



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 06:02 pm GMT

PDB ID : 7PJS
EMDB ID : EMD-13458
Title : Structure of the 70S ribosome with tRNAs in the classical pre-translocation state and apramycin (C)
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.
Deposited on : 2021-08-24
Resolution : 2.35 Å (reported)
Based on initial models : 5LZD, 6YSS, 4AQY

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

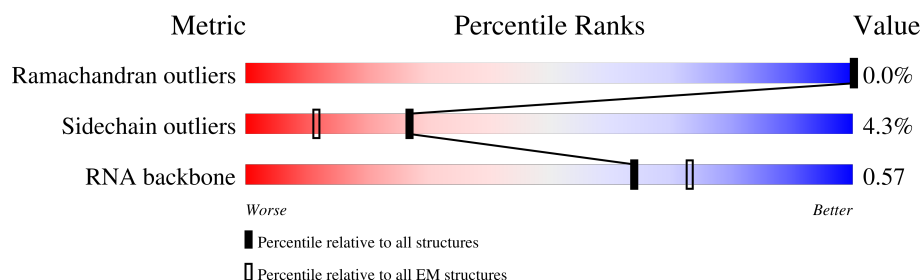
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.35 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.



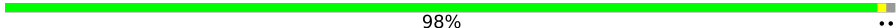
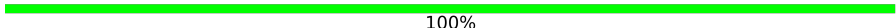

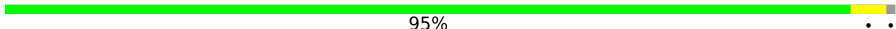
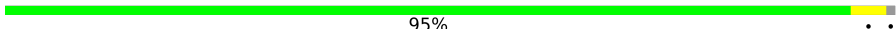

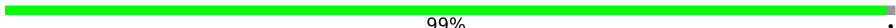
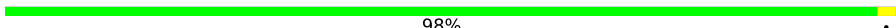
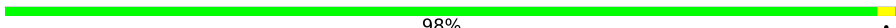
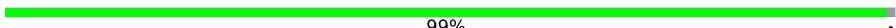
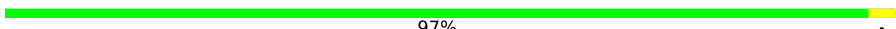

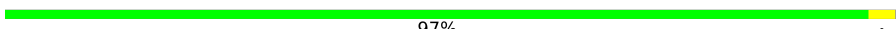
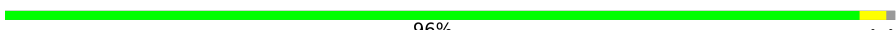
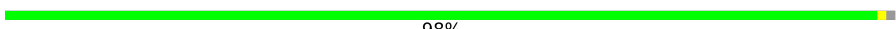

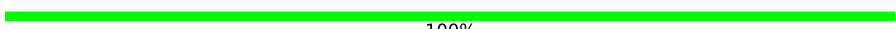


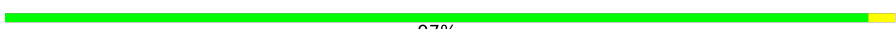


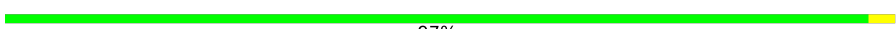


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 0 | 57 | |
| 2 | 1 | 55 | |
| 3 | 2 | 46 | |
| 4 | 3 | 65 | |
| 5 | 4 | 38 | |
| 6 | 5 | 165 | |
| 7 | 6 | 70 | |
| 8 | A | 2903 | |
| 9 | B | 120 | |



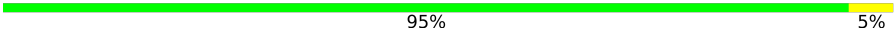



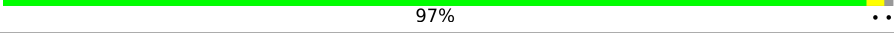



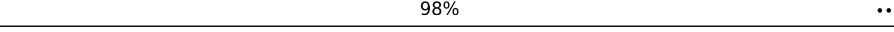

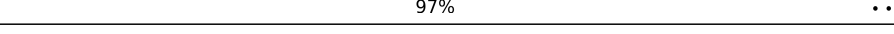
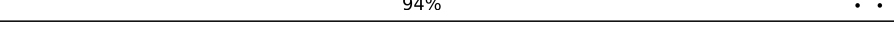
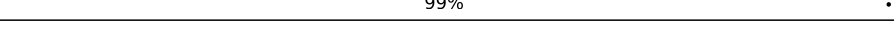
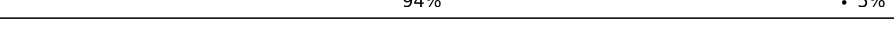


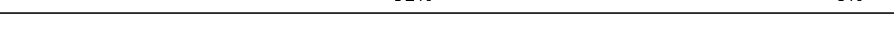
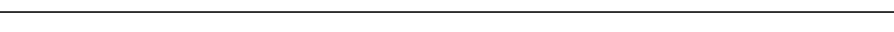




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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 10 | C | 273 |  98% .. |
| 11 | D | 209 |  100% |
| 12 | E | 201 |  100% |
| 13 | F | 179 |  95% . . |
| 14 | G | 177 |  95% . . |
| 15 | H | 149 |  90% 10% |
| 16 | I | 142 |  99% . |
| 17 | J | 142 |  98% . |
| 18 | K | 123 |  98% .. |
| 19 | L | 144 |  99% . |
| 20 | M | 136 |  97% . |
| 21 | N | 127 |  93% . 6% |
| 22 | O | 117 |  97% .. |
| 23 | P | 115 |  96% . . |
| 24 | Q | 118 |  98% .. |
| 25 | R | 103 |  94% 6% |
| 26 | S | 110 |  100% |
| 27 | T | 100 |  92% . 7% |
| 28 | U | 104 |  94% . . |
| 29 | V | 94 |  97% . |
| 30 | W | 85 |  88% 12% |
| 31 | X | 78 |  97% .. |
| 32 | Y | 63 |  97% . |
| 33 | Z | 59 |  95% . . |
| 34 | a | 1542 |  78% 21% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 35 | b | 240 |  88% 9% |
| 36 | c | 233 |  86% 12% |
| 37 | d | 206 |  95% 5% |
| 38 | e | 167 |  91% 6% |
| 39 | f | 135 |  70% 26% |
| 40 | g | 179 |  78% 7% 16% |
| 41 | h | 130 |  97% .. |
| 42 | i | 130 |  86% 12% . |
| 43 | j | 103 |  88% 7% 5% |
| 44 | k | 129 |  88% . 10% |
| 45 | l | 124 |  98% .. |
| 46 | m | 118 |  88% 8% . |
| 47 | n | 102 |  97% .. |
| 48 | o | 89 |  94% . . |
| 49 | p | 82 |  99% . |
| 50 | q | 84 |  94% . 5% |
| 51 | r | 75 |  84% . 13% |
| 52 | s | 92 |  84% 5% 11% |
| 53 | t | 87 |  92% 6% . |
| 54 | u | 71 |  89% . 8% |
| 55 | v | 77 |  71% 27% . |
| 56 | w | 76 |  68% 29% . |
| 57 | y | 2 |  100% |
| 58 | z | 33 |  27% . . 67% |

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 147741 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 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1 | 0 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

- Molecule 2 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 2 | 1 | 50 | Total | C | N | O | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | |

- Molecule 3 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3 | 2 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

- Molecule 4 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 4 | 3 | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 5 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5 | 4 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

- Molecule 6 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 6 | 5 | 131 | Total | C | N | O | 0 | 0 |
| | | | 647 | 385 | 131 | 131 | | |

- Molecule 7 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7 | 6 | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 522 | 323 | 99 | 94 | 6 | | |

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 8 | A | 2903 | Total | C | N | O | P | 0 | 0 |
| | | | 62338 | 27816 | 11471 | 20148 | 2903 | | |

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 9 | B | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2570 | 1144 | 468 | 838 | 120 | | |

- Molecule 10 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10 | C | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | |

- Molecule 11 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | D | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | |

- Molecule 12 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | E | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 13 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | F | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | |

- Molecule 14 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | G | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 15 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | H | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | |

- Molecule 16 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | I | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 693 | 411 | 141 | 141 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | J | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 18 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | K | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | |

- Molecule 19 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | L | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | |

- Molecule 20 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | M | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | |

- Molecule 21 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | N | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | |

- Molecule 22 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 22 | O | 116 | Total | C | N | O | | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | P | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 24 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 24 | Q | 117 | Total | C | N | O | | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | R | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 26 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | S | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 27 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | T | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | |

- Molecule 28 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 28 | U | 102 | Total | C | N | O | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | |

- Molecule 29 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | V | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 30 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | W | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 575 | 356 | 116 | 102 | 1 | | |

- Molecule 31 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | X | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

- Molecule 32 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32 | Y | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | |

- Molecule 33 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33 | Z | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 34 | a | 1540 | Total | C | N | O | P | 0 | 0 |
| | | | 33050 | 14748 | 6057 | 10705 | 1540 | | |

- Molecule 35 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35 | b | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | |

- Molecule 36 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36 | c | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | |

- Molecule 37 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37 | d | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | |

- Molecule 38 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | e | 157 | Total | C | N | O | S | 0 | 0 |
| | | | 1141 | 709 | 218 | 208 | 6 | | |

- Molecule 39 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | f | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | |

- Molecule 40 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | g | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1181 | 735 | 227 | 215 | 4 | | |

- Molecule 41 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | h | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | |

- Molecule 42 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | i | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | |

- Molecule 43 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | j | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | |

- Molecule 44 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | k | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 869 | 535 | 173 | 158 | 3 | | |

- Molecule 45 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | l | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | |

- Molecule 46 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | m | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 883 | 546 | 178 | 156 | 3 | | |

- Molecule 47 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47 | n | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 799 | 498 | 165 | 133 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| n | 35 | ALA | - | insertion | UNP C3SR07 |

- Molecule 48 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | o | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | |

- Molecule 49 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49 | p | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | |

- Molecule 50 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50 | q | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | |

- Molecule 51 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 51 | r | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 535 | 339 | 100 | 95 | 1 | | |

- Molecule 52 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52 | s | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 658 | 421 | 125 | 110 | 2 | | |

- Molecule 53 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | t | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | |

- Molecule 54 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 54 | u | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 506 | 313 | 105 | 87 | 1 | | |

- Molecule 55 is a RNA chain called P-site tRNA(fMet).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|---|
| 55 | v | 77 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1642 | 733 | 297 | 534 | 77 | 1 | | |

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|---|
| 56 | w | 76 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1631 | 731 | 291 | 531 | 76 | 2 | | |

- Molecule 57 is a protein called Dipeptide (FME-PHE).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---|---------|-------|
| 57 | y | 2 | Total | C | N | O | S | 0 | 0 |
| | | | 21 | 15 | 2 | 3 | 1 | | |

- Molecule 58 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 58 | z | 11 | Total | C | N | O | P | 0 | 0 |
| | | | 230 | 103 | 35 | 81 | 11 | | |

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 59 | 0 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 59 | A | 258 | Total | Mg | 0 |
| | | | 258 | 258 | |
| 59 | B | 4 | Total | Mg | 0 |
| | | | 4 | 4 | |
| 59 | C | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 59 | D | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 59 | N | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 59 | O | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 59 | P | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 59 | a | 92 | Total | Mg | 0 |
| | | | 92 | 92 | |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 59 | m | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 59 | n | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

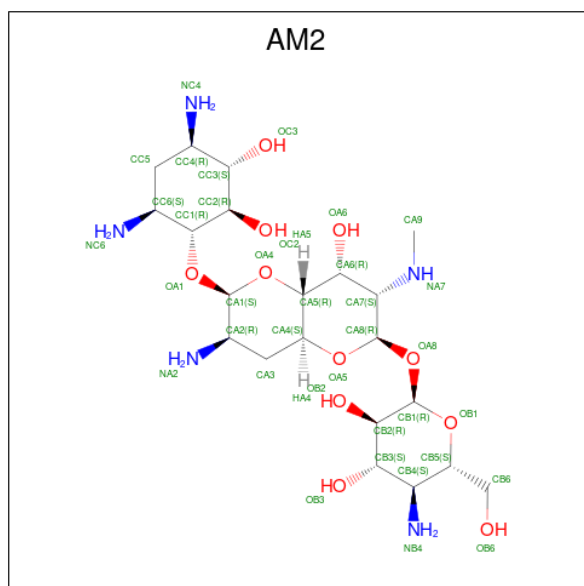
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 60 | 4 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 60 | 6 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 61 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 61 | A | 1 | Total | Na | 0 |
| | | | 1 | 1 | |
| 61 | B | 1 | Total | Na | 0 |
| | | | 1 | 1 | |

- Molecule 62 is APRAMYCIN (three-letter code: AM2) (formula: C₂₁H₄₁N₅O₁₁).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 62 | a | 1 | Total | C | N | O | 0 |
| | | | 37 | 21 | 5 | 11 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 62 | a | 1 | Total | C | N | O | 0 |
| | | | 37 | 21 | 5 | 11 | |
| 62 | a | 1 | Total | C | N | O | 0 |
| | | | 37 | 21 | 5 | 11 | |
| 62 | a | 1 | Total | C | N | O | 0 |
| | | | 37 | 21 | 5 | 11 | |

- Molecule 63 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 63 | A | 5 | Total | O | 0 |
| | | | 5 | 5 | |
| 63 | a | 15 | Total | O | 0 |
| | | | 15 | 15 | |
| 63 | z | 2 | Total | O | 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. 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. 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: 50S ribosomal protein L32

Chain 0:  96% ..




- Molecule 2: 50S ribosomal protein L33

Chain 1:  85% 5% 9%



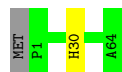
- Molecule 3: 50S ribosomal protein L34

Chain 2:  91% 9%



- Molecule 4: 50S ribosomal protein L35

Chain 3:  97% ..




