U |
| 49 | 2 | 1396 | A |
| 49 | 2 | 1397 | U |
| 49 | 2 | 1402 | A |
| 49 | 2 | 1404 | U |
| 49 | 2 | 1406 | G |
| 49 | 2 | 1428 | G |
| 49 | 2 | 1429 | G |
| 49 | 2 | 1439 | A |
| 49 | 2 | 1442 | U |
| 49 | 2 | 1449 | G |
| 49 | 2 | 1452 | A |
| 49 | 2 | 1454 | A |
| 49 | 2 | 1462 | U |
| 49 | 2 | 1463 | U |
| 49 | 2 | 1466 | G |
| 49 | 2 | 1475 | G |
| 49 | 2 | 1476 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 2 | 1477 | U |
| 49 | 2 | 1483 | A |
| 49 | 2 | 1489 | A |
| 49 | 2 | 1490 | G |
| 49 | 2 | 1492 | U |
| 49 | 2 | 1497 | G |
| 49 | 2 | 1498 | A |
| 49 | 2 | 1507 | G |
| 49 | 2 | 1508 | A |
| 49 | 2 | 1515 | G |
| 49 | 2 | 1520 | G |
| 49 | 2 | 1521 | C |
| 49 | 2 | 1533 | A |
| 49 | 2 | 1535 | U |
| 49 | 2 | 1536 | G |
| 49 | 2 | 1548 | G |
| 49 | 2 | 1551 | U |
| 49 | 2 | 1552 | G |
| 49 | 2 | 1553 | C |
| 49 | 2 | 1554 | C |
| 49 | 2 | 1556 | A |
| 49 | 2 | 1558 | C |
| 49 | 2 | 1560 | U |
| 49 | 2 | 1570 | G |
| 49 | 2 | 1573 | G |
| 49 | 2 | 1575 | G |
| 49 | 2 | 1578 | U |
| 49 | 2 | 1580 | A |
| 49 | 2 | 1584 | G |
| 49 | 2 | 1585 | U |
| 49 | 2 | 1588 | A |
| 49 | 2 | 1598 | G |
| 49 | 2 | 1601 | A |
| 49 | 2 | 1603 | G |
| 49 | 2 | 1604 | G |
| 49 | 2 | 1606 | G |
| 49 | 2 | 1621 | U |
| 49 | 2 | 1623 | A |
| 49 | 2 | 1637 | A |
| 49 | 2 | 1638 | G |
| 49 | 2 | 1647 | A |
| 49 | 2 | 1648 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 2 | 1654 | G |
| 49 | 2 | 1661 | A |
| 49 | 2 | 1665 | G |
| 49 | 2 | 1671 | G |
| 49 | 2 | 1678 | A |
| 49 | 2 | 1680 | G |
| 49 | 2 | 1683 | C |
| 49 | 2 | 1689 | C |
| 49 | 2 | 1692 | U |
| 49 | 2 | 1693 | G |
| 49 | 2 | 1695 | A |
| 49 | 2 | 1696 | C |
| 49 | 2 | 1697 | A |
| 49 | 2 | 1700 | C |
| 49 | 2 | 1701 | C |
| 49 | 2 | 1702 | G |
| 49 | 2 | 1721 | U |
| 49 | 2 | 1722 | G |
| 49 | 2 | 1725 | U |
| 49 | 2 | 1726 | G |
| 49 | 2 | 1744 | G |
| 49 | 2 | 1748 | G |
| 49 | 2 | 1753 | C |
| 49 | 2 | 1756 | C |
| 49 | 2 | 1757 | G |
| 49 | 2 | 1773 | C |
| 49 | 2 | 1776 | G |
| 49 | 2 | 1781 | A |
| 49 | 2 | 1783 | C |
| 49 | 2 | 1823 | A |
| 49 | 2 | 1824 | A |
| 49 | 2 | 1825 | A |
| 49 | 2 | 1831 | A |
| 49 | 2 | 1833 | C |
| 49 | 2 | 1834 | A |
| 49 | 2 | 1835 | A |
| 49 | 2 | 1836 | G |
| 49 | 2 | 1838 | U |
| 49 | 2 | 1849 | G |
| 49 | 2 | 1851 | A |
| 49 | 2 | 1852 | C |
| 49 | 2 | 1861 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 2 | 1862 | G |
| 49 | 2 | 1863 | A |
| 49 | 2 | 1865 | C |
| 49 | 2 | 1868 | U |
| 49 | 2 | 1869 | A |
| 83 | 3 | 8 | U |
| 83 | 3 | 9 | G |
| 83 | 3 | 10 | G |
| 83 | 3 | 13 | G |
| 83 | 3 | 16 | U |
| 83 | 3 | 17 | U |
| 83 | 3 | 18 | G |
| 83 | 3 | 19 | G |
| 83 | 3 | 20 | U |
| 83 | 3 | 21 | A |
| 83 | 3 | 22 | G |
| 83 | 3 | 23 | A |
| 83 | 3 | 24 | C |
| 83 | 3 | 26 | C |
| 83 | 3 | 46 | G |
| 83 | 3 | 49 | C |
| 83 | 3 | 51 | A |
| 83 | 3 | 54 | G |
| 83 | 3 | 55 | G |
| 83 | 3 | 58 | U |
| 83 | 3 | 71 | U |
| 83 | 3 | 77 | C |
| 83 | 3 | 82 | G |
| 83 | 3 | 85 | C |
| 83 | 3 | 86 | C |
| 85 | 4 | 6031 | A |
| 85 | 4 | 6032 | A |
| 85 | 4 | 6033 | A |
| 85 | 4 | 6036 | G |
| 85 | 4 | 6038 | G |
| 85 | 4 | 6040 | U |
| 85 | 4 | 6041 | C |
| 85 | 4 | 6042 | U |
| 85 | 4 | 6043 | U |
| 85 | 4 | 6044 | G |
| 85 | 4 | 6048 | G |
| 85 | 4 | 6050 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 85 | 4 | 6052 | A |
| 85 | 4 | 6054 | A |
| 85 | 4 | 6056 | A |
| 85 | 4 | 6057 | A |
| 85 | 4 | 6058 | U |
| 85 | 4 | 6059 | U |
| 85 | 4 | 6060 | U |
| 85 | 4 | 6061 | U |
| 85 | 4 | 6062 | G |
| 85 | 4 | 6063 | A |
| 85 | 4 | 6064 | G |
| 85 | 4 | 6065 | A |
| 85 | 4 | 6066 | G |
| 85 | 4 | 6067 | G |
| 85 | 4 | 6068 | U |
| 85 | 4 | 6069 | U |
| 85 | 4 | 6072 | U |
| 85 | 4 | 6073 | A |
| 85 | 4 | 6074 | A |
| 85 | 4 | 6075 | A |
| 85 | 4 | 6076 | U |
| 85 | 4 | 6077 | U |
| 85 | 4 | 6081 | A |
| 85 | 4 | 6083 | U |
| 85 | 4 | 6084 | A |
| 85 | 4 | 6085 | G |
| 85 | 4 | 6087 | G |
| 85 | 4 | 6088 | C |
| 85 | 4 | 6090 | A |
| 85 | 4 | 6094 | U |
| 85 | 4 | 6097 | U |
| 85 | 4 | 6098 | A |
| 85 | 4 | 6099 | U |
| 85 | 4 | 6100 | U |
| 85 | 4 | 6101 | U |
| 85 | 4 | 6105 | U |
| 85 | 4 | 6106 | U |
| 85 | 4 | 6107 | A |
| 85 | 4 | 6108 | G |
| 85 | 4 | 6113 | U |
| 85 | 4 | 6115 | A |
| 85 | 4 | 6116 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 85 | 4 | 6119 | U |
| 85 | 4 | 6121 | A |
| 85 | 4 | 6122 | C |
| 85 | 4 | 6123 | G |
| 85 | 4 | 6125 | U |
| 85 | 4 | 6126 | C |
| 85 | 4 | 6128 | A |
| 85 | 4 | 6129 | G |
| 85 | 4 | 6134 | C |
| 85 | 4 | 6136 | U |
| 85 | 4 | 6139 | U |
| 85 | 4 | 6140 | G |
| 85 | 4 | 6150 | C |
| 85 | 4 | 6151 | A |
| 85 | 4 | 6152 | A |
| 85 | 4 | 6154 | A |
| 85 | 4 | 6158 | A |
| 85 | 4 | 6162 | A |
| 85 | 4 | 6163 | G |
| 85 | 4 | 6164 | C |
| 85 | 4 | 6165 | C |
| 85 | 4 | 6166 | C |
| 85 | 4 | 6167 | U |
| 85 | 4 | 6168 | C |
| 85 | 4 | 6169 | U |
| 85 | 4 | 6170 | C |
| 85 | 4 | 6171 | U |
| 85 | 4 | 6172 | G |
| 85 | 4 | 6173 | C |
| 85 | 4 | 6174 | G |
| 85 | 4 | 6175 | G |
| 85 | 4 | 6176 | U |
| 85 | 4 | 6177 | U |
| 85 | 4 | 6178 | U |
| 85 | 4 | 6179 | U |
| 85 | 4 | 6180 | U |
| 85 | 4 | 6181 | C |
| 85 | 4 | 6182 | A |
| 85 | 4 | 6183 | G |
| 85 | 4 | 6185 | U |
| 85 | 4 | 6186 | U |
| 85 | 4 | 6187 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 85 | 4 | 6188 | G |
| 85 | 4 | 6189 | G |
| 85 | 4 | 6190 | U |
| 85 | 4 | 6191 | A |
| 85 | 4 | 6192 | G |
| 85 | 4 | 6193 | U |
| 85 | 4 | 6196 | A |
| 85 | 4 | 6197 | A |
| 85 | 4 | 6198 | A |
| 85 | 4 | 6199 | A |
| 85 | 4 | 6200 | A |
| 85 | 4 | 6202 | C |
| 85 | 4 | 6203 | U |
| 85 | 4 | 6204 | A |
| 85 | 4 | 6205 | A |
| 85 | 4 | 6206 | G |
| 85 | 4 | 6207 | A |
| 85 | 4 | 6208 | A |
| 85 | 4 | 6209 | A |
| 85 | 4 | 6210 | U |
| 85 | 4 | 6211 | U |
| 85 | 4 | 6212 | U |
| 85 | 4 | 6213 | A |
| 85 | 4 | 6214 | C |
| 85 | 4 | 6215 | C |
| 85 | 4 | 6216 | U |
| 85 | 4 | 6217 | C |