- Molecule 5: 50S ribosomal protein L36

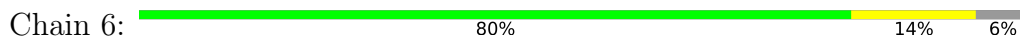
Chain 4:  95% 5%



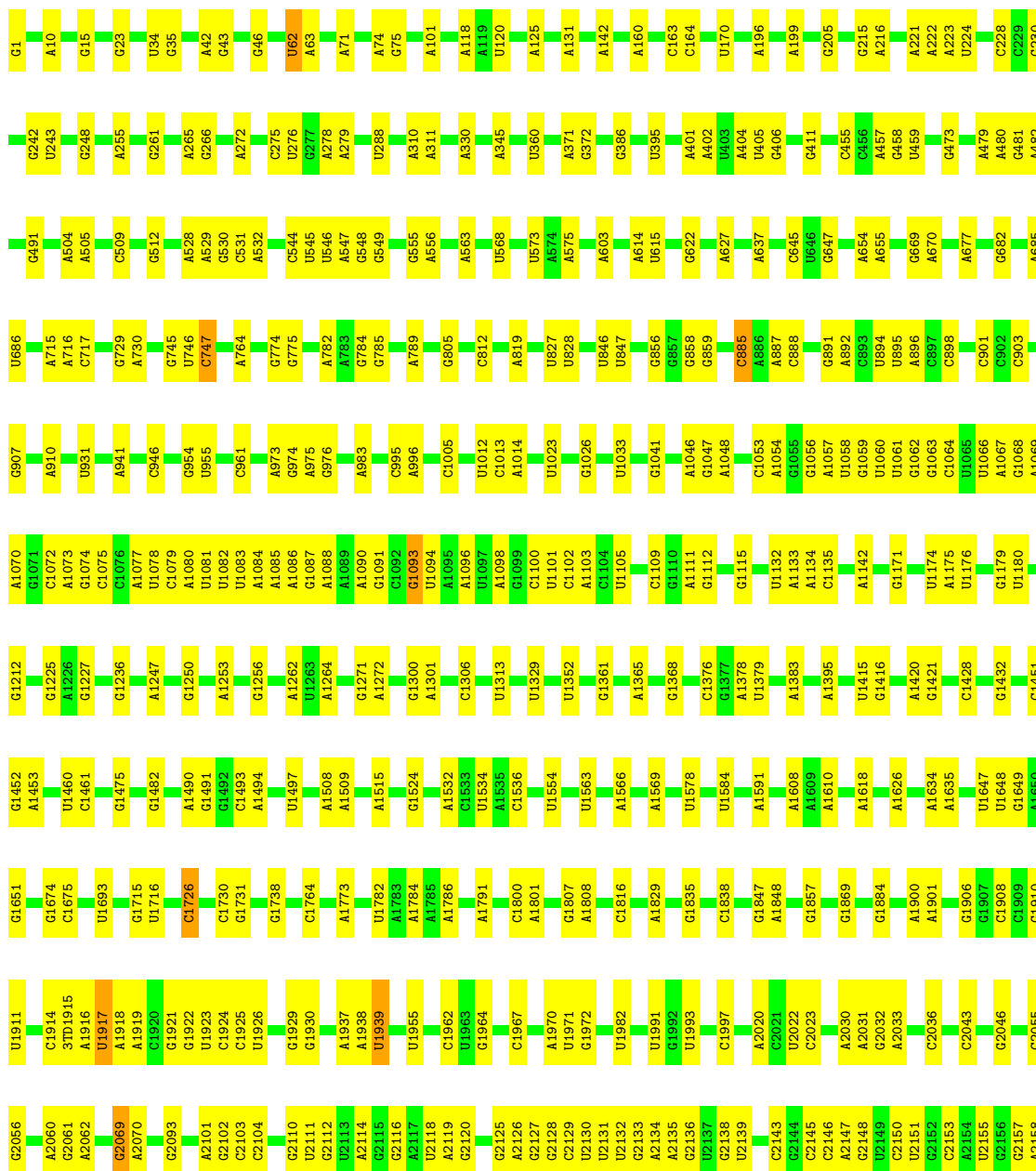
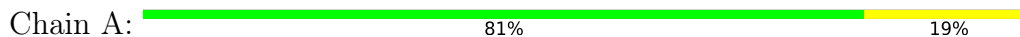
- Molecule 6: 50S ribosomal protein L10

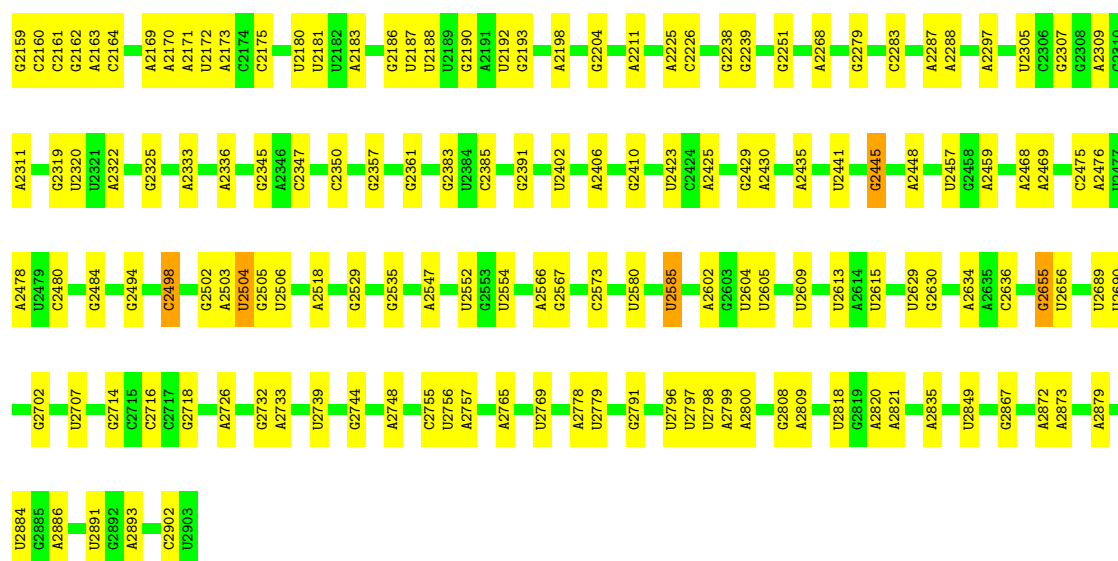
Chain 5:  79% 21%

- Molecule 7: 50S ribosomal protein L31



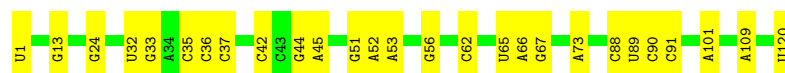
- Molecule 8: 23S ribosomal RNA





• Molecule 9: 5S ribosomal RNA

Chain B: 78% 22%



• Molecule 10: 50S ribosomal protein L2

Chain C: 98% ..



• Molecule 11: 50S ribosomal protein L3

Chain D: 100%



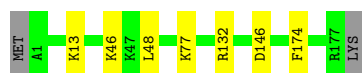
• Molecule 12: 50S ribosomal protein L4

Chain E: 100%



• Molecule 13: 50S ribosomal protein L5

Chain F: 95% ..



- Molecule 14: 50S ribosomal protein L6

Chain G: 95%



- Molecule 15: 50S ribosomal protein L9

Chain H: 90%



- Molecule 16: 50S ribosomal protein L11

Chain I: 99%



- Molecule 17: 50S ribosomal protein L13

Chain J: 98%



- Molecule 18: 50S ribosomal protein L14

Chain K: 98%



- Molecule 19: 50S ribosomal protein L15

Chain L: 99%



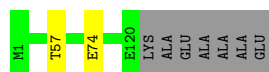
- Molecule 20: 50S ribosomal protein L16

Chain M: 97%



- Molecule 21: 50S ribosomal protein L17

Chain N: 93% 6%



- Molecule 22: 50S ribosomal protein L18

Chain O: 97% ..



- Molecule 23: 50S ribosomal protein L19

Chain P: 96% ..



- Molecule 24: 50S ribosomal protein L20

Chain Q: 98% ..



- Molecule 25: 50S ribosomal protein L21

Chain R: 94% 6%



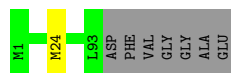
- Molecule 26: 50S ribosomal protein L22

Chain S: 100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L23

Chain T: 92% 7%



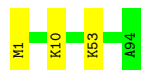
- Molecule 28: 50S ribosomal protein L24

Chain U:  94% . .



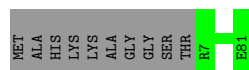
- Molecule 29: 50S ribosomal protein L25

Chain V:  97% .



- Molecule 30: 50S ribosomal protein L27

Chain W:  88% 12%



- Molecule 31: 50S ribosomal protein L28

Chain X:  97% . .



- Molecule 32: 50S ribosomal protein L29

Chain Y:  97% .




- Molecule 33: 50S ribosomal protein L30

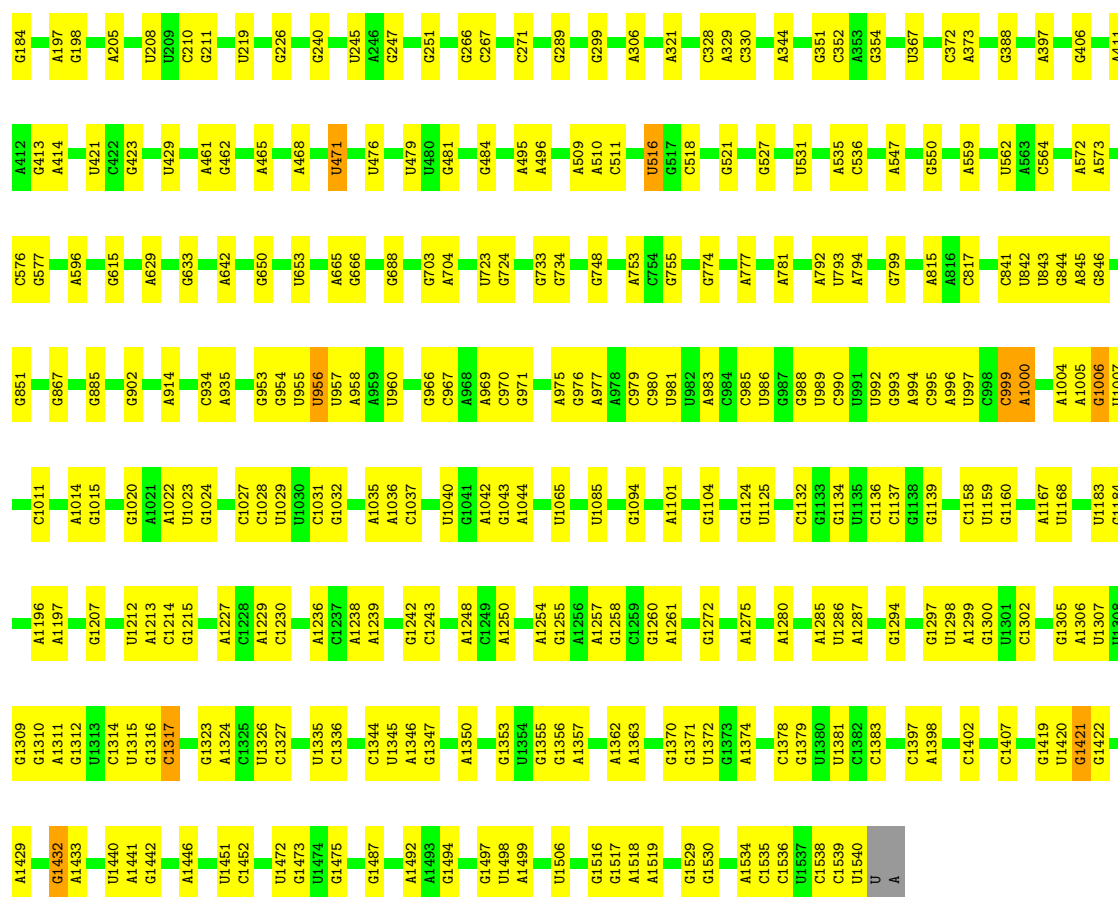
Chain Z:  95% . .



- Molecule 34: 16S ribosomal RNA

Chain a:  78% 21% .





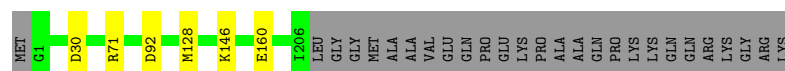
- Molecule 35: 30S ribosomal protein S2

Chain b: 88% 9%



- Molecule 36: 30S ribosomal protein S3

Chain c: 86% 12%




- Molecule 37: 30S ribosomal protein S4

Chain d: 95% 5%



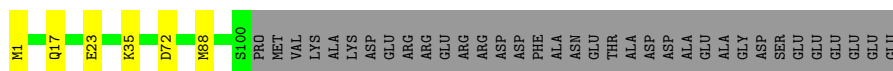
- Molecule 38: 30S ribosomal protein S5

Chain e:  91% • 6%




- Molecule 39: 30S ribosomal protein S6

Chain f:  70% • 26%



- Molecule 40: 30S ribosomal protein S7

Chain g:  78% 7% 16%




- Molecule 41: 30S ribosomal protein S8

Chain h:  97% ••




- Molecule 42: 30S ribosomal protein S9

Chain i:  86% 12% •



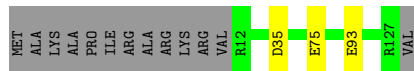
- Molecule 43: 30S ribosomal protein S10

Chain j:  88% 7% 5%



- Molecule 44: 30S ribosomal protein S11

Chain k:  88% • 10%



- Molecule 45: 30S ribosomal protein S12

Chain l:  98% ..



- Molecule 46: 30S ribosomal protein S13

Chain m:  88% 8% .



- Molecule 47: 30S ribosomal protein S14

Chain n:  97% ..



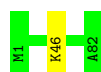
- Molecule 48: 30S ribosomal protein S15

Chain o:  94% . .



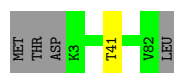
- Molecule 49: 30S ribosomal protein S16

Chain p:  99% .




- Molecule 50: 30S ribosomal protein S17

Chain q:  94% . 5%




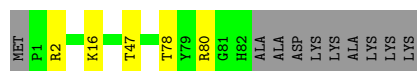
- Molecule 51: 30S ribosomal protein S18

Chain r:  84% . 13%



- Molecule 52: 30S ribosomal protein S19

Chain s:  84% 5% 11%




- Molecule 53: 30S ribosomal protein S20

Chain t:  92% 6% .



- Molecule 54: 30S ribosomal protein S21

Chain u:  89% . 8%



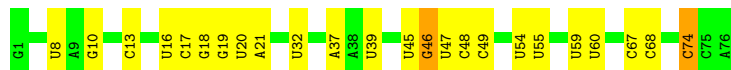
- Molecule 55: P-site tRNA(fMet)

Chain v:  71% 27% .



- Molecule 56: P-site fMet-Phe-tRNA(Phe)

Chain w:  68% 29% .



- Molecule 57: Dipeptide (FME-PHE)

Chain y:  100%



- Molecule 58: mRNA

Chain z:  27% . . 67%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 537761 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 30 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 1200 | Depositor |
| Magnification | 59000 | Depositor |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, FME, MG, 6MZ, MIA, 4OC, 3TD, 2MA, 2MG, OMC, NA, 1MG, UR3, 4SU, H2U, OMG, G7M, OMU, AM2, MA6, ZN, PSU, 5MC

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 | 0 | 0.31 | 0/450 | 0.65 | 1/599 (0.2%) |
| 2 | 1 | 0.31 | 0/416 | 0.53 | 0/554 |
| 3 | 2 | 0.29 | 0/380 | 0.66 | 0/498 |
| 4 | 3 | 0.30 | 0/513 | 0.53 | 0/676 |
| 5 | 4 | 0.32 | 0/303 | 0.61 | 0/397 |
| 6 | 5 | 0.24 | 0/646 | 0.43 | 0/898 |
| 7 | 6 | 0.31 | 0/531 | 0.71 | 0/709 |
| 8 | A | 0.59 | 1/69266 (0.0%) | 0.80 | 23/108055 (0.0%) |
| 9 | B | 0.54 | 1/2873 (0.0%) | 0.78 | 0/4478 |
| 10 | C | 0.34 | 0/2121 | 0.58 | 0/2852 |
| 11 | D | 0.33 | 0/1586 | 0.54 | 0/2134 |
| 12 | E | 0.31 | 0/1571 | 0.50 | 0/2113 |
| 13 | F | 0.31 | 0/1434 | 0.58 | 0/1926 |
| 14 | G | 0.29 | 0/1343 | 0.53 | 0/1816 |
| 15 | H | 0.32 | 0/1122 | 0.68 | 0/1515 |
| 16 | I | 0.25 | 0/692 | 0.45 | 0/960 |
| 17 | J | 0.33 | 0/1152 | 0.52 | 0/1551 |
| 18 | K | 0.33 | 0/947 | 0.60 | 0/1268 |
| 19 | L | 0.32 | 0/1054 | 0.60 | 0/1403 |
| 20 | M | 0.33 | 0/1093 | 0.58 | 0/1460 |
| 21 | N | 0.30 | 0/973 | 0.56 | 0/1301 |
| 22 | O | 0.31 | 0/902 | 0.60 | 0/1209 |
| 23 | P | 0.32 | 0/929 | 0.56 | 0/1242 |
| 24 | Q | 0.33 | 0/960 | 0.53 | 0/1278 |
| 25 | R | 0.34 | 0/829 | 0.59 | 0/1107 |
| 26 | S | 0.29 | 0/864 | 0.53 | 0/1156 |
| 27 | T | 0.31 | 0/744 | 0.55 | 0/994 |
| 28 | U | 0.31 | 0/787 | 0.52 | 0/1051 |
| 29 | V | 0.32 | 0/766 | 0.53 | 0/1025 |
| 30 | W | 0.32 | 0/582 | 0.54 | 0/769 |
| 31 | X | 0.33 | 0/635 | 0.59 | 0/848 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | Y | 0.30 | 0/510 | 0.58 | 0/677 |
| 33 | Z | 0.28 | 0/453 | 0.58 | 0/605 |
| 34 | a | 0.53 | 0/36725 | 0.83 | 25/57285 (0.0%) |
| 35 | b | 0.29 | 0/1735 | 0.57 | 1/2338 (0.0%) |
| 36 | c | 0.31 | 0/1651 | 0.55 | 0/2225 |
| 37 | d | 0.29 | 0/1665 | 0.55 | 0/2227 |
| 38 | e | 0.31 | 0/1154 | 0.55 | 0/1554 |
| 39 | f | 0.31 | 0/835 | 0.59 | 0/1128 |
| 40 | g | 0.28 | 0/1195 | 0.58 | 0/1602 |
| 41 | h | 0.30 | 0/989 | 0.50 | 0/1326 |
| 42 | i | 0.31 | 0/1034 | 0.64 | 0/1375 |
| 43 | j | 0.34 | 0/796 | 0.69 | 0/1077 |
| 44 | k | 0.31 | 0/885 | 0.63 | 0/1195 |
| 45 | l | 0.34 | 0/969 | 0.63 | 1/1300 (0.1%) |
| 46 | m | 0.30 | 0/892 | 0.62 | 0/1193 |
| 47 | n | 0.28 | 0/811 | 0.55 | 0/1081 |
| 48 | o | 0.27 | 0/722 | 0.55 | 0/964 |
| 49 | p | 0.31 | 0/659 | 0.58 | 0/884 |
| 50 | q | 0.32 | 0/657 | 0.58 | 0/881 |
| 51 | r | 0.33 | 0/544 | 0.56 | 0/731 |
| 52 | s | 0.31 | 0/675 | 0.59 | 0/908 |
| 53 | t | 0.27 | 0/671 | 0.48 | 0/888 |
| 54 | u | 0.33 | 0/512 | 0.60 | 0/683 |
| 55 | v | 0.51 | 1/1745 (0.1%) | 0.80 | 0/2716 |
| 56 | w | 0.36 | 0/1650 | 0.82 | 1/2569 (0.0%) |
| 57 | y | 0.43 | 0/11 | 0.26 | 0/13 |
| 58 | z | 0.49 | 0/255 | 1.18 | 3/394 (0.8%) |
| All | All | 0.51 | 3/158864 (0.0%) | 0.76 | 55/237661 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 9 | B | 1 | U | OP3-P | -10.68 | 1.48 | 1.61 |
| 55 | v | 1 | C | OP3-P | -10.66 | 1.48 | 1.61 |
| 8 | A | 1 | G | OP3-P | -10.60 | 1.48 | 1.61 |