All (92) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 48 | G |
| 45 | 5 | 125 | C |
| 45 | 5 | 275 | C |
| 45 | 5 | 481 | G |
| 45 | 5 | 504 | G |
| 45 | 5 | 930 | G |
| 45 | 5 | 1072 | C |
| 45 | 5 | 1211 | G |
| 45 | 5 | 1291 | G |
| 45 | 5 | 1445 | U |
| 45 | 5 | 1455 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 5 | 1633 | G |
| 45 | 5 | 2046 | G |
| 45 | 5 | 2089 | G |
| 45 | 5 | 2266 | C |
| 45 | 5 | 2502 | A |
| 45 | 5 | 2661 | U |
| 45 | 5 | 2695 | A |
| 45 | 5 | 3603 | G |
| 45 | 5 | 3625 | G |
| 45 | 5 | 4054 | C |
| 45 | 5 | 4170 | A |
| 45 | 5 | 4232 | U |
| 45 | 5 | 4448 | G |
| 45 | 5 | 4699 | U |
| 45 | 5 | 4719 | G |
| 45 | 5 | 4884 | G |
| 45 | 5 | 4925 | U |
| 45 | 5 | 4947 | U |
| 47 | 8 | 124 | U |
| 49 | 2 | 24 | C |
| 49 | 2 | 110 | U |
| 49 | 2 | 182 | C |
| 49 | 2 | 532 | C |
| 49 | 2 | 553 | U |
| 49 | 2 | 561 | A |
| 49 | 2 | 688 | U |
| 49 | 2 | 752 | G |
| 49 | 2 | 1137 | U |
| 49 | 2 | 1253 | A |
| 49 | 2 | 1395 | C |
| 49 | 2 | 1489 | A |
| 49 | 2 | 1637 | A |
| 49 | 2 | 1664 | A |
| 85 | 4 | 6057 | A |
| 85 | 4 | 6058 | U |
| 85 | 4 | 6059 | U |
| 85 | 4 | 6060 | U |
| 85 | 4 | 6061 | U |
| 85 | 4 | 6066 | G |
| 85 | 4 | 6067 | G |
| 85 | 4 | 6068 | U |
| 85 | 4 | 6072 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 85 | 4 | 6073 | A |
| 85 | 4 | 6076 | U |
| 85 | 4 | 6107 | A |
| 85 | 4 | 6150 | C |
| 85 | 4 | 6151 | A |
| 85 | 4 | 6163 | G |
| 85 | 4 | 6164 | C |
| 85 | 4 | 6165 | C |
| 85 | 4 | 6166 | C |
| 85 | 4 | 6167 | U |
| 85 | 4 | 6170 | C |
| 85 | 4 | 6171 | U |
| 85 | 4 | 6172 | G |
| 85 | 4 | 6173 | C |
| 85 | 4 | 6174 | G |
| 85 | 4 | 6175 | G |
| 85 | 4 | 6176 | U |
| 85 | 4 | 6179 | U |
| 85 | 4 | 6180 | U |
| 85 | 4 | 6181 | C |
| 85 | 4 | 6182 | A |
| 85 | 4 | 6183 | G |
| 85 | 4 | 6184 | A |
| 85 | 4 | 6185 | U |
| 85 | 4 | 6186 | U |
| 85 | 4 | 6187 | A |
| 85 | 4 | 6188 | G |
| 85 | 4 | 6189 | G |
| 85 | 4 | 6190 | U |
| 85 | 4 | 6196 | A |
| 85 | 4 | 6199 | A |
| 85 | 4 | 6206 | G |
| 85 | 4 | 6208 | A |
| 85 | 4 | 6209 | A |
| 85 | 4 | 6210 | U |
| 85 | 4 | 6211 | U |
| 85 | 4 | 6212 | U |
| 85 | 4 | 6213 | A |
| 85 | 4 | 6214 | C |

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 45 | 5 | 36 |
| 49 | 2 | 20 |
| 48 | K | 3 |
| 47 | 8 | 1 |
| 82 | hh | 1 |
| 14 | O | 1 |
| 3 | C | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | 5 | 2113:G | O3' | 2258:C | P | 41.98 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | 5 | 1252:C | O3' | 1271:G | P | 33.40 |
| 1 | 5 | 1696:C | O3' | 1720:C | P | 19.99 |
| 1 | 5 | 1219:G | O3' | 1233:G | P | 18.35 |
| 1 | 5 | 523:C | O3' | 638:G | P | 18.12 |
| 1 | 5 | 990:C | O3' | 1064:G | P | 18.08 |
| 1 | 2 | 756:C | O3' | 788:G | P | 17.83 |
| 1 | 5 | 4101:C | O3' | 4107:G | P | 17.76 |
| 1 | 5 | 4138:C | O3' | 4146:G | P | 17.64 |
| 1 | 2 | 834:C | O3' | 841:G | P | 17.63 |
| 1 | 2 | 697:G | O3' | 729:C | P | 17.51 |
| 1 | 5 | 3977:C | O3' | 4034:G | P | 17.44 |
| 1 | 2 | 1417:C | O3' | 1423:C | P | 15.35 |
| 1 | 5 | 5022:U | O3' | 5028:G | P | 14.94 |
| 1 | 2 | 1761:U | O3' | 1771:G | P | 14.63 |
| 1 | 5 | 4777:C | O3' | 4859:C | P | 14.47 |
| 1 | 5 | 760:G | O3' | 904:C | P | 14.39 |
| 1 | 2 | 130:G | O3' | 141:A | P | 13.98 |
| 1 | 5 | 1364:U | O3' | 1368:A | P | 13.51 |
| 1 | 2 | 323:C | O3' | 329:G | P | 12.90 |
| 1 | 5 | 1405:C | O3' | 1411(A):G | P | 12.67 |
| 1 | 5 | 4045:G | O3' | 4047:A | P | 12.53 |
| 1 | 5 | 2901:G | O3' | 3597:G | P | 11.66 |
| 1 | 5 | 182:G | O3' | 189:G | P | 10.37 |
| 1 | 5 | 4729:A | O3' | 4735:G | P | 9.24 |
| 1 | 5 | 1180:C | O3' | 1183:C | P | 8.44 |
| 1 | 5 | 971(A):G | O3' | 972:C | P | 8.39 |
| 1 | 2 | 689:U | O3' | 690:G | P | 8.38 |
| 1 | 8 | 79:G | O3' | 85:U | P | 7.62 |
| 1 | hh | 2:THR | C | 3:GLU | N | 7.52 |
| 1 | K | 194:LEU | C | 195:LYS | N | 7.40 |
| 1 | 5 | 737:C | O3' | 738(A):C | P | 7.09 |
| 1 | 5 | 970:G | O3' | 971:U | P | 6.80 |
| 1 | 5 | 500:G | O3' | 504:G | P | 6.70 |
| 1 | 2 | 736:C | O3' | 743:U | P | 6.55 |
| 1 | 5 | 1957:U | O3' | 1958:A | P | 6.11 |
| 1 | 2 | 225:G | O3' | 287:U | P | 5.99 |
| 1 | 5 | 751:G | O3' | 752:G | P | 5.86 |
| 1 | 5 | 4740:G | O3' | 4743:G | P | 5.52 |
| 1 | 5 | 971:U | O3' | 971(A):G | P | 5.18 |
| 1 | K | 9:THR | C | 10:LEU | N | 5.03 |
| 1 | 2 | 1432:U | O3' | 1438:A | P | 4.80 |
| 1 | 5 | 1239:C | O3' | 1244:G | P | 4.77 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | 2 | 322:C | O3' | 323:C | P | 4.73 |
| 1 | 5 | 512:U | O3' | 515:C | P | 4.66 |
| 1 | K | 172:VAL | C | 173:LYS | N | 4.60 |
| 1 | 5 | 1438:U | O3' | 1440:U | P | 4.48 |
| 1 | 5 | 170:C | O3' | 171:U | P | 4.34 |
| 1 | 2 | 745:C | O3' | 749:U | P | 4.21 |
| 1 | 2 | 1697:A | O3' | 1698:C | P | 4.16 |
| 1 | 2 | 886:A | O3' | 887:U | P | 4.06 |
| 1 | 2 | 304:C | O3' | 305:U | P | 4.01 |
| 1 | O | 109:PRO | C | 111:PRO | N | 3.99 |
| 1 | 2 | 903:A | O3' | 904:A | P | 3.93 |
| 1 | 5 | 4899:G | O3' | 4902:C | P | 3.53 |
| 1 | 2 | 798:G | O3' | 799:U | P | 3.35 |
| 1 | 5 | 1100:U | O3' | 1168:G | P | 3.34 |
| 1 | 5 | 738(A):C | O3' | 739:G | P | 3.31 |
| 1 | 5 | 267:G | O3' | 268:G | P | 3.29 |
| 1 | 2 | 902:G | O3' | 903:A | P | 3.29 |
| 1 | 2 | 1201:U | O3' | 1202:U | P | 3.27 |
| 1 | 5 | 5020:G | O3' | 5021:C | P | 3.24 |
| 1 | C | 132:ALA | C | 133:LEU | N | 3.22 |

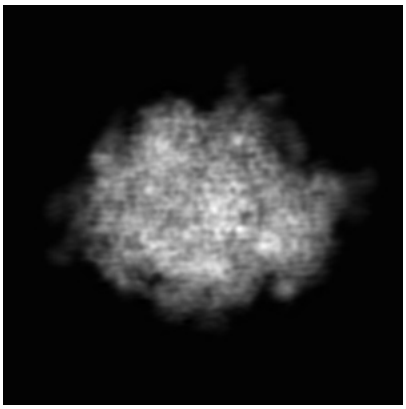
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7836. These allow visual inspection of the internal detail of the map and identification of artifacts.

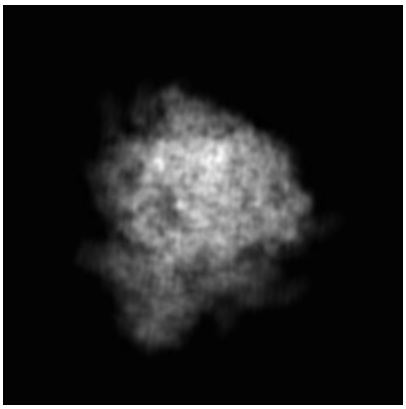
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

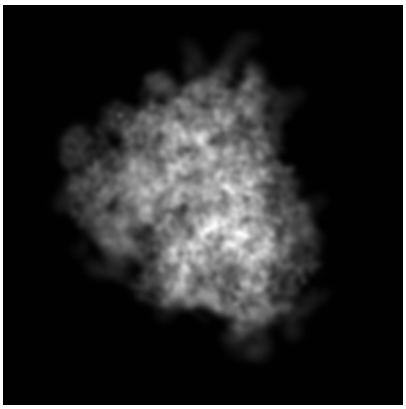
### 6.1.1 Primary map



X

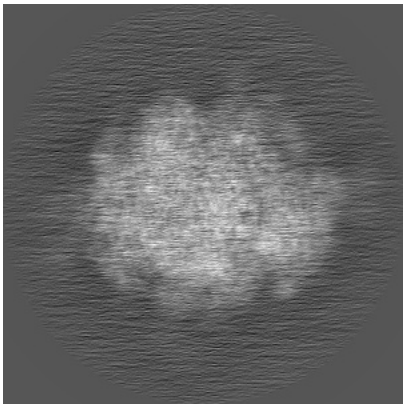


Y

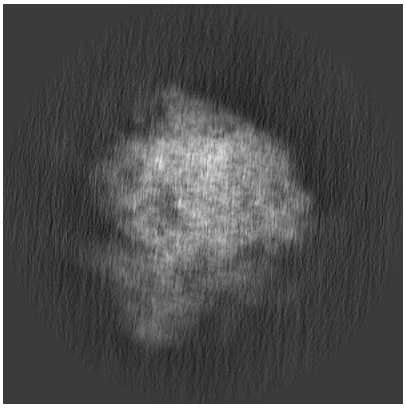


Z

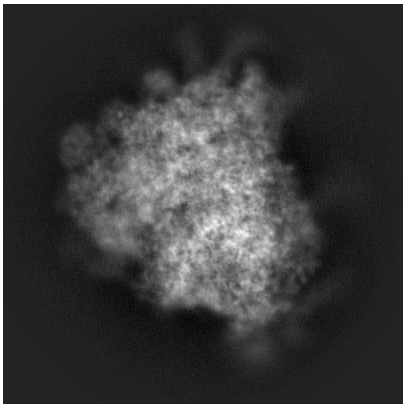
### 6.1.2 Raw map



X



Y

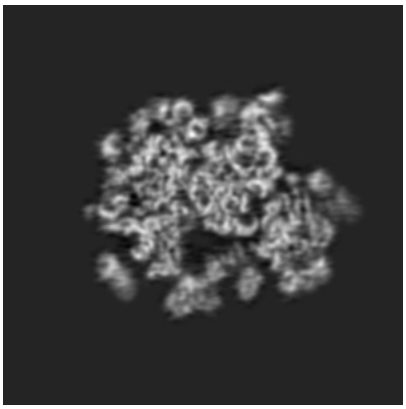


Z

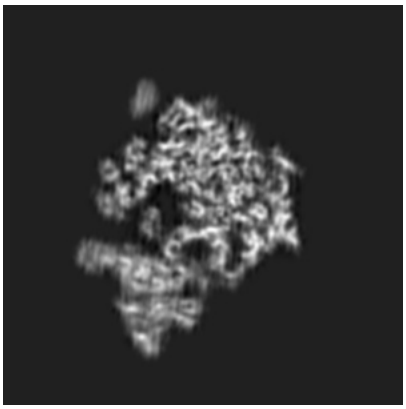
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