All (55) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 58 | z | -1 | C | OP2-P-O3' | -10.72 | 81.61 | 105.20 |
| 58 | z | -1 | C | OP1-P-O3' | -10.70 | 81.67 | 105.20 |
| 34 | a | 999 | C | C2-N1-C1' | 9.50 | 129.25 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | a | 999 | C | C6-N1-C1' | -7.77 | 111.47 | 120.80 |
| 8 | A | 2506 | U | C2-N1-C1' | 7.61 | 126.83 | 117.70 |
| 8 | A | 512 | G | O4'-C1'-N9 | 7.60 | 114.28 | 108.20 |
| 8 | A | 2585 | U | C2-N1-C1' | 7.53 | 126.73 | 117.70 |
| 58 | z | 0 | U | OP1-P-OP2 | 7.18 | 130.37 | 119.60 |
| 8 | A | 1313 | U | C2-N1-C1' | 7.04 | 126.14 | 117.70 |
| 1 | 0 | 45 | ASP | CB-CG-OD1 | 6.86 | 124.47 | 118.30 |
| 34 | a | 1006 | G | O4'-C1'-N9 | 6.74 | 113.59 | 108.20 |
| 34 | a | 1421 | G | O5'-P-OP1 | -6.70 | 99.67 | 105.70 |
| 34 | a | 999 | C | N1-C2-O2 | 6.70 | 122.92 | 118.90 |
| 34 | a | 1000 | A | OP1-P-OP2 | -6.61 | 109.69 | 119.60 |
| 8 | A | 2585 | U | N1-C2-O2 | 6.53 | 127.37 | 122.80 |
| 8 | A | 2506 | U | N1-C2-O2 | 6.40 | 127.28 | 122.80 |
| 8 | A | 2585 | U | N3-C2-O2 | -6.33 | 117.77 | 122.20 |
| 8 | A | 528 | A | C2-N3-C4 | -5.75 | 107.73 | 110.60 |
| 34 | a | 1158 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 34 | a | 1420 | U | P-O3'-C3' | -5.67 | 112.90 | 119.70 |
| 34 | a | 471 | U | N3-C2-O2 | -5.64 | 118.25 | 122.20 |
| 8 | A | 901 | C | C2-N1-C1' | 5.60 | 124.96 | 118.80 |
| 56 | w | 74 | C | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 8 | A | 1914 | C | C2-N1-C1' | 5.57 | 124.93 | 118.80 |
| 34 | a | 970 | C | C2-N1-C1' | 5.56 | 124.92 | 118.80 |
| 34 | a | 1317 | C | C2-N1-C1' | 5.54 | 124.90 | 118.80 |
| 8 | A | 1313 | U | N1-C2-O2 | 5.52 | 126.67 | 122.80 |
| 34 | a | 956 | U | C2-N1-C1' | 5.43 | 124.22 | 117.70 |
| 8 | A | 1726 | C | C2-N1-C1' | 5.42 | 124.76 | 118.80 |
| 34 | a | 979 | C | N3-C2-O2 | -5.40 | 118.12 | 121.90 |
| 8 | A | 2506 | U | N3-C2-O2 | -5.38 | 118.43 | 122.20 |
| 8 | A | 62 | U | C2-N1-C1' | 5.38 | 124.16 | 117.70 |
| 34 | a | 476 | U | C2-N1-C1' | 5.35 | 124.12 | 117.70 |
| 8 | A | 2506 | U | C6-N1-C1' | -5.33 | 113.74 | 121.20 |
| 34 | a | 999 | C | C5-C6-N1 | 5.32 | 123.66 | 121.00 |
| 34 | a | 1326 | U | C2-N1-C1' | 5.28 | 124.03 | 117.70 |
| 34 | a | 1327 | C | C2-N1-C1' | 5.27 | 124.60 | 118.80 |
| 8 | A | 1921 | G | P-O3'-C3' | -5.26 | 113.38 | 119.70 |
| 34 | a | 471 | U | N1-C2-O2 | 5.21 | 126.45 | 122.80 |
| 34 | a | 1432 | G | C4-N9-C1' | 5.20 | 133.25 | 126.50 |
| 8 | A | 1093 | G | C3'-C2'-C1' | 5.19 | 105.66 | 101.50 |
| 8 | A | 1675 | C | N3-C2-O2 | -5.18 | 118.27 | 121.90 |
| 34 | a | 1158 | C | C2-N1-C1' | 5.18 | 124.50 | 118.80 |
| 34 | a | 981 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 8 | A | 1914 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 34 | a | 979 | C | C2-N1-C1' | 5.15 | 124.47 | 118.80 |
| 8 | A | 1675 | C | C2-N1-C1' | 5.14 | 124.46 | 118.80 |
| 34 | a | 1432 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 8 | A | 2391 | G | O4'-C1'-N9 | 5.13 | 112.31 | 108.20 |
| 34 | a | 481 | G | C4-N9-C1' | 5.11 | 133.15 | 126.50 |
| 45 | l | 102 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 |
| 34 | a | 1327 | C | N3-C2-O2 | -5.09 | 118.34 | 121.90 |
| 35 | b | 9 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 8 | A | 885 | C | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 8 | A | 2655 | G | P-O3'-C3' | 5.01 | 125.72 | 119.70 |

There are no chirality outliers.

There are no planarity outliers.

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 | 0 | 54/57 (95%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 2 | 1 | 48/55 (87%) | 48 (100%) | 0 | 0 | 100 | 100 |
| 3 | 2 | 44/46 (96%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | 3 | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 5 | 4 | 36/38 (95%) | 33 (92%) | 3 (8%) | 0 | 100 | 100 |
| 6 | 5 | 129/165 (78%) | 116 (90%) | 13 (10%) | 0 | 100 | 100 |
| 7 | 6 | 64/70 (91%) | 57 (89%) | 7 (11%) | 0 | 100 | 100 |
| 10 | C | 269/273 (98%) | 256 (95%) | 13 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 11 | D | 207/209 (99%) | 197 (95%) | 10 (5%) | 0 | 100 | 100 |
| 12 | E | 199/201 (99%) | 197 (99%) | 2 (1%) | 0 | 100 | 100 |
| 13 | F | 175/179 (98%) | 161 (92%) | 14 (8%) | 0 | 100 | 100 |
| 14 | G | 174/177 (98%) | 172 (99%) | 2 (1%) | 0 | 100 | 100 |
| 15 | H | 147/149 (99%) | 128 (87%) | 19 (13%) | 0 | 100 | 100 |
| 16 | I | 139/142 (98%) | 130 (94%) | 9 (6%) | 0 | 100 | 100 |
| 17 | J | 140/142 (99%) | 138 (99%) | 2 (1%) | 0 | 100 | 100 |
| 18 | K | 120/123 (98%) | 116 (97%) | 4 (3%) | 0 | 100 | 100 |
| 19 | L | 141/144 (98%) | 133 (94%) | 8 (6%) | 0 | 100 | 100 |
| 20 | M | 134/136 (98%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 21 | N | 118/127 (93%) | 113 (96%) | 5 (4%) | 0 | 100 | 100 |
| 22 | O | 114/117 (97%) | 112 (98%) | 2 (2%) | 0 | 100 | 100 |
| 23 | P | 112/115 (97%) | 110 (98%) | 2 (2%) | 0 | 100 | 100 |
| 24 | Q | 115/118 (98%) | 113 (98%) | 2 (2%) | 0 | 100 | 100 |
| 25 | R | 101/103 (98%) | 95 (94%) | 5 (5%) | 1 (1%) | 13 | 13 |
| 26 | S | 108/110 (98%) | 106 (98%) | 2 (2%) | 0 | 100 | 100 |
| 27 | T | 91/100 (91%) | 91 (100%) | 0 | 0 | 100 | 100 |
| 28 | U | 100/104 (96%) | 92 (92%) | 8 (8%) | 0 | 100 | 100 |
| 29 | V | 92/94 (98%) | 90 (98%) | 2 (2%) | 0 | 100 | 100 |
| 30 | W | 73/85 (86%) | 69 (94%) | 4 (6%) | 0 | 100 | 100 |
| 31 | X | 75/78 (96%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 32 | Y | 61/63 (97%) | 61 (100%) | 0 | 0 | 100 | 100 |
| 33 | Z | 56/59 (95%) | 56 (100%) | 0 | 0 | 100 | 100 |
| 35 | b | 216/240 (90%) | 203 (94%) | 13 (6%) | 0 | 100 | 100 |
| 36 | c | 204/233 (88%) | 195 (96%) | 9 (4%) | 0 | 100 | 100 |
| 37 | d | 203/206 (98%) | 190 (94%) | 13 (6%) | 0 | 100 | 100 |
| 38 | e | 155/167 (93%) | 152 (98%) | 3 (2%) | 0 | 100 | 100 |
| 39 | f | 98/135 (73%) | 94 (96%) | 4 (4%) | 0 | 100 | 100 |
| 40 | g | 149/179 (83%) | 145 (97%) | 4 (3%) | 0 | 100 | 100 |
| 41 | h | 127/130 (98%) | 125 (98%) | 2 (2%) | 0 | 100 | 100 |
| 42 | i | 125/130 (96%) | 122 (98%) | 3 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 43 | j | 96/103 (93%) | 85 (88%) | 11 (12%) | 0 | 100 | 100 |
| 44 | k | 114/129 (88%) | 106 (93%) | 8 (7%) | 0 | 100 | 100 |
| 45 | l | 121/124 (98%) | 116 (96%) | 5 (4%) | 0 | 100 | 100 |
| 46 | m | 112/118 (95%) | 108 (96%) | 4 (4%) | 0 | 100 | 100 |
| 47 | n | 99/102 (97%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 48 | o | 86/89 (97%) | 80 (93%) | 6 (7%) | 0 | 100 | 100 |
| 49 | p | 80/82 (98%) | 76 (95%) | 4 (5%) | 0 | 100 | 100 |
| 50 | q | 78/84 (93%) | 76 (97%) | 2 (3%) | 0 | 100 | 100 |
| 51 | r | 63/75 (84%) | 61 (97%) | 2 (3%) | 0 | 100 | 100 |
| 52 | s | 80/92 (87%) | 79 (99%) | 1 (1%) | 0 | 100 | 100 |
| 53 | t | 83/87 (95%) | 81 (98%) | 2 (2%) | 0 | 100 | 100 |
| 54 | u | 63/71 (89%) | 61 (97%) | 2 (3%) | 0 | 100 | 100 |
| All | All | 5850/6220 (94%) | 5602 (96%) | 247 (4%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | R | 51 | VAL |

5.3.2 Protein sidechains ⓘ

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 | 0 | 47/48 (98%) | 47 (100%) | 0 | 100 | 100 |
| 2 | 1 | 45/49 (92%) | 42 (93%) | 3 (7%) | 13 | 14 |
| 3 | 2 | 38/38 (100%) | 34 (90%) | 4 (10%) | 5 | 5 |
| 4 | 3 | 51/52 (98%) | 50 (98%) | 1 (2%) | 50 | 63 |
| 5 | 4 | 34/34 (100%) | 32 (94%) | 2 (6%) | 16 | 18 |
| 7 | 6 | 59/62 (95%) | 49 (83%) | 10 (17%) | 1 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 10 | C | 216/218 (99%) | 213 (99%) | 3 (1%) | 62 | 75 |
| 11 | D | 164/164 (100%) | 163 (99%) | 1 (1%) | 84 | 91 |
| 12 | E | 165/165 (100%) | 164 (99%) | 1 (1%) | 84 | 91 |
| 13 | F | 148/150 (99%) | 141 (95%) | 7 (5%) | 22 | 27 |
| 14 | G | 137/138 (99%) | 130 (95%) | 7 (5%) | 20 | 24 |
| 15 | H | 114/114 (100%) | 99 (87%) | 15 (13%) | 3 | 3 |
| 17 | J | 116/116 (100%) | 113 (97%) | 3 (3%) | 41 | 52 |
| 18 | K | 103/104 (99%) | 101 (98%) | 2 (2%) | 52 | 65 |
| 19 | L | 102/103 (99%) | 102 (100%) | 0 | 100 | 100 |
| 20 | M | 109/109 (100%) | 105 (96%) | 4 (4%) | 29 | 38 |
| 21 | N | 100/103 (97%) | 98 (98%) | 2 (2%) | 50 | 63 |
| 22 | O | 86/87 (99%) | 83 (96%) | 3 (4%) | 31 | 40 |
| 23 | P | 99/100 (99%) | 95 (96%) | 4 (4%) | 27 | 34 |
| 24 | Q | 89/90 (99%) | 88 (99%) | 1 (1%) | 70 | 81 |
| 25 | R | 84/84 (100%) | 79 (94%) | 5 (6%) | 16 | 18 |
| 26 | S | 93/93 (100%) | 93 (100%) | 0 | 100 | 100 |
| 27 | T | 80/84 (95%) | 79 (99%) | 1 (1%) | 65 | 77 |
| 28 | U | 83/85 (98%) | 79 (95%) | 4 (5%) | 21 | 26 |
| 29 | V | 78/78 (100%) | 75 (96%) | 3 (4%) | 28 | 37 |
| 30 | W | 57/63 (90%) | 57 (100%) | 0 | 100 | 100 |
| 31 | X | 67/68 (98%) | 66 (98%) | 1 (2%) | 60 | 73 |
| 32 | Y | 55/55 (100%) | 53 (96%) | 2 (4%) | 30 | 39 |
| 33 | Z | 48/49 (98%) | 46 (96%) | 2 (4%) | 25 | 32 |
| 35 | b | 180/198 (91%) | 173 (96%) | 7 (4%) | 27 | 36 |
| 36 | c | 170/190 (90%) | 164 (96%) | 6 (4%) | 31 | 40 |
| 37 | d | 172/173 (99%) | 162 (94%) | 10 (6%) | 17 | 19 |
| 38 | e | 114/126 (90%) | 109 (96%) | 5 (4%) | 24 | 30 |
| 39 | f | 87/116 (75%) | 81 (93%) | 6 (7%) | 13 | 13 |
| 40 | g | 124/147 (84%) | 112 (90%) | 12 (10%) | 6 | 6 |
| 41 | h | 104/105 (99%) | 101 (97%) | 3 (3%) | 37 | 48 |
| 42 | i | 105/107 (98%) | 90 (86%) | 15 (14%) | 2 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 43 | j | 86/90 (96%) | 79 (92%) | 7 (8%) | 9 | 9 |
| 44 | k | 89/99 (90%) | 86 (97%) | 3 (3%) | 32 | 41 |
| 45 | l | 103/104 (99%) | 103 (100%) | 0 | 100 | 100 |
| 46 | m | 92/96 (96%) | 82 (89%) | 10 (11%) | 5 | 4 |
| 47 | n | 79/84 (94%) | 77 (98%) | 2 (2%) | 42 | 53 |
| 48 | o | 76/77 (99%) | 72 (95%) | 4 (5%) | 19 | 23 |
| 49 | p | 65/65 (100%) | 64 (98%) | 1 (2%) | 60 | 73 |
| 50 | q | 74/78 (95%) | 73 (99%) | 1 (1%) | 62 | 75 |
| 51 | r | 56/65 (86%) | 54 (96%) | 2 (4%) | 30 | 39 |
| 52 | s | 72/79 (91%) | 67 (93%) | 5 (7%) | 13 | 13 |
| 53 | t | 65/66 (98%) | 60 (92%) | 5 (8%) | 10 | 10 |
| 54 | u | 46/61 (75%) | 44 (96%) | 2 (4%) | 25 | 31 |
| 57 | y | 1/1 (100%) | 0 | 1 (100%) | 0 | 0 |
| All | All | 4627/4830 (96%) | 4429 (96%) | 198 (4%) | 27 | 31 |

All (198) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 1 | 7 | LYS |
| 2 | 1 | 27 | ARG |
| 2 | 1 | 52 | LYS |
| 3 | 2 | 15 | SER |
| 3 | 2 | 24 | THR |
| 3 | 2 | 25 | LYS |
| 3 | 2 | 41 | ARG |
| 4 | 3 | 30 | HIS |
| 5 | 4 | 4 | ARG |
| 5 | 4 | 12 | ARG |
| 7 | 6 | 3 | LYS |
| 7 | 6 | 4 | ASP |
| 7 | 6 | 10 | GLU |
| 7 | 6 | 39 | LYS |
| 7 | 6 | 47 | LYS |
| 7 | 6 | 49 | ARG |
| 7 | 6 | 50 | ASP |
| 7 | 6 | 59 | ARG |
| 7 | 6 | 62 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | 6 | 66 | ILE |
| 10 | C | 86 | ARG |
| 10 | C | 259 | ASN |
| 10 | C | 263 | ASP |
| 11 | D | 128 | ARG |
| 12 | E | 116 | ASP |
| 13 | F | 13 | LYS |
| 13 | F | 46 | LYS |
| 13 | F | 48 | LEU |
| 13 | F | 77 | LYS |
| 13 | F | 132 | ARG |
| 13 | F | 146 | ASP |
| 13 | F | 174 | PHE |
| 14 | G | 41 | GLU |
| 14 | G | 47 | ASN |
| 14 | G | 94 | ARG |
| 14 | G | 151 | ARG |
| 14 | G | 152 | ARG |
| 14 | G | 165 | ASP |
| 14 | G | 175 | LYS |
| 15 | H | 7 | ASP |
| 15 | H | 8 | LYS |
| 15 | H | 17 | ASP |
| 15 | H | 41 | LYS |
| 15 | H | 46 | PHE |
| 15 | H | 51 | ARG |
| 15 | H | 53 | GLU |
| 15 | H | 57 | LYS |
| 15 | H | 68 | ARG |
| 15 | H | 70 | GLU |
| 15 | H | 101 | ASP |
| 15 | H | 110 | VAL |
| 15 | H | 112 | LYS |
| 15 | H | 131 | SER |
| 15 | H | 132 | PHE |
| 17 | J | 1 | MET |
| 17 | J | 71 | ASP |
| 17 | J | 129 | GLU |
| 18 | K | 40 | LYS |
| 18 | K | 49 | ARG |
| 20 | M | 6 | ARG |
| 20 | M | 58 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | M | 110 | GLU |
| 20 | M | 127 | LYS |
| 21 | N | 57 | THR |
| 21 | N | 74 | GLU |
| 22 | O | 46 | GLU |
| 22 | O | 88 | LYS |
| 22 | O | 89 | ASP |
| 23 | P | 6 | GLN |
| 23 | P | 9 | GLN |
| 23 | P | 18 | SER |
| 23 | P | 64 | SER |
| 24 | Q | 12 | ARG |
| 25 | R | 1 | MET |
| 25 | R | 43 | ASN |
| 25 | R | 60 | LYS |
| 25 | R | 70 | GLU |
| 25 | R | 73 | LYS |
| 27 | T | 24 | MET |
| 28 | U | 23 | LYS |
| 28 | U | 73 | ASN |
| 28 | U | 99 | SER |
| 28 | U | 100 | GLU |
| 29 | V | 1 | MET |
| 29 | V | 10 | LYS |
| 29 | V | 53 | LYS |
| 31 | X | 34 | SER |
| 32 | Y | 8 | GLU |
| 32 | Y | 34 | SER |
| 33 | Z | 30 | ARG |
| 33 | Z | 36 | GLU |
| 35 | b | 61 | SER |
| 35 | b | 73 | ARG |
| 35 | b | 77 | GLU |
| 35 | b | 120 | SER |
| 35 | b | 125 | PHE |
| 35 | b | 127 | LYS |
| 35 | b | 196 | ASP |
| 36 | c | 30 | ASP |
| 36 | c | 71 | ARG |
| 36 | c | 92 | ASP |
| 36 | c | 128 | MET |
| 36 | c | 146 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | c | 160 | GLU |
| 37 | d | 12 | ARG |
| 37 | d | 28 | ASP |
| 37 | d | 44 | LYS |
| 37 | d | 49 | ASP |
| 37 | d | 70 | GLN |
| 37 | d | 140 | ASP |
| 37 | d | 150 | LYS |
| 37 | d | 184 | LYS |
| 37 | d | 189 | ASP |
| 37 | d | 205 | LYS |
| 38 | e | 21 | SER |
| 38 | e | 44 | ARG |
| 38 | e | 75 | LEU |
| 38 | e | 147 | ASN |
| 38 | e | 158 | LYS |
| 39 | f | 1 | MET |
| 39 | f | 17 | GLN |
| 39 | f | 23 | GLU |
| 39 | f | 35 | LYS |
| 39 | f | 72 | ASP |
| 39 | f | 88 | MET |
| 40 | g | 3 | ARG |
| 40 | g | 4 | ARG |
| 40 | g | 36 | SER |
| 40 | g | 42 | VAL |
| 40 | g | 48 | THR |
| 40 | g | 51 | GLN |
| 40 | g | 52 | ARG |
| 40 | g | 55 | LYS |
| 40 | g | 56 | SER |
| 40 | g | 110 | ARG |
| 40 | g | 114 | SER |
| 40 | g | 119 | LEU |
| 41 | h | 37 | ASN |
| 41 | h | 42 | GLU |
| 41 | h | 49 | LYS |
| 42 | i | 11 | ARG |
| 42 | i | 13 | SER |
| 42 | i | 26 | LYS |
| 42 | i | 28 | VAL |
| 42 | i | 55 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | i | 58 | GLU |
| 42 | i | 65 | THR |
| 42 | i | 71 | ILE |
| 42 | i | 79 | ARG |
| 42 | i | 84 | ARG |
| 42 | i | 96 | GLU |
| 42 | i | 98 | ARG |
| 42 | i | 104 | THR |
| 42 | i | 105 | ARG |
| 42 | i | 128 | LYS |
| 43 | j | 20 | GLN |
| 43 | j | 24 | GLU |
| 43 | j | 35 | GLN |
| 43 | j | 46 | LYS |
| 43 | j | 78 | GLU |
| 43 | j | 82 | LYS |
| 43 | j | 88 | MET |
| 44 | k | 35 | ASP |
| 44 | k | 75 | GLU |
| 44 | k | 93 | GLU |
| 46 | m | 2 | ARG |
| 46 | m | 15 | VAL |
| 46 | m | 26 | LYS |
| 46 | m | 30 | LYS |
| 46 | m | 42 | VAL |
| 46 | m | 49 | GLU |
| 46 | m | 53 | ASP |
| 46 | m | 59 | VAL |
| 46 | m | 77 | LYS |
| 46 | m | 113 | LYS |
| 47 | n | 25 | GLU |
| 47 | n | 45 | VAL |
| 48 | o | 13 | GLU |
| 48 | o | 17 | ASP |
| 48 | o | 57 | ARG |
| 48 | o | 87 | ARG |
| 49 | p | 46 | LYS |
| 50 | q | 41 | THR |
| 51 | r | 11 | ARG |
| 51 | r | 47 | ARG |
| 52 | s | 2 | ARG |
| 52 | s | 16 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | s | 47 | THR |
| 52 | s | 78 | THR |
| 52 | s | 80 | ARG |
| 53 | t | 13 | SER |
| 53 | t | 14 | GLU |
| 53 | t | 23 | ARG |
| 53 | t | 27 | MET |
| 53 | t | 81 | GLN |
| 54 | u | 6 | ARG |
| 54 | u | 12 | ASP |
| 57 | y | 102 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | Y | 15 | ASN |
| 32 | Y | 36 | GLN |
| 32 | Y | 45 | GLN |
| 36 | c | 99 | GLN |
| 39 | f | 3 | HIS |
| 47 | n | 49 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 34 | a | 1536/1542 (99%) | 312 (20%) | 0 |
| 55 | v | 76/77 (98%) | 18 (23%) | 0 |
| 56 | w | 74/76 (97%) | 18 (24%) | 0 |
| 58 | z | 10/33 (30%) | 1 (10%) | 0 |
| 8 | A | 2898/2903 (99%) | 517 (17%) | 37 (1%) |
| 9 | B | 119/120 (99%) | 23 (19%) | 4 (3%) |
| All | All | 4713/4751 (99%) | 889 (18%) | 41 (0%) |