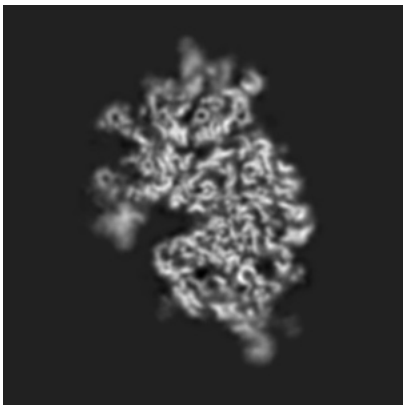
### 6.2.1 Primary map



X Index: 200

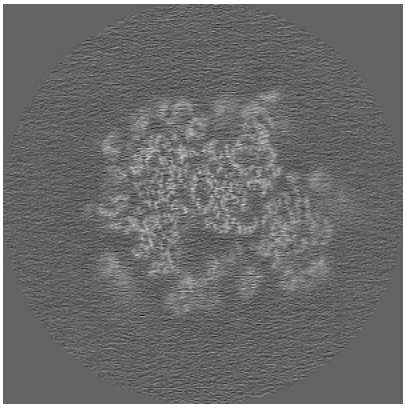


Y Index: 200

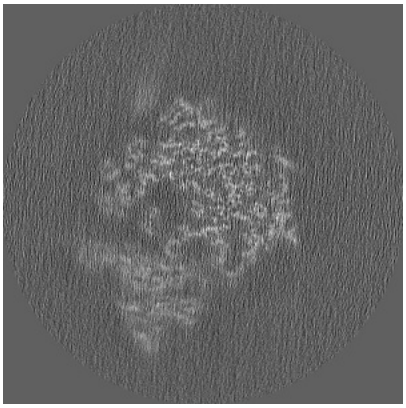


Z Index: 200

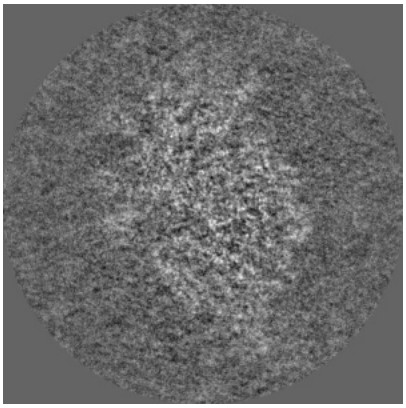
### 6.2.2 Raw map



X Index: 200



Y Index: 200

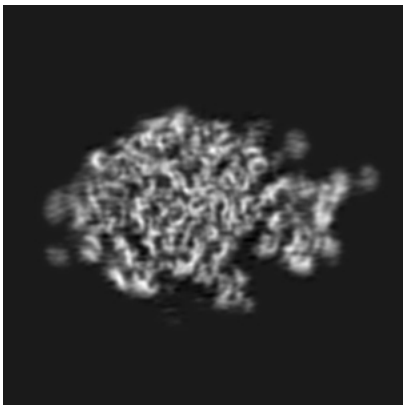


Z Index: 200

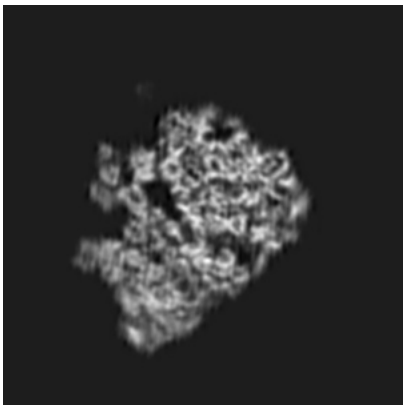
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