All (889) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | A | 10 | A |
| 8 | A | 15 | G |
| 8 | A | 23 | G |
| 8 | A | 34 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | A | 35 | G |
| 8 | A | 42 | A |
| 8 | A | 43 | G |
| 8 | A | 46 | G |
| 8 | A | 62 | U |
| 8 | A | 63 | A |
| 8 | A | 71 | A |
| 8 | A | 74 | A |
| 8 | A | 75 | G |
| 8 | A | 101 | A |
| 8 | A | 118 | A |
| 8 | A | 120 | U |
| 8 | A | 125 | A |
| 8 | A | 131 | A |
| 8 | A | 142 | A |
| 8 | A | 160 | A |
| 8 | A | 163 | C |
| 8 | A | 164 | C |
| 8 | A | 170 | U |
| 8 | A | 196 | A |
| 8 | A | 199 | A |
| 8 | A | 205 | G |
| 8 | A | 215 | G |
| 8 | A | 216 | A |
| 8 | A | 221 | A |
| 8 | A | 222 | A |
| 8 | A | 223 | A |
| 8 | A | 224 | U |
| 8 | A | 228 | C |
| 8 | A | 230 | G |
| 8 | A | 242 | G |
| 8 | A | 243 | U |
| 8 | A | 248 | G |
| 8 | A | 255 | A |
| 8 | A | 261 | G |
| 8 | A | 265 | A |
| 8 | A | 266 | G |
| 8 | A | 272 | A |
| 8 | A | 275 | C |
| 8 | A | 276 | U |
| 8 | A | 278 | A |
| 8 | A | 279 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | A | 288 | U |
| 8 | A | 311 | A |
| 8 | A | 330 | A |
| 8 | A | 345 | A |
| 8 | A | 360 | U |
| 8 | A | 371 | A |
| 8 | A | 372 | G |
| 8 | A | 386 | G |
| 8 | A | 395 | U |
| 8 | A | 401 | A |
| 8 | A | 402 | A |
| 8 | A | 404 | A |
| 8 | A | 405 | U |
| 8 | A | 406 | G |
| 8 | A | 411 | G |
| 8 | A | 455 | C |
| 8 | A | 457 | A |
| 8 | A | 458 | G |
| 8 | A | 459 | U |
| 8 | A | 473 | G |
| 8 | A | 480 | A |
| 8 | A | 481 | G |
| 8 | A | 482 | A |
| 8 | A | 491 | G |
| 8 | A | 504 | A |
| 8 | A | 505 | A |
| 8 | A | 509 | C |
| 8 | A | 529 | A |
| 8 | A | 530 | G |
| 8 | A | 531 | C |
| 8 | A | 532 | A |
| 8 | A | 544 | C |
| 8 | A | 545 | U |
| 8 | A | 546 | U |
| 8 | A | 547 | A |
| 8 | A | 548 | G |
| 8 | A | 549 | G |
| 8 | A | 556 | A |
| 8 | A | 563 | A |
| 8 | A | 568 | U |
| 8 | A | 573 | U |
| 8 | A | 575 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | A | 603 | A |
| 8 | A | 614 | A |
| 8 | A | 615 | U |
| 8 | A | 622 | G |
| 8 | A | 627 | A |
| 8 | A | 637 | A |
| 8 | A | 645 | C |
| 8 | A | 647 | G |
| 8 | A | 654 | A |
| 8 | A | 655 | A |
| 8 | A | 669 | G |
| 8 | A | 670 | A |
| 8 | A | 677 | A |
| 8 | A | 682 | G |
| 8 | A | 685 | A |
| 8 | A | 686 | U |
| 8 | A | 715 | A |
| 8 | A | 716 | A |
| 8 | A | 717 | C |
| 8 | A | 729 | G |
| 8 | A | 730 | A |
| 8 | A | 747 | 5MC |
| 8 | A | 764 | A |
| 8 | A | 775 | G |
| 8 | A | 782 | A |
| 8 | A | 784 | G |
| 8 | A | 785 | G |
| 8 | A | 789 | A |
| 8 | A | 805 | G |
| 8 | A | 812 | C |
| 8 | A | 819 | A |
| 8 | A | 827 | U |
| 8 | A | 828 | U |
| 8 | A | 846 | U |
| 8 | A | 847 | U |
| 8 | A | 856 | G |
| 8 | A | 858 | G |
| 8 | A | 859 | G |
| 8 | A | 885 | C |
| 8 | A | 887 | A |
| 8 | A | 888 | C |
| 8 | A | 891 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 892 | A |
| 8 | A | 894 | U |
| 8 | A | 895 | U |
| 8 | A | 896 | A |
| 8 | A | 898 | C |
| 8 | A | 903 | C |
| 8 | A | 907 | G |
| 8 | A | 910 | A |
| 8 | A | 931 | U |
| 8 | A | 941 | A |
| 8 | A | 946 | C |
| 8 | A | 961 | C |
| 8 | A | 973 | A |
| 8 | A | 974 | G |
| 8 | A | 975 | A |
| 8 | A | 983 | A |
| 8 | A | 995 | C |
| 8 | A | 996 | A |
| 8 | A | 1005 | C |
| 8 | A | 1012 | U |
| 8 | A | 1013 | C |
| 8 | A | 1026 | G |
| 8 | A | 1033 | U |
| 8 | A | 1041 | G |
| 8 | A | 1046 | A |
| 8 | A | 1047 | G |
| 8 | A | 1048 | A |
| 8 | A | 1053 | C |
| 8 | A | 1054 | A |
| 8 | A | 1056 | G |
| 8 | A | 1057 | A |
| 8 | A | 1058 | U |
| 8 | A | 1059 | G |
| 8 | A | 1060 | U |
| 8 | A | 1061 | U |
| 8 | A | 1062 | G |
| 8 | A | 1063 | G |
| 8 | A | 1064 | C |
| 8 | A | 1066 | U |
| 8 | A | 1067 | A |
| 8 | A | 1068 | G |
| 8 | A | 1069 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 1070 | A |
| 8 | A | 1072 | C |
| 8 | A | 1073 | A |
| 8 | A | 1074 | G |
| 8 | A | 1075 | C |
| 8 | A | 1077 | A |
| 8 | A | 1078 | U |
| 8 | A | 1079 | C |
| 8 | A | 1080 | A |
| 8 | A | 1081 | U |
| 8 | A | 1082 | U |
| 8 | A | 1083 | U |
| 8 | A | 1084 | A |
| 8 | A | 1085 | A |
| 8 | A | 1086 | A |
| 8 | A | 1087 | G |
| 8 | A | 1088 | A |
| 8 | A | 1090 | A |
| 8 | A | 1091 | G |
| 8 | A | 1093 | G |
| 8 | A | 1094 | U |
| 8 | A | 1096 | A |
| 8 | A | 1098 | A |
| 8 | A | 1100 | C |
| 8 | A | 1101 | U |
| 8 | A | 1102 | C |
| 8 | A | 1103 | A |
| 8 | A | 1105 | U |
| 8 | A | 1109 | C |
| 8 | A | 1111 | A |
| 8 | A | 1112 | G |
| 8 | A | 1115 | G |
| 8 | A | 1132 | U |
| 8 | A | 1133 | A |
| 8 | A | 1134 | A |
| 8 | A | 1135 | C |
| 8 | A | 1142 | A |
| 8 | A | 1171 | G |
| 8 | A | 1174 | U |
| 8 | A | 1175 | A |
| 8 | A | 1176 | U |
| 8 | A | 1179 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 1180 | U |
| 8 | A | 1212 | G |
| 8 | A | 1225 | G |
| 8 | A | 1227 | G |
| 8 | A | 1236 | G |
| 8 | A | 1247 | A |
| 8 | A | 1250 | G |
| 8 | A | 1253 | A |
| 8 | A | 1256 | G |
| 8 | A | 1262 | A |
| 8 | A | 1264 | A |
| 8 | A | 1271 | G |
| 8 | A | 1272 | A |
| 8 | A | 1300 | G |
| 8 | A | 1301 | A |
| 8 | A | 1306 | C |
| 8 | A | 1329 | U |
| 8 | A | 1352 | U |
| 8 | A | 1365 | A |
| 8 | A | 1368 | G |
| 8 | A | 1376 | C |
| 8 | A | 1378 | A |
| 8 | A | 1379 | U |
| 8 | A | 1383 | A |
| 8 | A | 1395 | A |
| 8 | A | 1415 | U |
| 8 | A | 1416 | G |
| 8 | A | 1420 | A |
| 8 | A | 1421 | G |
| 8 | A | 1428 | C |
| 8 | A | 1432 | G |
| 8 | A | 1452 | G |
| 8 | A | 1453 | A |
| 8 | A | 1460 | U |
| 8 | A | 1461 | C |
| 8 | A | 1475 | G |
| 8 | A | 1482 | G |
| 8 | A | 1490 | A |
| 8 | A | 1491 | G |
| 8 | A | 1493 | C |
| 8 | A | 1494 | A |
| 8 | A | 1497 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 1508 | A |
| 8 | A | 1509 | A |
| 8 | A | 1515 | A |
| 8 | A | 1524 | G |
| 8 | A | 1532 | A |
| 8 | A | 1534 | U |
| 8 | A | 1536 | C |
| 8 | A | 1554 | U |
| 8 | A | 1563 | U |
| 8 | A | 1566 | A |
| 8 | A | 1569 | A |
| 8 | A | 1578 | U |
| 8 | A | 1584 | U |
| 8 | A | 1591 | A |
| 8 | A | 1608 | A |
| 8 | A | 1610 | A |
| 8 | A | 1626 | A |
| 8 | A | 1634 | A |
| 8 | A | 1635 | A |
| 8 | A | 1647 | U |
| 8 | A | 1648 | U |
| 8 | A | 1649 | G |
| 8 | A | 1651 | G |
| 8 | A | 1674 | G |
| 8 | A | 1693 | U |
| 8 | A | 1715 | G |
| 8 | A | 1716 | U |
| 8 | A | 1726 | C |
| 8 | A | 1730 | C |
| 8 | A | 1731 | G |
| 8 | A | 1738 | G |
| 8 | A | 1764 | C |
| 8 | A | 1773 | A |
| 8 | A | 1782 | U |
| 8 | A | 1784 | A |
| 8 | A | 1786 | A |
| 8 | A | 1791 | A |
| 8 | A | 1800 | C |
| 8 | A | 1801 | A |
| 8 | A | 1807 | G |
| 8 | A | 1808 | A |
| 8 | A | 1816 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 1829 | A |
| 8 | A | 1838 | C |
| 8 | A | 1847 | G |
| 8 | A | 1848 | A |
| 8 | A | 1857 | G |
| 8 | A | 1869 | G |
| 8 | A | 1884 | G |
| 8 | A | 1900 | A |
| 8 | A | 1901 | A |
| 8 | A | 1906 | G |
| 8 | A | 1908 | C |
| 8 | A | 1910 | G |
| 8 | A | 1916 | A |
| 8 | A | 1917 | PSU |
| 8 | A | 1918 | A |
| 8 | A | 1919 | A |
| 8 | A | 1922 | G |
| 8 | A | 1923 | U |
| 8 | A | 1924 | C |
| 8 | A | 1925 | C |
| 8 | A | 1926 | U |
| 8 | A | 1929 | G |
| 8 | A | 1930 | G |
| 8 | A | 1937 | A |
| 8 | A | 1938 | A |
| 8 | A | 1939 | 5MU |
| 8 | A | 1955 | U |
| 8 | A | 1964 | G |
| 8 | A | 1967 | C |
| 8 | A | 1970 | A |
| 8 | A | 1971 | U |
| 8 | A | 1972 | G |
| 8 | A | 1982 | U |
| 8 | A | 1991 | U |
| 8 | A | 1993 | U |
| 8 | A | 1997 | C |
| 8 | A | 2020 | A |
| 8 | A | 2022 | U |
| 8 | A | 2023 | C |
| 8 | A | 2031 | A |
| 8 | A | 2032 | G |
| 8 | A | 2033 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 2036 | C |
| 8 | A | 2043 | C |
| 8 | A | 2046 | G |
| 8 | A | 2055 | C |
| 8 | A | 2056 | G |
| 8 | A | 2060 | A |
| 8 | A | 2061 | G |
| 8 | A | 2062 | A |
| 8 | A | 2069 | G7M |
| 8 | A | 2070 | A |
| 8 | A | 2093 | G |
| 8 | A | 2101 | A |
| 8 | A | 2102 | G |
| 8 | A | 2103 | C |
| 8 | A | 2104 | C |
| 8 | A | 2110 | G |
| 8 | A | 2111 | U |
| 8 | A | 2112 | G |
| 8 | A | 2114 | A |
| 8 | A | 2116 | G |
| 8 | A | 2118 | U |
| 8 | A | 2119 | A |
| 8 | A | 2120 | G |
| 8 | A | 2125 | G |
| 8 | A | 2126 | A |
| 8 | A | 2127 | G |
| 8 | A | 2128 | G |
| 8 | A | 2129 | C |
| 8 | A | 2130 | U |
| 8 | A | 2131 | U |
| 8 | A | 2132 | U |
| 8 | A | 2133 | G |
| 8 | A | 2134 | A |
| 8 | A | 2135 | A |
| 8 | A | 2136 | G |
| 8 | A | 2138 | G |
| 8 | A | 2139 | U |
| 8 | A | 2143 | C |
| 8 | A | 2145 | C |
| 8 | A | 2146 | C |
| 8 | A | 2147 | A |
| 8 | A | 2148 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 2150 | C |
| 8 | A | 2151 | U |
| 8 | A | 2153 | C |
| 8 | A | 2155 | U |
| 8 | A | 2157 | G |
| 8 | A | 2159 | G |
| 8 | A | 2160 | C |
| 8 | A | 2161 | C |
| 8 | A | 2162 | G |
| 8 | A | 2163 | A |
| 8 | A | 2164 | C |
| 8 | A | 2169 | A |
| 8 | A | 2170 | A |
| 8 | A | 2171 | A |
| 8 | A | 2172 | U |
| 8 | A | 2173 | A |
| 8 | A | 2175 | C |
| 8 | A | 2180 | U |
| 8 | A | 2181 | U |
| 8 | A | 2183 | A |
| 8 | A | 2186 | G |
| 8 | A | 2187 | U |
| 8 | A | 2188 | U |
| 8 | A | 2190 | G |
| 8 | A | 2193 | G |
| 8 | A | 2198 | A |
| 8 | A | 2204 | G |
| 8 | A | 2211 | A |
| 8 | A | 2225 | A |
| 8 | A | 2226 | C |
| 8 | A | 2238 | G |
| 8 | A | 2239 | G |
| 8 | A | 2268 | A |
| 8 | A | 2279 | G |
| 8 | A | 2283 | C |
| 8 | A | 2287 | A |
| 8 | A | 2288 | A |
| 8 | A | 2297 | A |
| 8 | A | 2305 | U |
| 8 | A | 2307 | G |
| 8 | A | 2309 | A |
| 8 | A | 2311 | A |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 2320 | U |
| 8 | A | 2322 | A |
| 8 | A | 2325 | G |
| 8 | A | 2333 | A |
| 8 | A | 2336 | A |
| 8 | A | 2345 | G |
| 8 | A | 2347 | C |
| 8 | A | 2350 | C |
| 8 | A | 2357 | G |
| 8 | A | 2361 | G |
| 8 | A | 2383 | G |
| 8 | A | 2385 | C |
| 8 | A | 2402 | U |
| 8 | A | 2406 | A |
| 8 | A | 2410 | G |
| 8 | A | 2423 | U |
| 8 | A | 2425 | A |
| 8 | A | 2429 | G |
| 8 | A | 2430 | A |
| 8 | A | 2435 | A |
| 8 | A | 2441 | U |
| 8 | A | 2445 | 2MG |
| 8 | A | 2448 | A |
| 8 | A | 2459 | A |
| 8 | A | 2469 | A |
| 8 | A | 2475 | C |
| 8 | A | 2476 | A |
| 8 | A | 2478 | A |
| 8 | A | 2480 | C |
| 8 | A | 2484 | G |
| 8 | A | 2494 | G |
| 8 | A | 2498 | OMC |
| 8 | A | 2502 | G |
| 8 | A | 2504 | PSU |
| 8 | A | 2505 | G |
| 8 | A | 2518 | A |
| 8 | A | 2529 | G |
| 8 | A | 2535 | G |
| 8 | A | 2547 | A |
| 8 | A | 2554 | U |
| 8 | A | 2566 | A |
| 8 | A | 2567 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 2573 | C |
| 8 | A | 2585 | U |
| 8 | A | 2602 | A |
| 8 | A | 2609 | U |
| 8 | A | 2613 | U |
| 8 | A | 2615 | U |
| 8 | A | 2629 | U |
| 8 | A | 2630 | G |
| 8 | A | 2634 | A |
| 8 | A | 2636 | C |
| 8 | A | 2656 | U |
| 8 | A | 2689 | U |
| 8 | A | 2690 | U |
| 8 | A | 2702 | G |
| 8 | A | 2707 | U |
| 8 | A | 2714 | G |
| 8 | A | 2716 | C |
| 8 | A | 2718 | G |
| 8 | A | 2726 | A |
| 8 | A | 2732 | G |
| 8 | A | 2733 | A |
| 8 | A | 2739 | U |
| 8 | A | 2744 | G |
| 8 | A | 2748 | A |
| 8 | A | 2755 | C |
| 8 | A | 2757 | A |
| 8 | A | 2765 | A |
| 8 | A | 2769 | U |
| 8 | A | 2778 | A |
| 8 | A | 2779 | U |
| 8 | A | 2791 | G |
| 8 | A | 2796 | U |
| 8 | A | 2797 | U |
| 8 | A | 2798 | U |
| 8 | A | 2799 | A |
| 8 | A | 2800 | A |
| 8 | A | 2809 | A |
| 8 | A | 2818 | U |
| 8 | A | 2820 | A |
| 8 | A | 2821 | A |
| 8 | A | 2835 | A |
| 8 | A | 2849 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 2867 | G |
| 8 | A | 2872 | A |
| 8 | A | 2873 | A |
| 8 | A | 2879 | A |
| 8 | A | 2884 | U |
| 8 | A | 2886 | A |
| 8 | A | 2891 | U |
| 8 | A | 2893 | A |
| 8 | A | 2902 | C |
| 9 | B | 13 | G |
| 9 | B | 24 | G |
| 9 | B | 32 | U |
| 9 | B | 33 | G |
| 9 | B | 35 | C |
| 9 | B | 37 | C |
| 9 | B | 42 | C |
| 9 | B | 44 | G |
| 9 | B | 45 | A |
| 9 | B | 51 | G |
| 9 | B | 53 | A |
| 9 | B | 56 | G |
| 9 | B | 62 | C |
| 9 | B | 65 | U |
| 9 | B | 67 | G |
| 9 | B | 73 | A |
| 9 | B | 88 | C |
| 9 | B | 89 | U |
| 9 | B | 90 | C |
| 9 | B | 91 | C |
| 9 | B | 101 | A |
| 9 | B | 109 | A |
| 9 | B | 120 | U |
| 34 | a | 6 | G |
| 34 | a | 7 | A |
| 34 | a | 9 | G |
| 34 | a | 22 | G |
| 34 | a | 32 | A |
| 34 | a | 39 | G |
| 34 | a | 47 | C |
| 34 | a | 48 | C |
| 34 | a | 50 | A |
| 34 | a | 51 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | a | 70 | U |
| 34 | a | 71 | A |
| 34 | a | 76 | G |
| 34 | a | 77 | A |
| 34 | a | 78 | A |
| 34 | a | 80 | A |
| 34 | a | 81 | A |
| 34 | a | 83 | C |
| 34 | a | 84 | U |
| 34 | a | 85 | U |
| 34 | a | 86 | G |
| 34 | a | 89 | U |
| 34 | a | 90 | C |
| 34 | a | 94 | G |
| 34 | a | 96 | U |
| 34 | a | 119 | A |
| 34 | a | 121 | U |
| 34 | a | 130 | A |
| 34 | a | 141 | G |
| 34 | a | 144 | G |
| 34 | a | 163 | C |
| 34 | a | 164 | G |
| 34 | a | 165 | G |
| 34 | a | 166 | U |
| 34 | a | 173 | U |
| 34 | a | 182 | A |
| 34 | a | 183 | C |
| 34 | a | 184 | G |
| 34 | a | 197 | A |
| 34 | a | 198 | G |
| 34 | a | 205 | A |
| 34 | a | 208 | U |
| 34 | a | 210 | C |
| 34 | a | 211 | G |
| 34 | a | 219 | U |
| 34 | a | 226 | G |
| 34 | a | 240 | G |
| 34 | a | 245 | U |
| 34 | a | 247 | G |
| 34 | a | 251 | G |
| 34 | a | 266 | G |
| 34 | a | 267 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | a | 271 | C |
| 34 | a | 289 | G |
| 34 | a | 299 | G |
| 34 | a | 306 | A |
| 34 | a | 321 | A |
| 34 | a | 328 | C |
| 34 | a | 329 | A |
| 34 | a | 330 | C |
| 34 | a | 344 | A |
| 34 | a | 351 | G |
| 34 | a | 352 | C |
| 34 | a | 354 | G |
| 34 | a | 367 | U |
| 34 | a | 372 | C |
| 34 | a | 373 | A |
| 34 | a | 388 | G |
| 34 | a | 397 | A |
| 34 | a | 406 | G |
| 34 | a | 411 | A |
| 34 | a | 413 | G |
| 34 | a | 414 | A |
| 34 | a | 421 | U |
| 34 | a | 423 | G |
| 34 | a | 429 | U |
| 34 | a | 461 | A |
| 34 | a | 462 | G |
| 34 | a | 465 | A |
| 34 | a | 468 | A |
| 34 | a | 471 | U |
| 34 | a | 479 | U |
| 34 | a | 484 | G |
| 34 | a | 495 | A |
| 34 | a | 496 | A |
| 34 | a | 509 | A |
| 34 | a | 510 | A |
| 34 | a | 511 | C |
| 34 | a | 516 | PSU |
| 34 | a | 518 | C |
| 34 | a | 521 | G |
| 34 | a | 531 | U |
| 34 | a | 535 | A |
| 34 | a | 536 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | a | 547 | A |
| 34 | a | 550 | G |
| 34 | a | 559 | A |
| 34 | a | 562 | U |
| 34 | a | 564 | C |
| 34 | a | 572 | A |
| 34 | a | 573 | A |
| 34 | a | 576 | C |
| 34 | a | 577 | G |
| 34 | a | 596 | A |
| 34 | a | 615 | G |
| 34 | a | 629 | A |
| 34 | a | 633 | G |
| 34 | a | 642 | A |
| 34 | a | 650 | G |
| 34 | a | 653 | U |
| 34 | a | 665 | A |
| 34 | a | 666 | G |
| 34 | a | 688 | G |
| 34 | a | 703 | G |
| 34 | a | 704 | A |
| 34 | a | 723 | U |
| 34 | a | 724 | G |
| 34 | a | 733 | G |
| 34 | a | 734 | G |
| 34 | a | 748 | G |
| 34 | a | 753 | A |
| 34 | a | 755 | G |
| 34 | a | 774 | G |
| 34 | a | 777 | A |
| 34 | a | 781 | A |
| 34 | a | 792 | A |
| 34 | a | 793 | U |
| 34 | a | 794 | A |
| 34 | a | 799 | G |
| 34 | a | 815 | A |
| 34 | a | 817 | C |
| 34 | a | 841 | C |
| 34 | a | 842 | U |
| 34 | a | 843 | U |
| 34 | a | 844 | G |
| 34 | a | 845 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | a | 846 | G |
| 34 | a | 851 | G |
| 34 | a | 867 | G |
| 34 | a | 885 | G |
| 34 | a | 902 | G |
| 34 | a | 914 | A |
| 34 | a | 934 | C |
| 34 | a | 935 | A |
| 34 | a | 953 | G |
| 34 | a | 954 | G |
| 34 | a | 955 | U |
| 34 | a | 956 | U |
| 34 | a | 957 | U |
| 34 | a | 958 | A |
| 34 | a | 960 | U |
| 34 | a | 969 | A |
| 34 | a | 971 | G |
| 34 | a | 975 | A |
| 34 | a | 976 | G |
| 34 | a | 977 | A |
| 34 | a | 980 | C |
| 34 | a | 983 | A |
| 34 | a | 985 | C |
| 34 | a | 986 | U |
| 34 | a | 988 | G |
| 34 | a | 989 | U |
| 34 | a | 990 | C |
| 34 | a | 992 | U |
| 34 | a | 993 | G |
| 34 | a | 994 | A |
| 34 | a | 995 | C |
| 34 | a | 996 | A |
| 34 | a | 997 | U |
| 34 | a | 999 | C |
| 34 | a | 1000 | A |
| 34 | a | 1004 | A |
| 34 | a | 1005 | A |
| 34 | a | 1006 | G |
| 34 | a | 1007 | U |
| 34 | a | 1011 | C |
| 34 | a | 1014 | A |
| 34 | a | 1015 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | a | 1020 | G |
| 34 | a | 1022 | A |
| 34 | a | 1023 | U |
| 34 | a | 1024 | G |
| 34 | a | 1027 | C |
| 34 | a | 1028 | C |
| 34 | a | 1029 | U |
| 34 | a | 1031 | C |
| 34 | a | 1032 | G |
| 34 | a | 1035 | A |
| 34 | a | 1036 | A |
| 34 | a | 1037 | C |
| 34 | a | 1040 | U |
| 34 | a | 1042 | A |
| 34 | a | 1043 | G |
| 34 | a | 1044 | A |
| 34 | a | 1065 | U |
| 34 | a | 1085 | U |
| 34 | a | 1094 | G |
| 34 | a | 1101 | A |
| 34 | a | 1104 | G |
| 34 | a | 1124 | G |
| 34 | a | 1125 | U |
| 34 | a | 1132 | C |
| 34 | a | 1134 | G |
| 34 | a | 1136 | C |
| 34 | a | 1137 | C |
| 34 | a | 1139 | G |
| 34 | a | 1159 | U |
| 34 | a | 1160 | G |
| 34 | a | 1167 | A |
| 34 | a | 1168 | U |
| 34 | a | 1183 | U |
| 34 | a | 1184 | G |
| 34 | a | 1196 | A |
| 34 | a | 1197 | A |
| 34 | a | 1212 | U |
| 34 | a | 1213 | A |
| 34 | a | 1214 | C |
| 34 | a | 1215 | G |
| 34 | a | 1227 | A |
| 34 | a | 1229 | A |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | a | 1230 | C |
| 34 | a | 1236 | A |
| 34 | a | 1238 | A |
| 34 | a | 1239 | A |
| 34 | a | 1242 | G |
| 34 | a | 1243 | C |
| 34 | a | 1248 | A |
| 34 | a | 1250 | A |
| 34 | a | 1254 | A |
| 34 | a | 1255 | G |
| 34 | a | 1257 | A |
| 34 | a | 1258 | G |
| 34 | a | 1260 | G |
| 34 | a | 1261 | A |
| 34 | a | 1272 | G |
| 34 | a | 1275 | A |
| 34 | a | 1280 | A |
| 34 | a | 1285 | A |
| 34 | a | 1286 | U |
| 34 | a | 1287 | A |
| 34 | a | 1294 | G |
| 34 | a | 1297 | G |
| 34 | a | 1298 | U |
| 34 | a | 1299 | A |
| 34 | a | 1300 | G |
| 34 | a | 1302 | C |
| 34 | a | 1305 | G |
| 34 | a | 1306 | A |
| 34 | a | 1307 | U |
| 34 | a | 1309 | G |
| 34 | a | 1310 | G |
| 34 | a | 1311 | A |
| 34 | a | 1312 | G |
| 34 | a | 1314 | C |
| 34 | a | 1315 | U |
| 34 | a | 1316 | G |
| 34 | a | 1317 | C |
| 34 | a | 1323 | G |
| 34 | a | 1324 | A |
| 34 | a | 1335 | U |
| 34 | a | 1336 | C |
| 34 | a | 1344 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | a | 1345 | U |
| 34 | a | 1346 | A |
| 34 | a | 1347 | G |
| 34 | a | 1350 | A |
| 34 | a | 1353 | G |
| 34 | a | 1355 | G |
| 34 | a | 1356 | G |
| 34 | a | 1357 | A |
| 34 | a | 1362 | A |
| 34 | a | 1363 | A |
| 34 | a | 1370 | G |
| 34 | a | 1371 | G |
| 34 | a | 1372 | U |
| 34 | a | 1374 | A |
| 34 | a | 1378 | C |
| 34 | a | 1379 | G |
| 34 | a | 1381 | U |
| 34 | a | 1383 | C |
| 34 | a | 1397 | C |
| 34 | a | 1398 | A |
| 34 | a | 1419 | G |
| 34 | a | 1421 | G |
| 34 | a | 1422 | G |
| 34 | a | 1429 | A |
| 34 | a | 1432 | G |
| 34 | a | 1433 | A |
| 34 | a | 1440 | U |
| 34 | a | 1441 | A |
| 34 | a | 1442 | G |
| 34 | a | 1446 | A |
| 34 | a | 1451 | U |
| 34 | a | 1452 | C |
| 34 | a | 1472 | U |
| 34 | a | 1473 | G |
| 34 | a | 1475 | G |
| 34 | a | 1487 | G |
| 34 | a | 1492 | A |
| 34 | a | 1494 | G |
| 34 | a | 1497 | G |
| 34 | a | 1499 | A |
| 34 | a | 1506 | U |
| 34 | a | 1517 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | a | 1529 | G |
| 34 | a | 1530 | G |
| 34 | a | 1534 | A |
| 34 | a | 1535 | C |
| 34 | a | 1536 | C |
| 34 | a | 1538 | C |
| 34 | a | 1539 | C |
| 34 | a | 1540 | U |
| 55 | v | 9 | G |
| 55 | v | 18 | G |
| 55 | v | 19 | G |
| 55 | v | 20 | H2U |
| 55 | v | 21 | A |
| 55 | v | 30 | G |
| 55 | v | 33 | U |
| 55 | v | 34 | C |
| 55 | v | 37 | A |
| 55 | v | 44 | A |
| 55 | v | 45 | G |
| 55 | v | 47 | U |
| 55 | v | 48 | C |
| 55 | v | 52 | G |
| 55 | v | 56 | C |
| 55 | v | 70 | G |
| 55 | v | 74 | C |
| 55 | v | 76 | A |
| 56 | w | 10 | G |
| 56 | w | 13 | C |
| 56 | w | 16 | U |
| 56 | w | 17 | C |
| 56 | w | 18 | G |
| 56 | w | 19 | G |
| 56 | w | 20 | U |
| 56 | w | 21 | A |
| 56 | w | 45 | U |
| 56 | w | 46 | G7M |
| 56 | w | 47 | U |
| 56 | w | 48 | C |
| 56 | w | 49 | C |
| 56 | w | 59 | U |
| 56 | w | 60 | U |
| 56 | w | 67 | C |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56 | w | 68 | C |
| 56 | w | 74 | C |
| 58 | z | 0 | U |