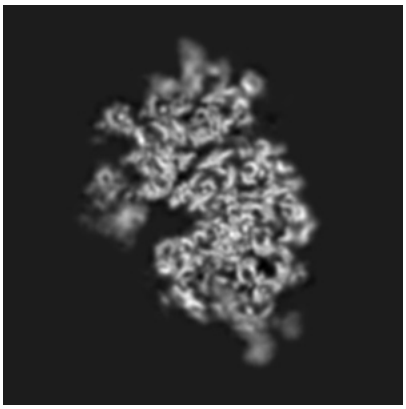
### 6.3.1 Primary map



X Index: 248

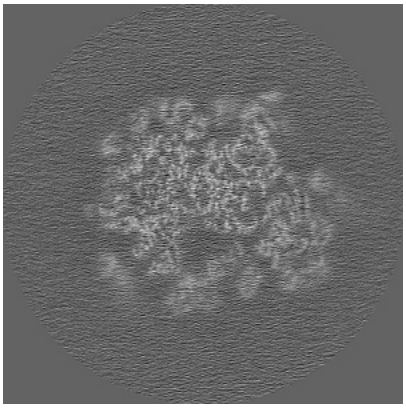


Y Index: 213

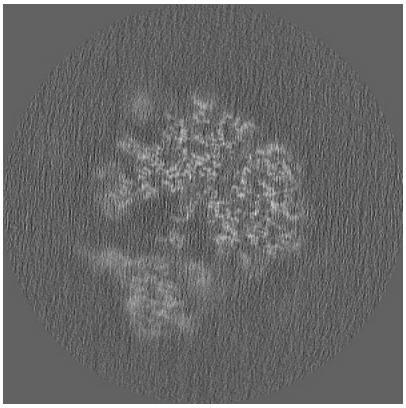


Z Index: 197

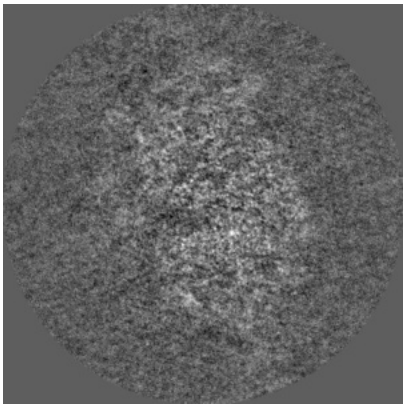
### 6.3.2 Raw map



X Index: 201



Y Index: 189

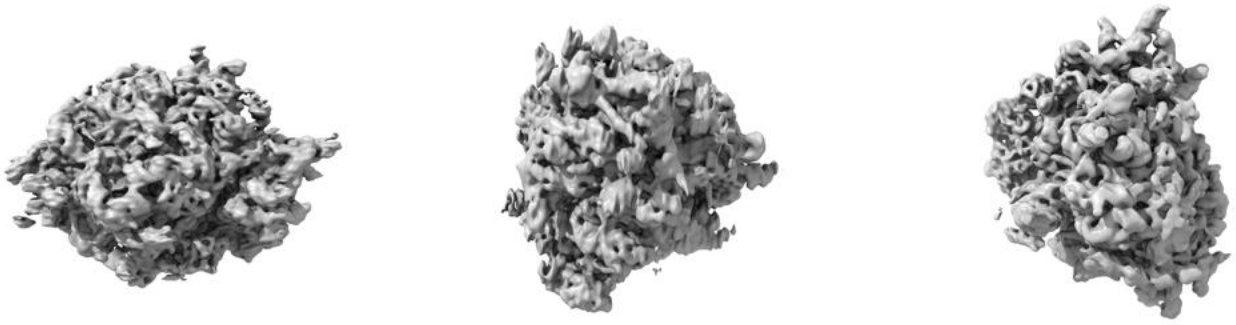


Z Index: 198

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

## 6.4 Orthogonal surface views (i)

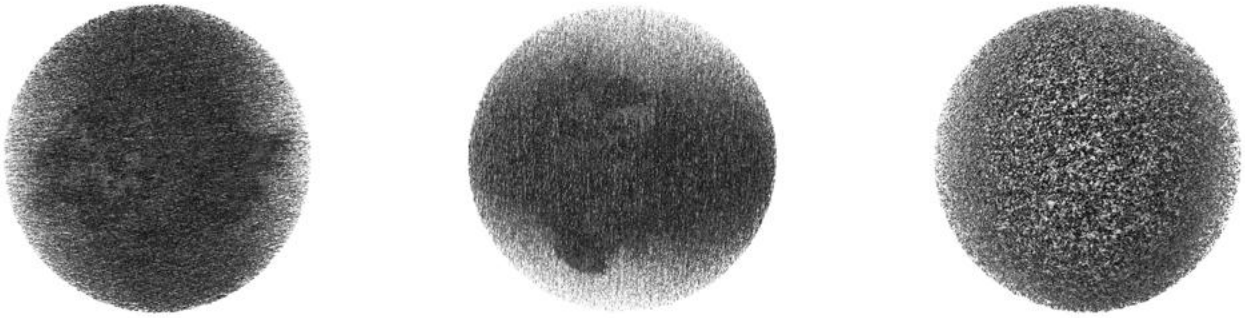
### 6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



X Y Z

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

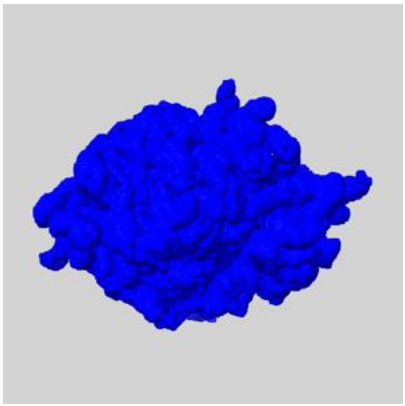
## 6.5 Mask visualisation

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

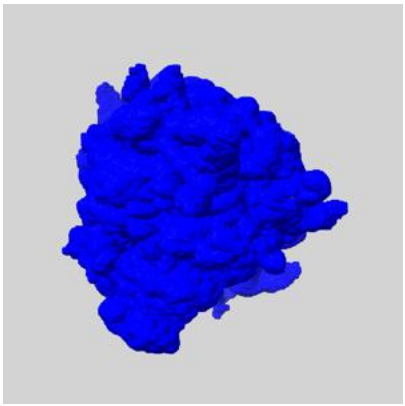
A mask typically either:

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

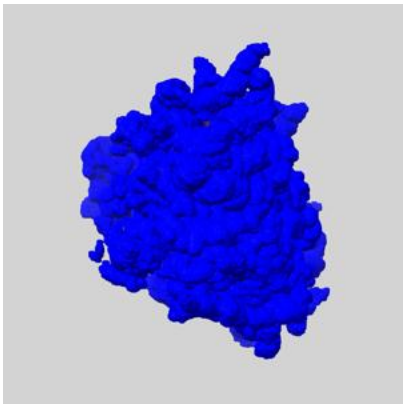
### 6.5.1 emd_7836_msk_1.map



X



Y

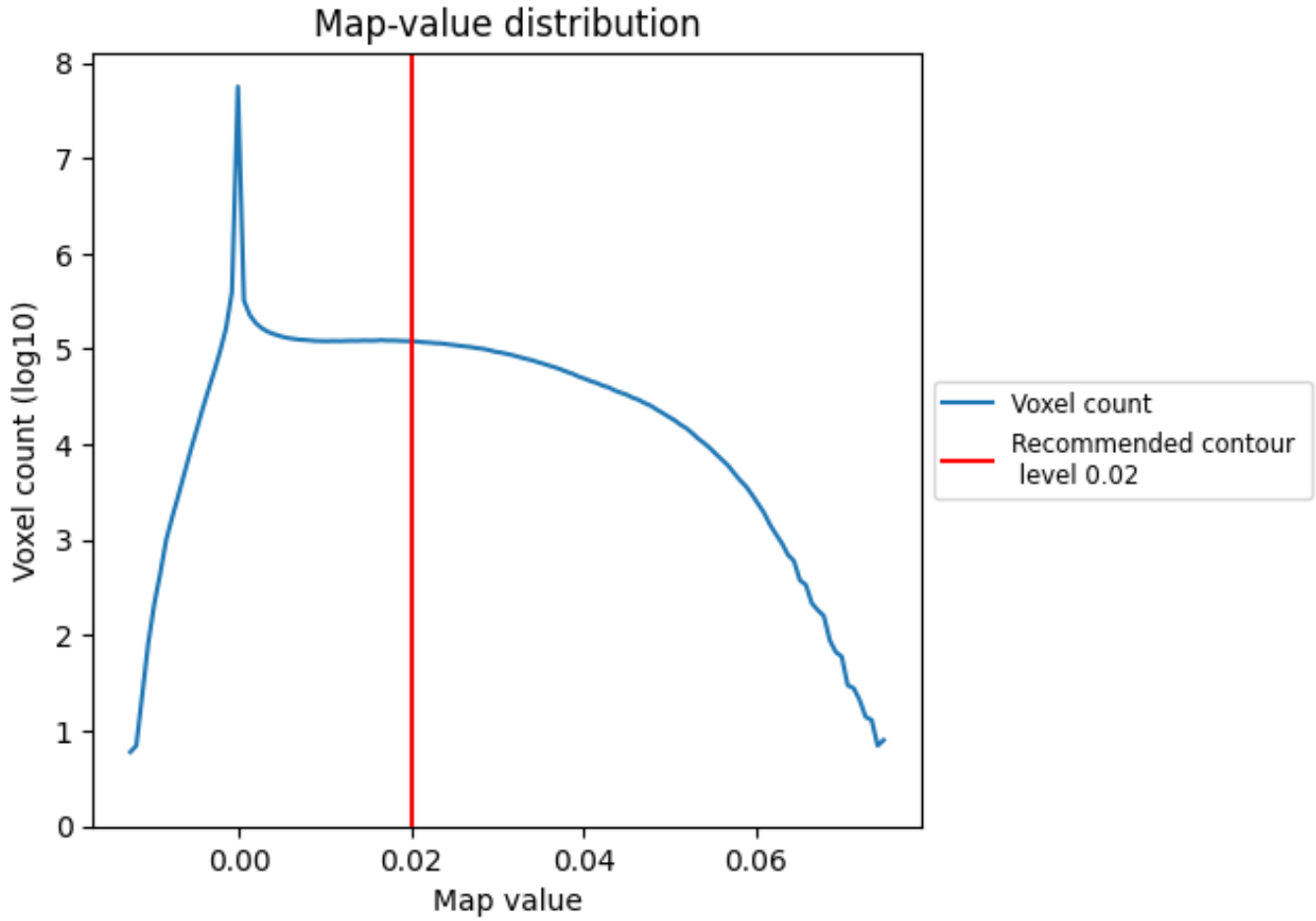


Z

# 7 Map analysis

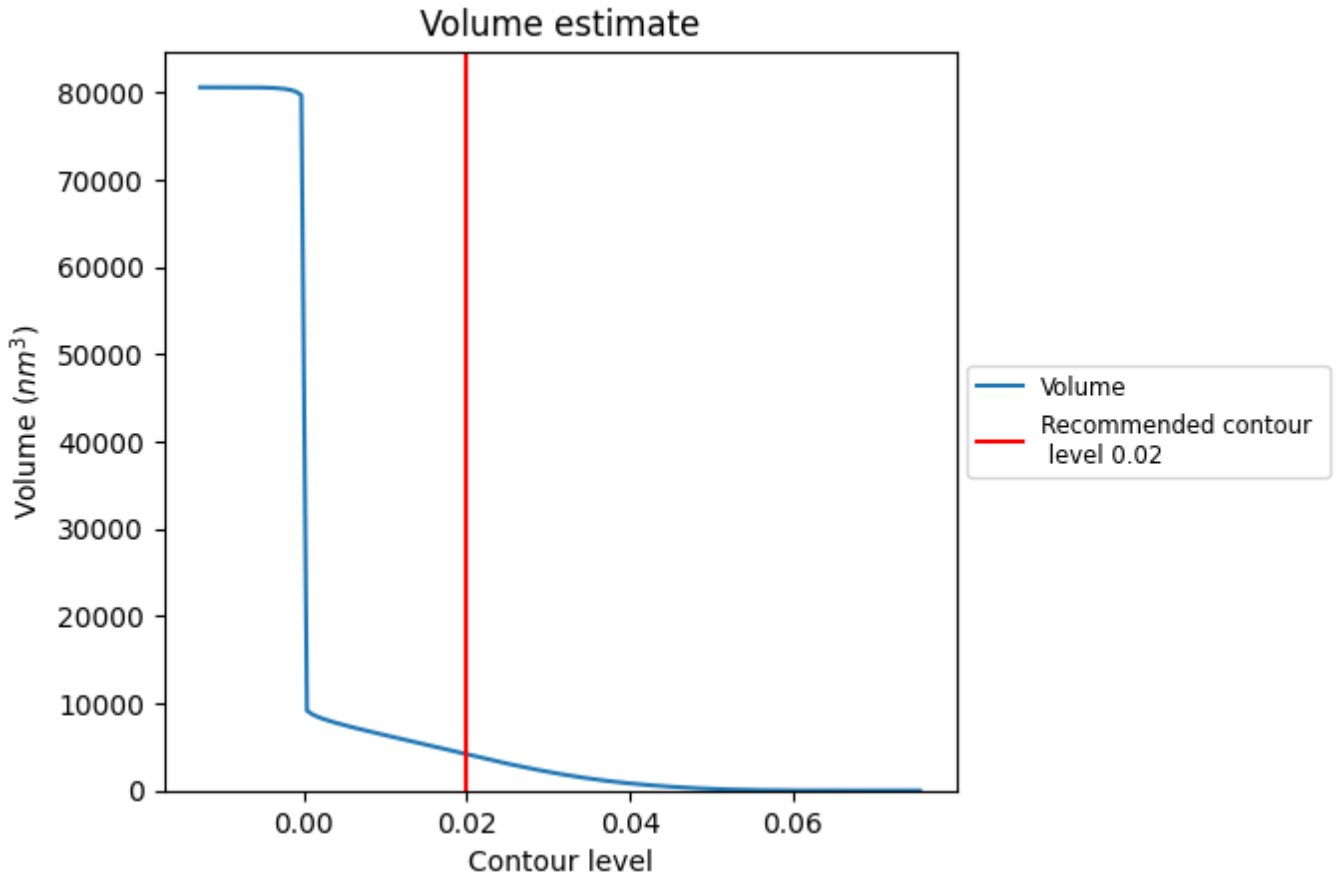
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

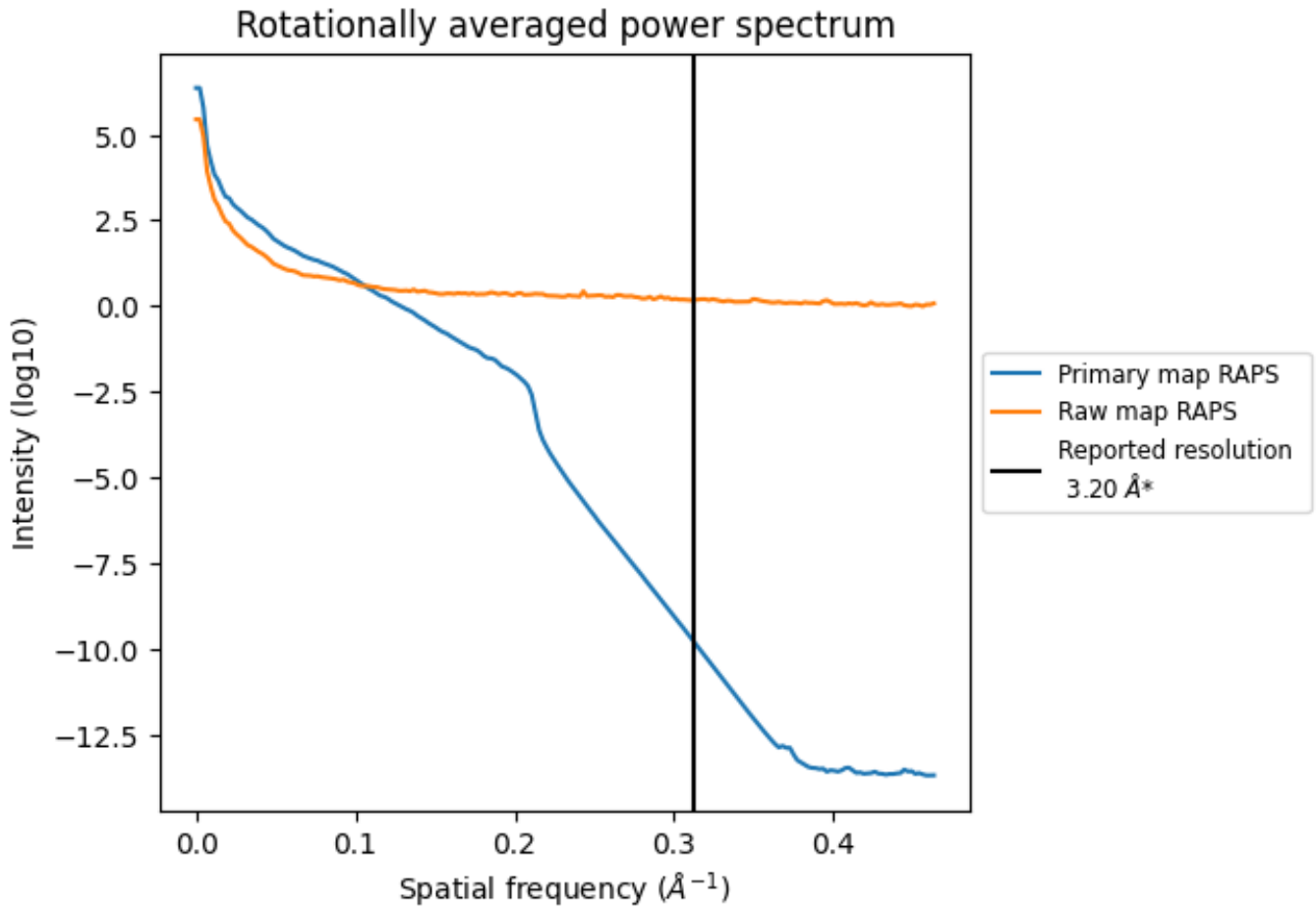
## 7.2 Volume estimate




The volume at the recommended contour level is 4136 $nm^3$; this corresponds to an approximate mass of 3736 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)