All (41) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 242 | G |
| 8 | A | 310 | A |
| 8 | A | 458 | G |
| 8 | A | 479 | A |
| 8 | A | 481 | G |
| 8 | A | 504 | A |
| 8 | A | 545 | U |
| 8 | A | 555 | G |
| 8 | A | 715 | A |
| 8 | A | 774 | G |
| 8 | A | 784 | G |
| 8 | A | 887 | A |
| 8 | A | 954 | G |
| 8 | A | 976 | G |
| 8 | A | 1014 | A |
| 8 | A | 1023 | U |
| 8 | A | 1062 | G |
| 8 | A | 1082 | U |
| 8 | A | 1090 | A |
| 8 | A | 1093 | G |
| 8 | A | 1361 | G |
| 8 | A | 1432 | G |
| 8 | A | 1451 | C |
| 8 | A | 1490 | A |
| 8 | A | 1715 | G |
| 8 | A | 1730 | C |
| 8 | A | 1847 | G |
| 8 | A | 2150 | C |
| 8 | A | 2158 | A |
| 8 | A | 2192 | U |
| 8 | A | 2287 | A |
| 8 | A | 2319 | G |
| 8 | A | 2468 | A |
| 8 | A | 2655 | G |
| 8 | A | 2756 | U |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | A | 2796 | U |
| 8 | A | 2808 | G |
| 9 | B | 36 | C |
| 9 | B | 44 | G |
| 9 | B | 52 | A |
| 9 | B | 66 | A |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|---------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 56 | PSU | w | 55 | 56 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.97 | 5 (22%) |
| 8 | PSU | A | 955 | 8 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.86 | 5 (22%) |
| 8 | 2MG | A | 2445 | 8 | 18,26,27 | 2.58 | 7 (38%) | 16,38,41 | 1.37 | 4 (25%) |
| 8 | 6MZ | A | 1618 | 8 | 18,25,26 | 2.14 | 3 (16%) | 16,36,39 | 1.85 | 3 (18%) |
| 8 | 5MC | A | 747 | 8 | 18,22,23 | 3.65 | 7 (38%) | 26,32,35 | 1.09 | 2 (7%) |
| 8 | 2MA | A | 2503 | 8,59 | 19,25,26 | 3.29 | 6 (31%) | 21,37,40 | 1.73 | 3 (14%) |
| 34 | PSU | a | 516 | 59,34 | 18,21,22 | 0.98 | 1 (5%) | 22,30,33 | 1.70 | 5 (22%) |
| 34 | 4OC | a | 1402 | 34 | 20,23,24 | 2.97 | 8 (40%) | 26,32,35 | 0.90 | 1 (3%) |
| 8 | PSU | A | 1917 | 8 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 1.75 | 5 (22%) |
| 34 | 2MG | a | 966 | 34 | 18,26,27 | 2.58 | 7 (38%) | 16,38,41 | 1.49 | 4 (25%) |
| 34 | 2MG | a | 1207 | 34 | 18,26,27 | 2.60 | 7 (38%) | 16,38,41 | 1.38 | 3 (18%) |
| 56 | G7M | w | 46 | 56 | 20,26,27 | 2.46 | 7 (35%) | 17,39,42 | 1.15 | 1 (5%) |
| 8 | PSU | A | 1911 | 8 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.80 | 4 (18%) |
| 8 | 2MG | A | 1835 | 8 | 18,26,27 | 2.59 | 7 (38%) | 16,38,41 | 1.39 | 4 (25%) |
| 34 | MA6 | a | 1519 | 34 | 18,26,27 | 0.98 | 1 (5%) | 19,38,41 | 2.69 | 2 (10%) |
| 8 | OMG | A | 2251 | 8,55,59 | 18,26,27 | 2.48 | 8 (44%) | 19,38,41 | 1.51 | 4 (21%) |
| 34 | 5MC | a | 967 | 34 | 18,22,23 | 3.68 | 7 (38%) | 26,32,35 | 1.00 | 2 (7%) |
| 8 | PSU | A | 746 | 8,59 | 18,21,22 | 1.05 | 1 (5%) | 22,30,33 | 1.71 | 4 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 56 | PSU | w | 32 | 56 | 18,21,22 | 1.02 | 1 (5%) | 22,30,33 | 1.70 | 4 (18%) |
| 8 | PSU | A | 2580 | 8 | 18,21,22 | 1.10 | 2 (11%) | 22,30,33 | 1.90 | 6 (27%) |
| 8 | PSU | A | 2504 | 8 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.78 | 4 (18%) |
| 55 | PSU | v | 55 | 55 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.68 | 4 (18%) |
| 8 | OMU | A | 2552 | 8,59 | 19,22,23 | 2.89 | 8 (42%) | 26,31,34 | 1.76 | 5 (19%) |
| 8 | G7M | A | 2069 | 8 | 20,26,27 | 2.38 | 7 (35%) | 17,39,42 | 1.45 | 2 (11%) |
| 8 | 1MG | A | 745 | 8 | 18,26,27 | 2.63 | 5 (27%) | 19,39,42 | 1.43 | 3 (15%) |
| 8 | PSU | A | 2457 | 8 | 18,21,22 | 1.06 | 1 (5%) | 22,30,33 | 1.86 | 5 (22%) |
| 8 | 5MC | A | 1962 | 8 | 18,22,23 | 3.65 | 7 (38%) | 26,32,35 | 1.04 | 2 (7%) |
| 56 | 4SU | w | 8 | 56 | 18,21,22 | 3.56 | 7 (38%) | 26,30,33 | 2.20 | 4 (15%) |
| 34 | 5MC | a | 1407 | 34 | 18,22,23 | 3.69 | 7 (38%) | 26,32,35 | 1.03 | 2 (7%) |
| 34 | MA6 | a | 1518 | 34 | 18,26,27 | 0.99 | 1 (5%) | 19,38,41 | 2.64 | 2 (10%) |
| 34 | G7M | a | 527 | 34 | 20,26,27 | 2.40 | 7 (35%) | 17,39,42 | 1.12 | 1 (5%) |
| 8 | 6MZ | A | 2030 | 8 | 18,25,26 | 2.05 | 3 (16%) | 16,36,39 | 2.30 | 3 (18%) |
| 56 | 5MU | w | 54 | 56 | 19,22,23 | 4.79 | 7 (36%) | 28,32,35 | 3.65 | 9 (32%) |
| 55 | 4SU | v | 8 | 55 | 18,21,22 | 3.59 | 7 (38%) | 26,30,33 | 2.22 | 4 (15%) |
| 8 | OMC | A | 2498 | 8,59 | 19,22,23 | 2.86 | 7 (36%) | 26,31,34 | 0.75 | 0 |
| 57 | FME | y | 101 | 57 | 8,9,10 | 0.88 | 0 | 7,9,11 | 1.81 | 2 (28%) |
| 34 | 2MG | a | 1516 | 34 | 18,26,27 | 2.61 | 7 (38%) | 16,38,41 | 1.43 | 4 (25%) |
| 55 | H2U | v | 20 | 55 | 18,21,22 | 3.08 | 5 (27%) | 21,30,33 | 1.98 | 5 (23%) |
| 8 | PSU | A | 2604 | 8 | 18,21,22 | 1.01 | 1 (5%) | 22,30,33 | 1.85 | 4 (18%) |
| 8 | 3TD | A | 1915 | 8 | 18,22,23 | 4.25 | 5 (27%) | 22,32,35 | 1.65 | 2 (9%) |
| 56 | MIA | w | 37 | 56 | 24,31,32 | 2.51 | 4 (16%) | 26,44,47 | 3.11 | 9 (34%) |
| 55 | 5MU | v | 54 | 55 | 19,22,23 | 4.81 | 7 (36%) | 28,32,35 | 3.66 | 9 (32%) |
| 8 | PSU | A | 2605 | 8 | 18,21,22 | 1.04 | 1 (5%) | 22,30,33 | 1.81 | 4 (18%) |
| 56 | PSU | w | 39 | 56 | 18,21,22 | 1.09 | 1 (5%) | 22,30,33 | 1.71 | 3 (13%) |
| 34 | UR3 | a | 1498 | 34 | 19,22,23 | 2.68 | 7 (36%) | 26,32,35 | 1.37 | 3 (11%) |
| 8 | 5MU | A | 1939 | 8 | 19,22,23 | 4.76 | 7 (36%) | 28,32,35 | 3.79 | 10 (35%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 56 | PSU | w | 55 | 56 | - | 1/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|---------|---------|-----------|---------|
| 8 | PSU | A | 955 | 8 | - | 0/7/25/26 | 0/2/2/2 |
| 8 | 2MG | A | 2445 | 8 | - | 2/5/27/28 | 0/3/3/3 |
| 8 | 6MZ | A | 1618 | 8 | - | 0/5/27/28 | 0/3/3/3 |
| 8 | 5MC | A | 747 | 8 | - | 0/7/25/26 | 0/2/2/2 |
| 8 | 2MA | A | 2503 | 8,59 | - | 2/3/25/26 | 0/3/3/3 |
| 34 | PSU | a | 516 | 59,34 | - | 0/7/25/26 | 0/2/2/2 |
| 34 | 4OC | a | 1402 | 34 | - | 2/9/29/30 | 0/2/2/2 |
| 8 | PSU | A | 1917 | 8 | - | 1/7/25/26 | 0/2/2/2 |
| 34 | 2MG | a | 966 | 34 | - | 0/5/27/28 | 0/3/3/3 |
| 34 | 2MG | a | 1207 | 34 | - | 0/5/27/28 | 0/3/3/3 |
| 56 | G7M | w | 46 | 56 | - | 0/3/25/26 | 0/3/3/3 |
| 8 | PSU | A | 1911 | 8 | - | 0/7/25/26 | 0/2/2/2 |
| 8 | 2MG | A | 1835 | 8 | - | 2/5/27/28 | 0/3/3/3 |
| 34 | MA6 | a | 1519 | 34 | - | 1/7/29/30 | 0/3/3/3 |
| 8 | OMG | A | 2251 | 8,55,59 | - | 1/5/27/28 | 0/3/3/3 |
| 34 | 5MC | a | 967 | 34 | - | 0/7/25/26 | 0/2/2/2 |
| 8 | PSU | A | 746 | 8,59 | - | 2/7/25/26 | 0/2/2/2 |
| 56 | PSU | w | 32 | 56 | - | 3/7/25/26 | 0/2/2/2 |
| 8 | PSU | A | 2580 | 8 | - | 0/7/25/26 | 0/2/2/2 |
| 8 | PSU | A | 2504 | 8 | - | 2/7/25/26 | 0/2/2/2 |
| 55 | PSU | v | 55 | 55 | - | 2/7/25/26 | 0/2/2/2 |
| 8 | OMU | A | 2552 | 8,59 | - | 3/9/27/28 | 0/2/2/2 |
| 8 | G7M | A | 2069 | 8 | - | 1/3/25/26 | 0/3/3/3 |
| 8 | 1MG | A | 745 | 8 | - | 0/3/25/26 | 0/3/3/3 |
| 8 | PSU | A | 2457 | 8 | - | 0/7/25/26 | 0/2/2/2 |
| 8 | 5MC | A | 1962 | 8 | - | 2/7/25/26 | 0/2/2/2 |
| 56 | 4SU | w | 8 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 34 | 5MC | a | 1407 | 34 | - | 0/7/25/26 | 0/2/2/2 |
| 34 | MA6 | a | 1518 | 34 | - | 0/7/29/30 | 0/3/3/3 |
| 34 | G7M | a | 527 | 34 | - | 1/3/25/26 | 0/3/3/3 |
| 8 | 6MZ | A | 2030 | 8 | - | 2/5/27/28 | 0/3/3/3 |
| 56 | 5MU | w | 54 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 4SU | v | 8 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 8 | OMC | A | 2498 | 8,59 | - | 2/9/27/28 | 0/2/2/2 |
| 57 | FME | y | 101 | 57 | - | 5/7/9/11 | - |
| 34 | 2MG | a | 1516 | 34 | - | 0/5/27/28 | 0/3/3/3 |
| 55 | H2U | v | 20 | 55 | - | 3/7/38/39 | 0/2/2/2 |
| 8 | PSU | A | 2604 | 8 | - | 0/7/25/26 | 0/2/2/2 |
| 8 | 3TD | A | 1915 | 8 | - | 3/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 56 | MIA | w | 37 | 56 | - | 2/11/33/34 | 0/3/3/3 |
| 55 | 5MU | v | 54 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 8 | PSU | A | 2605 | 8 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | PSU | w | 39 | 56 | - | 3/7/25/26 | 0/2/2/2 |
| 34 | UR3 | a | 1498 | 34 | - | 2/7/25/26 | 0/2/2/2 |
| 8 | 5MU | A | 1939 | 8 | - | 2/7/25/26 | 0/2/2/2 |

All (205) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8 | A | 1915 | 3TD | C6-C5 | 12.88 | 1.50 | 1.35 |
| 55 | v | 54 | 5MU | C2-N1 | 11.06 | 1.56 | 1.38 |
| 56 | w | 54 | 5MU | C2-N1 | 10.96 | 1.56 | 1.38 |
| 55 | v | 54 | 5MU | C6-N1 | 10.38 | 1.55 | 1.38 |
| 8 | A | 1939 | 5MU | C2-N1 | 10.36 | 1.55 | 1.38 |
| 56 | w | 54 | 5MU | C6-N1 | 10.36 | 1.55 | 1.38 |
| 8 | A | 1939 | 5MU | C6-N1 | 10.27 | 1.55 | 1.38 |
| 55 | v | 54 | 5MU | C4-C5 | 10.10 | 1.61 | 1.44 |
| 8 | A | 1939 | 5MU | C4-C5 | 9.87 | 1.61 | 1.44 |
| 56 | w | 54 | 5MU | C4-C5 | 9.86 | 1.61 | 1.44 |
| 55 | v | 20 | H2U | C2-N1 | 9.43 | 1.49 | 1.35 |
| 34 | a | 1407 | 5MC | C6-C5 | 9.38 | 1.50 | 1.34 |
| 8 | A | 1915 | 3TD | C2-N1 | 9.23 | 1.49 | 1.37 |
| 34 | a | 967 | 5MC | C6-C5 | 9.19 | 1.49 | 1.34 |
| 8 | A | 1962 | 5MC | C6-C5 | 9.18 | 1.49 | 1.34 |
| 8 | A | 747 | 5MC | C6-C5 | 9.17 | 1.49 | 1.34 |
| 8 | A | 2503 | 2MA | C4-N3 | 8.81 | 1.49 | 1.35 |
| 8 | A | 1939 | 5MU | C4-N3 | -8.16 | 1.23 | 1.38 |
| 55 | v | 8 | 4SU | C4-N3 | 7.95 | 1.46 | 1.37 |
| 56 | w | 8 | 4SU | C4-N3 | 7.90 | 1.46 | 1.37 |
| 56 | w | 54 | 5MU | C4-N3 | -7.86 | 1.24 | 1.38 |
| 55 | v | 54 | 5MU | C4-N3 | -7.72 | 1.24 | 1.38 |
| 8 | A | 1618 | 6MZ | C6-N6 | 7.62 | 1.47 | 1.35 |
| 55 | v | 8 | 4SU | C2-N1 | 7.34 | 1.50 | 1.38 |
| 56 | w | 8 | 4SU | C2-N1 | 7.25 | 1.50 | 1.38 |
| 8 | A | 2030 | 6MZ | C6-N6 | 7.21 | 1.46 | 1.35 |
| 56 | w | 37 | MIA | C13-C14 | 7.19 | 1.53 | 1.32 |
| 8 | A | 745 | 1MG | C2-N2 | 7.18 | 1.47 | 1.34 |
| 56 | w | 37 | MIA | C2-S10 | 7.01 | 1.81 | 1.75 |
| 8 | A | 1962 | 5MC | C4-N3 | 6.83 | 1.45 | 1.34 |
| 34 | a | 1498 | UR3 | C2-N1 | 6.82 | 1.48 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 34 | a | 967 | 5MC | C4-N3 | 6.81 | 1.45 | 1.34 |
| 8 | A | 2503 | 2MA | C2-N3 | 6.80 | 1.46 | 1.34 |
| 8 | A | 2552 | OMU | C2-N1 | 6.74 | 1.49 | 1.38 |
| 8 | A | 747 | 5MC | C4-N3 | 6.69 | 1.45 | 1.34 |
| 34 | a | 1407 | 5MC | C4-N3 | 6.67 | 1.45 | 1.34 |
| 34 | a | 1402 | 4OC | C4-N3 | 6.56 | 1.44 | 1.32 |
| 55 | v | 20 | H2U | C2-N3 | 6.49 | 1.49 | 1.38 |
| 8 | A | 2552 | OMU | C2-N3 | 6.30 | 1.49 | 1.38 |
| 34 | a | 1207 | 2MG | C2-N2 | 6.27 | 1.47 | 1.33 |
| 34 | a | 1516 | 2MG | C2-N2 | 6.25 | 1.47 | 1.33 |
| 34 | a | 967 | 5MC | C2-N3 | 6.23 | 1.49 | 1.36 |
| 8 | A | 2498 | OMC | C6-C5 | 6.21 | 1.49 | 1.35 |
| 8 | A | 1835 | 2MG | C2-N2 | 6.20 | 1.47 | 1.33 |
| 8 | A | 1962 | 5MC | C2-N3 | 6.17 | 1.48 | 1.36 |
| 34 | a | 966 | 2MG | C2-N2 | 6.14 | 1.47 | 1.33 |
| 8 | A | 2445 | 2MG | C2-N2 | 6.12 | 1.47 | 1.33 |
| 34 | a | 1498 | UR3 | C6-C5 | 6.10 | 1.49 | 1.35 |
| 8 | A | 747 | 5MC | C2-N3 | 6.10 | 1.48 | 1.36 |
| 34 | a | 1407 | 5MC | C2-N3 | 6.07 | 1.48 | 1.36 |
| 34 | a | 1402 | 4OC | C6-C5 | 6.02 | 1.49 | 1.35 |
| 8 | A | 1939 | 5MU | C6-C5 | 5.94 | 1.44 | 1.34 |
| 56 | w | 8 | 4SU | C6-C5 | 5.88 | 1.48 | 1.35 |
| 8 | A | 2498 | OMC | C2-N3 | 5.87 | 1.48 | 1.36 |
| 55 | v | 8 | 4SU | C6-C5 | 5.83 | 1.48 | 1.35 |
| 55 | v | 54 | 5MU | C6-C5 | 5.77 | 1.44 | 1.34 |
| 8 | A | 2503 | 2MA | C2-N1 | 5.69 | 1.44 | 1.34 |
| 56 | w | 54 | 5MU | C6-C5 | 5.67 | 1.43 | 1.34 |
| 8 | A | 1915 | 3TD | C6-N1 | 5.66 | 1.45 | 1.36 |
| 56 | w | 46 | G7M | C2-N3 | 5.65 | 1.46 | 1.33 |
| 56 | w | 37 | MIA | C6-N6 | 5.61 | 1.44 | 1.34 |
| 34 | a | 1402 | 4OC | C2-N3 | 5.60 | 1.47 | 1.36 |
| 34 | a | 527 | G7M | C2-N3 | 5.59 | 1.46 | 1.33 |
| 55 | v | 8 | 4SU | C2-N3 | 5.57 | 1.47 | 1.38 |
| 8 | A | 2552 | OMU | C6-C5 | 5.53 | 1.47 | 1.35 |
| 8 | A | 2498 | OMC | C4-N3 | 5.52 | 1.45 | 1.34 |
| 8 | A | 745 | 1MG | C2-N3 | 5.49 | 1.44 | 1.34 |
| 56 | w | 8 | 4SU | C2-N3 | 5.44 | 1.47 | 1.38 |
| 8 | A | 2069 | G7M | C2-N3 | 5.32 | 1.46 | 1.33 |
| 8 | A | 2251 | OMG | C2-N3 | 5.18 | 1.45 | 1.33 |
| 56 | w | 8 | 4SU | C4-S4 | -5.16 | 1.58 | 1.68 |
| 8 | A | 2503 | 2MA | C6-N1 | 5.14 | 1.43 | 1.33 |
| 55 | v | 8 | 4SU | C4-S4 | -5.13 | 1.58 | 1.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 8 | A | 1835 | 2MG | C4-N3 | 4.97 | 1.49 | 1.37 |
| 55 | v | 20 | H2U | C4-N3 | 4.97 | 1.46 | 1.37 |
| 34 | a | 966 | 2MG | C4-N3 | 4.96 | 1.49 | 1.37 |
| 34 | a | 1207 | 2MG | C4-N3 | 4.95 | 1.49 | 1.37 |
| 34 | a | 527 | G7M | C4-N3 | 4.94 | 1.49 | 1.37 |
| 8 | A | 1915 | 3TD | C2-N3 | 4.92 | 1.49 | 1.38 |
| 8 | A | 745 | 1MG | C4-N3 | 4.90 | 1.49 | 1.37 |
| 56 | w | 46 | G7M | C4-N3 | 4.88 | 1.49 | 1.37 |
| 34 | a | 1516 | 2MG | C4-N3 | 4.84 | 1.49 | 1.37 |
| 8 | A | 2069 | G7M | C4-N3 | 4.80 | 1.49 | 1.37 |
| 34 | a | 967 | 5MC | C4-N4 | 4.79 | 1.46 | 1.34 |
| 8 | A | 2445 | 2MG | C4-N3 | 4.79 | 1.49 | 1.37 |
| 8 | A | 747 | 5MC | C4-N4 | 4.74 | 1.46 | 1.34 |
| 8 | A | 2251 | OMG | C4-N3 | 4.74 | 1.48 | 1.37 |
| 8 | A | 1962 | 5MC | C4-N4 | 4.73 | 1.46 | 1.34 |
| 34 | a | 1407 | 5MC | C4-N4 | 4.73 | 1.46 | 1.34 |
| 34 | a | 1498 | UR3 | C2-N3 | 4.61 | 1.47 | 1.39 |
| 34 | a | 1407 | 5MC | C6-N1 | 4.56 | 1.45 | 1.38 |
| 8 | A | 2251 | OMG | C2-N2 | 4.49 | 1.44 | 1.34 |
| 34 | a | 967 | 5MC | C6-N1 | 4.49 | 1.45 | 1.38 |
| 8 | A | 747 | 5MC | C6-N1 | 4.41 | 1.45 | 1.38 |
| 34 | a | 966 | 2MG | C2-N1 | 4.40 | 1.43 | 1.36 |
| 34 | a | 1516 | 2MG | C2-N1 | 4.39 | 1.43 | 1.36 |
| 34 | a | 1207 | 2MG | C2-N1 | 4.38 | 1.43 | 1.36 |
| 8 | A | 1835 | 2MG | C2-N1 | 4.33 | 1.43 | 1.36 |
| 56 | w | 46 | G7M | C2-N2 | 4.29 | 1.44 | 1.34 |
| 8 | A | 1962 | 5MC | C6-N1 | 4.28 | 1.45 | 1.38 |
| 8 | A | 2445 | 2MG | C2-N1 | 4.27 | 1.43 | 1.36 |
| 34 | a | 527 | G7M | C2-N2 | 4.23 | 1.44 | 1.34 |
| 34 | a | 1407 | 5MC | C2-N1 | 4.19 | 1.49 | 1.40 |
| 8 | A | 2069 | G7M | C2-N2 | 4.13 | 1.44 | 1.34 |
| 8 | A | 747 | 5MC | C2-N1 | 4.11 | 1.48 | 1.40 |
| 34 | a | 967 | 5MC | C2-N1 | 4.08 | 1.48 | 1.40 |
| 8 | A | 1962 | 5MC | C2-N1 | 4.06 | 1.48 | 1.40 |
| 34 | a | 1402 | 4OC | C4-N4 | 4.02 | 1.44 | 1.35 |
| 56 | w | 46 | G7M | C6-N1 | 3.82 | 1.43 | 1.37 |
| 34 | a | 1402 | 4OC | C5-C4 | 3.80 | 1.48 | 1.40 |
| 34 | a | 1402 | 4OC | C2-N1 | 3.78 | 1.48 | 1.40 |
| 8 | A | 2498 | OMC | C4-N4 | 3.73 | 1.42 | 1.33 |
| 8 | A | 2498 | OMC | C2-N1 | 3.57 | 1.47 | 1.40 |
| 8 | A | 2069 | G7M | C6-N1 | 3.57 | 1.43 | 1.37 |
| 55 | v | 55 | PSU | C6-C5 | 3.53 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 8 | A | 2498 | OMC | C6-N1 | 3.50 | 1.46 | 1.38 |
| 56 | w | 46 | G7M | C5-C6 | 3.50 | 1.54 | 1.45 |
| 8 | A | 747 | 5MC | O2-C2 | -3.44 | 1.17 | 1.23 |
| 34 | a | 527 | G7M | C6-N1 | 3.41 | 1.43 | 1.37 |
| 34 | a | 1407 | 5MC | O2-C2 | -3.40 | 1.17 | 1.23 |
| 8 | A | 2504 | PSU | C6-C5 | 3.40 | 1.39 | 1.35 |
| 8 | A | 2552 | OMU | C4-N3 | 3.36 | 1.44 | 1.38 |
| 34 | a | 1516 | 2MG | C6-N1 | 3.36 | 1.42 | 1.37 |
| 34 | a | 527 | G7M | C5-C6 | 3.31 | 1.54 | 1.45 |
| 8 | A | 2251 | OMG | C6-N1 | 3.30 | 1.42 | 1.37 |
| 34 | a | 966 | 2MG | C6-N1 | 3.29 | 1.42 | 1.37 |
| 8 | A | 1962 | 5MC | O2-C2 | -3.29 | 1.17 | 1.23 |
| 56 | w | 55 | PSU | C6-C5 | 3.28 | 1.39 | 1.35 |
| 8 | A | 1911 | PSU | C6-C5 | 3.26 | 1.39 | 1.35 |
| 56 | w | 39 | PSU | C6-C5 | 3.26 | 1.39 | 1.35 |
| 55 | v | 8 | 4SU | C5-C4 | 3.25 | 1.46 | 1.42 |
| 34 | a | 967 | 5MC | O2-C2 | -3.24 | 1.17 | 1.23 |
| 8 | A | 1835 | 2MG | C6-N1 | 3.24 | 1.42 | 1.37 |
| 8 | A | 2069 | G7M | C5-C6 | 3.22 | 1.53 | 1.45 |
| 56 | w | 32 | PSU | C6-C5 | 3.22 | 1.39 | 1.35 |
| 8 | A | 2445 | 2MG | C6-N1 | 3.20 | 1.42 | 1.37 |
| 34 | a | 1207 | 2MG | C6-N1 | 3.20 | 1.42 | 1.37 |
| 56 | w | 8 | 4SU | C5-C4 | 3.19 | 1.46 | 1.42 |
| 8 | A | 2445 | 2MG | O6-C6 | -3.17 | 1.16 | 1.23 |
| 8 | A | 1835 | 2MG | O6-C6 | -3.16 | 1.16 | 1.23 |
| 8 | A | 2552 | OMU | O4-C4 | -3.14 | 1.18 | 1.24 |
| 8 | A | 2498 | OMC | O2-C2 | -3.13 | 1.17 | 1.23 |
| 8 | A | 746 | PSU | C6-C5 | 3.11 | 1.38 | 1.35 |
| 34 | a | 1402 | 4OC | O2-C2 | -3.10 | 1.18 | 1.23 |
| 8 | A | 1917 | PSU | C6-C5 | 3.10 | 1.38 | 1.35 |
| 34 | a | 966 | 2MG | O6-C6 | -3.08 | 1.17 | 1.23 |
| 8 | A | 2030 | 6MZ | C5-C4 | -3.08 | 1.32 | 1.40 |
| 8 | A | 2457 | PSU | C6-C5 | 3.07 | 1.38 | 1.35 |
| 8 | A | 2605 | PSU | C6-C5 | 3.07 | 1.38 | 1.35 |
| 34 | a | 1516 | 2MG | C5-C4 | -3.07 | 1.35 | 1.43 |
| 8 | A | 1915 | 3TD | C4-N3 | 3.06 | 1.47 | 1.40 |
| 34 | a | 1207 | 2MG | O6-C6 | -3.06 | 1.17 | 1.23 |
| 34 | a | 1516 | 2MG | O6-C6 | -3.04 | 1.17 | 1.23 |
| 8 | A | 2580 | PSU | C6-C5 | 3.02 | 1.38 | 1.35 |
| 8 | A | 2445 | 2MG | C5-C4 | -3.00 | 1.35 | 1.43 |
| 8 | A | 2604 | PSU | C6-C5 | 3.00 | 1.38 | 1.35 |
| 34 | a | 1402 | 4OC | C6-N1 | 3.00 | 1.45 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 8 | A | 955 | PSU | C6-C5 | 2.98 | 1.38 | 1.35 |
| 8 | A | 1618 | 6MZ | C5-C4 | -2.94 | 1.33 | 1.40 |
| 34 | a | 1207 | 2MG | C5-C6 | 2.94 | 1.53 | 1.47 |
| 8 | A | 2445 | 2MG | C5-C6 | 2.92 | 1.53 | 1.47 |
| 34 | a | 966 | 2MG | C5-C4 | -2.92 | 1.35 | 1.43 |
| 34 | a | 1207 | 2MG | C5-C4 | -2.92 | 1.35 | 1.43 |
| 34 | a | 1498 | UR3 | C6-N1 | 2.91 | 1.45 | 1.38 |
| 34 | a | 1516 | 2MG | C5-C6 | 2.90 | 1.53 | 1.47 |
| 8 | A | 1835 | 2MG | C5-C4 | -2.90 | 1.35 | 1.43 |
| 34 | a | 516 | PSU | C6-C5 | 2.88 | 1.38 | 1.35 |
| 8 | A | 2251 | OMG | C5-C4 | -2.88 | 1.35 | 1.43 |
| 8 | A | 1939 | 5MU | O4-C4 | -2.87 | 1.18 | 1.23 |
| 8 | A | 745 | 1MG | C5-C4 | -2.87 | 1.35 | 1.43 |
| 8 | A | 1939 | 5MU | O2-C2 | -2.86 | 1.17 | 1.23 |
| 56 | w | 37 | MIA | C5-C4 | -2.85 | 1.33 | 1.40 |
| 8 | A | 2552 | OMU | O2-C2 | -2.81 | 1.17 | 1.23 |
| 8 | A | 2251 | OMG | C5-C6 | 2.81 | 1.53 | 1.47 |
| 8 | A | 1835 | 2MG | C5-C6 | 2.79 | 1.53 | 1.47 |
| 56 | w | 54 | 5MU | O4-C4 | -2.77 | 1.18 | 1.23 |
| 56 | w | 46 | G7M | C2-N1 | 2.76 | 1.44 | 1.37 |
| 34 | a | 966 | 2MG | C5-C6 | 2.73 | 1.53 | 1.47 |
| 34 | a | 1518 | MA6 | C5-C4 | -2.70 | 1.33 | 1.40 |
| 55 | v | 8 | 4SU | O2-C2 | -2.69 | 1.18 | 1.23 |
| 8 | A | 2503 | 2MA | C6-C5 | 2.69 | 1.53 | 1.43 |
| 34 | a | 1519 | MA6 | C5-C4 | -2.64 | 1.33 | 1.40 |
| 55 | v | 54 | 5MU | O4-C4 | -2.64 | 1.18 | 1.23 |
| 8 | A | 1618 | 6MZ | C2-N3 | 2.58 | 1.36 | 1.32 |
| 8 | A | 2552 | OMU | C6-N1 | 2.57 | 1.44 | 1.38 |
| 8 | A | 2069 | G7M | C2-N1 | 2.55 | 1.44 | 1.37 |
| 56 | w | 8 | 4SU | O2-C2 | -2.54 | 1.18 | 1.23 |
| 34 | a | 1498 | UR3 | O2-C2 | -2.51 | 1.17 | 1.22 |
| 8 | A | 2069 | G7M | O6-C6 | -2.51 | 1.18 | 1.23 |
| 56 | w | 54 | 5MU | O2-C2 | -2.50 | 1.18 | 1.23 |
| 34 | a | 527 | G7M | C2-N1 | 2.50 | 1.43 | 1.37 |
| 34 | a | 527 | G7M | O6-C6 | -2.49 | 1.18 | 1.23 |
| 8 | A | 2251 | OMG | C2-N1 | 2.47 | 1.43 | 1.37 |
| 8 | A | 2251 | OMG | O6-C6 | -2.46 | 1.18 | 1.23 |
| 34 | a | 1498 | UR3 | O4-C4 | -2.43 | 1.18 | 1.23 |
| 8 | A | 2503 | 2MA | C6-N6 | -2.37 | 1.25 | 1.34 |
| 8 | A | 2030 | 6MZ | C2-N3 | 2.35 | 1.35 | 1.32 |
| 55 | v | 54 | 5MU | O2-C2 | -2.34 | 1.18 | 1.23 |
| 55 | v | 20 | H2U | O4-C4 | -2.31 | 1.18 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55 | v | 20 | H2U | O2-C2 | -2.27 | 1.18 | 1.23 |
| 56 | w | 46 | G7M | O6-C6 | -2.25 | 1.18 | 1.23 |
| 8 | A | 2580 | PSU | O4'-C1' | -2.24 | 1.40 | 1.43 |
| 8 | A | 2552 | OMU | C5-C4 | 2.13 | 1.48 | 1.43 |
| 8 | A | 745 | 1MG | C6-N1 | 2.05 | 1.43 | 1.39 |
| 34 | a | 1498 | UR3 | C5-C4 | 2.03 | 1.49 | 1.43 |