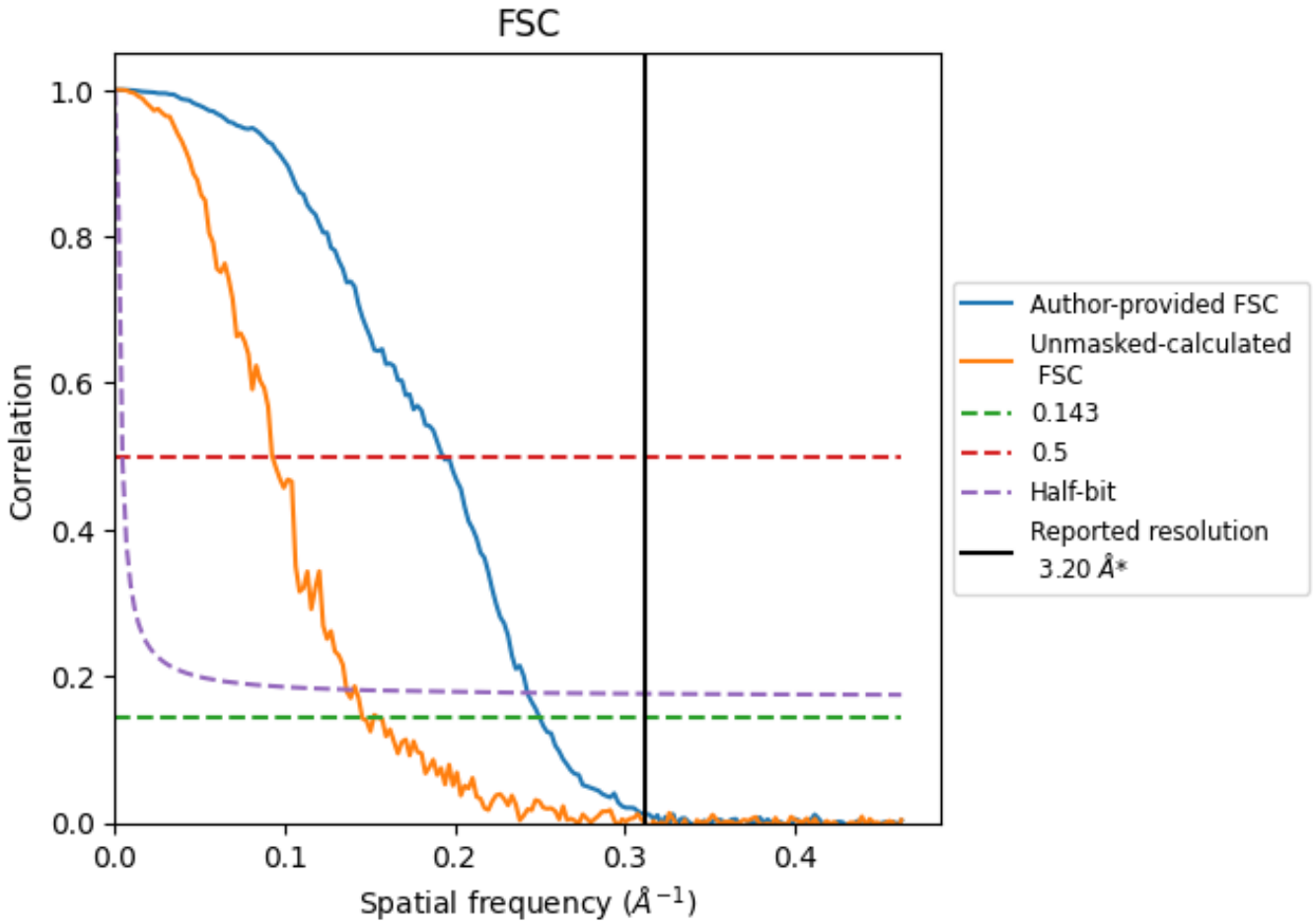



*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

# 8 Fourier-Shell correlation

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

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.312 Å$^{-1}$

## 8.2 Resolution estimates (i)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.20 | - | - |
| Author-provided FSC curve | 4.00 | 5.17 | 4.12 |
| Unmasked-calculated* | 6.86 | 10.79 | 7.33 |

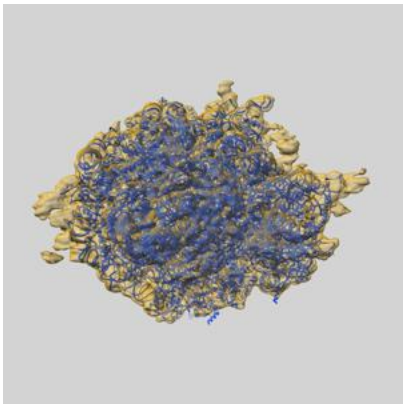
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.86 differs from the reported value 3.2 by more than 10 %

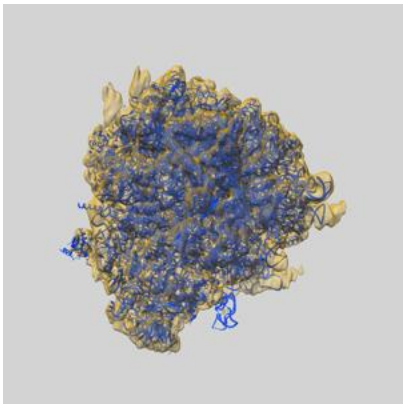
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7836 and PDB model 6D9J. Per-residue inclusion information can be found in section 3 on page 21.

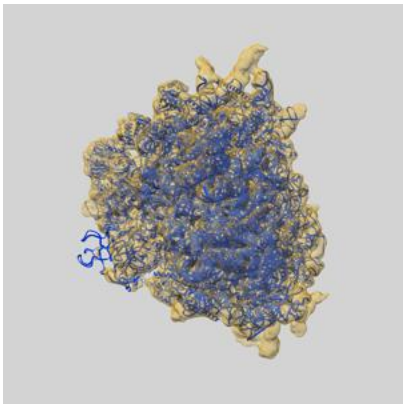
## 9.1 Map-model overlay



X



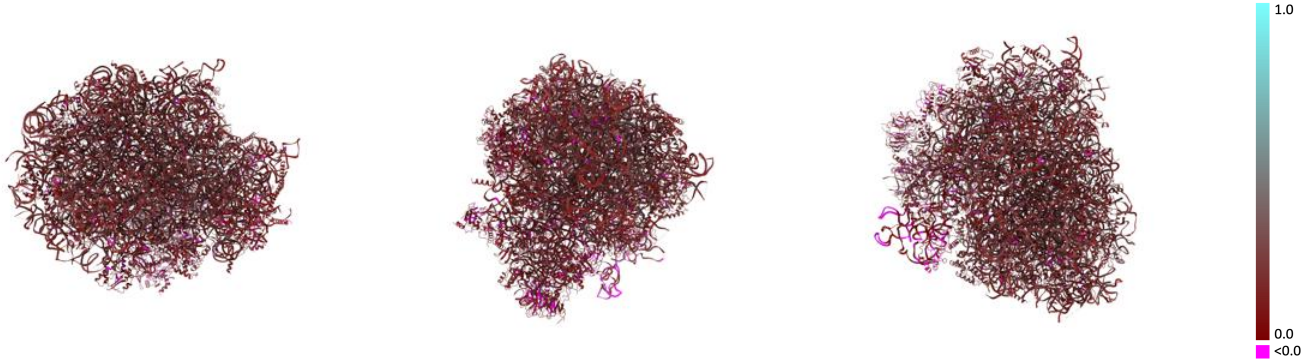
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

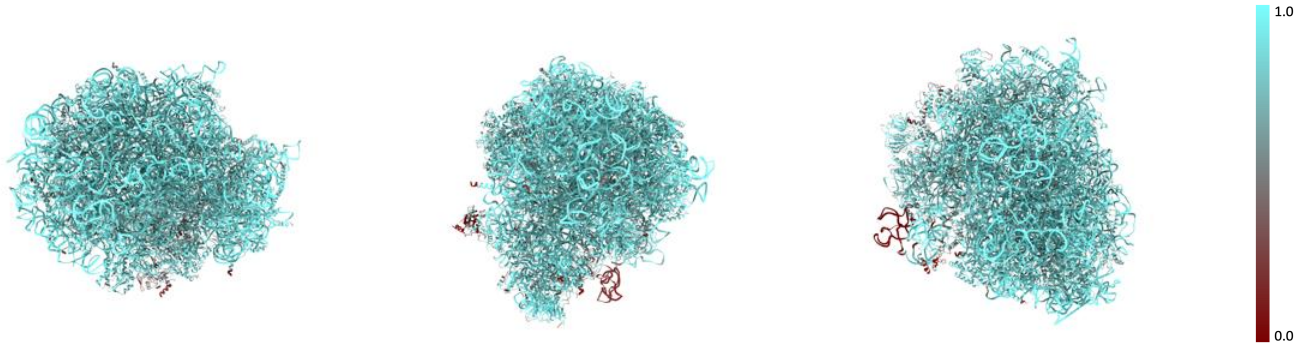
## 9.2 Q-score mapped to coordinate model




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.

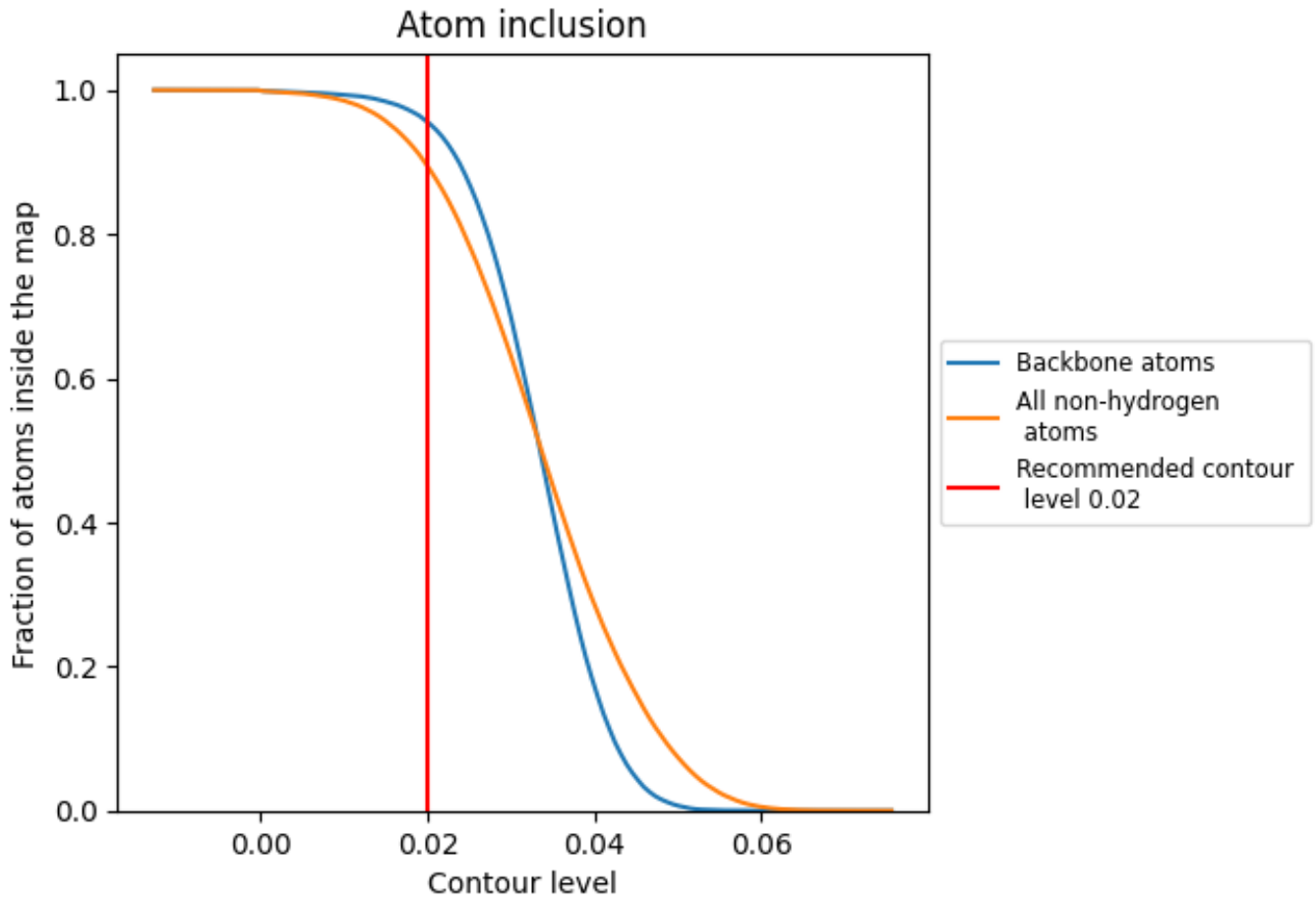
## 9.3 Atom inclusion mapped to coordinate model




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 (0.02).

## 9.4 Atom inclusion (i)




At the recommended contour level, 96% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8948 | 0.1880 |
| 2 | 0.9769 | 0.2060 |
| 3 | 0.7774 | 0.1720 |
| 4 | 0.5296 | 0.0620 |
| 5 | 0.9830 | 0.2280 |
| 7 | 0.9961 | 0.2340 |
| 8 | 0.9804 | 0.2140 |
| 9 | 0.7334 | 0.1480 |
| A | 0.8352 | 0.1770 |
| B | 0.8227 | 0.1750 |
| BB | 0.7879 | 0.1530 |
| C | 0.8351 | 0.1610 |
| CC | 0.8570 | 0.1640 |
| D | 0.8944 | 0.1680 |
| DD | 0.8005 | 0.1630 |
| E | 0.8523 | 0.1690 |
| EE | 0.7809 | 0.1540 |
| F | 0.7993 | 0.1610 |
| FF | 0.8578 | 0.1500 |
| G | 0.8268 | 0.1690 |
| GG | 0.8031 | 0.1470 |
| H | 0.8072 | 0.1740 |
| HH | 0.8571 | 0.1460 |
| I | 0.8203 | 0.1700 |
| II | 0.7960 | 0.1670 |
| J | 0.8448 | 0.1570 |
| JJ | 0.8494 | 0.1540 |
| K | 0.5691 | 0.0670 |
| KK | 0.8150 | 0.1510 |
| L | 0.8354 | 0.1780 |
| LL | 0.8608 | 0.1400 |
| M | 0.9020 | 0.1660 |
| MM | 0.8123 | 0.1870 |
| N | 0.8414 | 0.1420 |
| NN | 0.3300 | 0.0790 |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| Chain | Atom inclusion | Q-score |
|---|---|---|
| O | 0.8032 | 0.1710 |
| OO | 0.8122 | 0.1750 |
| P | 0.8723 | 0.1570 |
| PP | 0.8460 | 0.1530 |
| Q | 0.8000 | 0.1630 |
| QQ | 0.8197 | 0.1090 |
| R | 0.8244 | 0.1720 |
| RR | 0.8205 | 0.1110 |
| S | 0.8487 | 0.1750 |
| SS | 0.5973 | 0.0840 |
| T | 0.8036 | 0.1790 |
| TT | 0.7459 | 0.1390 |
| U | 0.8407 | 0.1780 |
| UU | 0.8594 | 0.1220 |
| V | 0.7687 | 0.1790 |
| VV | 0.7842 | 0.1220 |
| W | 0.8387 | 0.1680 |
| WW | 0.7910 | 0.1510 |
| X | 0.8170 | 0.1620 |
| XX | 0.8149 | 0.1770 |
| Y | 0.8822 | 0.1560 |
| YY | 0.7554 | 0.1600 |
| Z | 0.8910 | 0.1650 |
| ZZ | 0.8787 | 0.1410 |
| a | 0.8812 | 0.1550 |
| aa | 0.7496 | 0.1480 |
| b | 0.8074 | 0.1590 |
| bb | 0.8248 | 0.1560 |
| c | 0.8669 | 0.1750 |
| cc | 0.8138 | 0.1780 |
| d | 0.8483 | 0.1750 |
| dd | 0.7404 | 0.1430 |
| e | 0.8279 | 0.1830 |
| ee | 0.9048 | 0.1340 |
| f | 0.8302 | 0.1700 |
| ff | 0.7841 | 0.1470 |
| g | 0.8481 | 0.1460 |
| gg | 0.5009 | 0.0810 |
| h | 0.8315 | 0.1750 |
| hh | 0.8708 | 0.1260 |
| i | 0.8128 | 0.1780 |
| j | 0.8720 | 0.1320 |

*Continued on next page...*

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| k | 0.8259 | 0.1720 |
| l | 0.8337 | 0.1610 |
| m | 0.8072 | 0.1570 |
| n | 0.7661 | 0.1230 |
| o | 0.8752 | 0.1730 |
| p | 0.8200 | 0.1710 |
| r | 0.8454 | 0.1740 |
| s | 0.7697 | 0.1380 |
| t | 0.6520 | 0.0890 |