All (176) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 8 | A | 1939 | 5MU | C5-C4-N3 | 12.47 | 125.95 | 115.31 |
| 55 | v | 54 | 5MU | C5-C4-N3 | 12.28 | 125.80 | 115.31 |
| 56 | w | 54 | 5MU | C5-C4-N3 | 12.28 | 125.79 | 115.31 |
| 8 | A | 1939 | 5MU | C5-C6-N1 | -11.03 | 111.99 | 123.34 |
| 55 | v | 54 | 5MU | C5-C6-N1 | -10.10 | 112.95 | 123.34 |
| 34 | a | 1519 | MA6 | N1-C6-N6 | -10.03 | 106.50 | 117.06 |
| 56 | w | 54 | 5MU | C5-C6-N1 | -9.80 | 113.25 | 123.34 |
| 34 | a | 1518 | MA6 | N1-C6-N6 | -9.73 | 106.81 | 117.06 |
| 56 | w | 37 | MIA | C12-C13-C14 | -9.05 | 109.52 | 127.14 |
| 56 | w | 37 | MIA | C11-S10-C2 | 8.78 | 108.82 | 102.27 |
| 55 | v | 8 | 4SU | C4-N3-C2 | -7.73 | 119.83 | 127.34 |
| 56 | w | 8 | 4SU | C4-N3-C2 | -7.67 | 119.89 | 127.34 |
| 55 | v | 20 | H2U | C4-N3-C2 | -6.66 | 120.27 | 125.79 |
| 8 | A | 2030 | 6MZ | C9-N6-C6 | -5.88 | 117.81 | 122.87 |
| 8 | A | 2503 | 2MA | C2-N3-C4 | 5.80 | 120.23 | 115.52 |
| 8 | A | 2030 | 6MZ | N3-C2-N1 | -5.70 | 119.76 | 128.68 |
| 34 | a | 1518 | MA6 | N3-C2-N1 | -5.69 | 119.79 | 128.68 |
| 34 | a | 1519 | MA6 | N3-C2-N1 | -5.57 | 119.98 | 128.68 |
| 56 | w | 8 | 4SU | C5-C4-N3 | 5.54 | 119.83 | 114.69 |
| 8 | A | 1618 | 6MZ | N3-C2-N1 | -5.40 | 120.23 | 128.68 |
| 55 | v | 8 | 4SU | C5-C4-N3 | 5.40 | 119.70 | 114.69 |
| 8 | A | 1939 | 5MU | C4-N3-C2 | -5.29 | 120.50 | 127.35 |
| 8 | A | 2552 | OMU | C4-N3-C2 | -5.25 | 119.66 | 126.58 |
| 8 | A | 1915 | 3TD | N1-C2-N3 | 5.24 | 120.27 | 116.14 |
| 56 | w | 54 | 5MU | O4-C4-C5 | -5.15 | 118.93 | 124.90 |
| 55 | v | 54 | 5MU | O4-C4-C5 | -5.12 | 118.97 | 124.90 |
| 56 | w | 55 | PSU | N1-C2-N3 | 4.94 | 120.73 | 115.13 |
| 8 | A | 1939 | 5MU | O4-C4-C5 | -4.88 | 119.24 | 124.90 |
| 8 | A | 2604 | PSU | C4-N3-C2 | -4.88 | 119.31 | 126.34 |
| 8 | A | 2457 | PSU | C4-N3-C2 | -4.87 | 119.31 | 126.34 |
| 56 | w | 54 | 5MU | C4-N3-C2 | -4.86 | 121.06 | 127.35 |
| 55 | v | 54 | 5MU | C4-N3-C2 | -4.81 | 121.12 | 127.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8 | A | 955 | PSU | N1-C2-N3 | 4.78 | 120.55 | 115.13 |
| 8 | A | 955 | PSU | C4-N3-C2 | -4.78 | 119.45 | 126.34 |
| 8 | A | 2604 | PSU | N1-C2-N3 | 4.73 | 120.49 | 115.13 |
| 8 | A | 2605 | PSU | C4-N3-C2 | -4.72 | 119.53 | 126.34 |
| 8 | A | 2457 | PSU | N1-C2-N3 | 4.71 | 120.47 | 115.13 |
| 8 | A | 1939 | 5MU | N3-C2-N1 | 4.71 | 121.15 | 114.89 |
| 8 | A | 2580 | PSU | N1-C2-N3 | 4.70 | 120.45 | 115.13 |
| 56 | w | 37 | MIA | C15-C14-C13 | -4.65 | 109.22 | 122.65 |
| 8 | A | 1911 | PSU | N1-C2-N3 | 4.64 | 120.38 | 115.13 |
| 8 | A | 1911 | PSU | C4-N3-C2 | -4.63 | 119.67 | 126.34 |
| 8 | A | 2504 | PSU | C4-N3-C2 | -4.62 | 119.69 | 126.34 |
| 56 | w | 37 | MIA | C16-C14-C13 | -4.60 | 109.35 | 122.65 |
| 8 | A | 2605 | PSU | N1-C2-N3 | 4.60 | 120.34 | 115.13 |
| 56 | w | 39 | PSU | C4-N3-C2 | -4.59 | 119.72 | 126.34 |
| 8 | A | 746 | PSU | C4-N3-C2 | -4.59 | 119.72 | 126.34 |
| 8 | A | 2504 | PSU | N1-C2-N3 | 4.58 | 120.32 | 115.13 |
| 8 | A | 2580 | PSU | C4-N3-C2 | -4.58 | 119.75 | 126.34 |
| 8 | A | 1917 | PSU | N1-C2-N3 | 4.55 | 120.29 | 115.13 |
| 55 | v | 55 | PSU | C4-N3-C2 | -4.50 | 119.86 | 126.34 |
| 56 | w | 39 | PSU | N1-C2-N3 | 4.49 | 120.22 | 115.13 |
| 56 | w | 32 | PSU | C4-N3-C2 | -4.47 | 119.90 | 126.34 |
| 8 | A | 746 | PSU | N1-C2-N3 | 4.44 | 120.16 | 115.13 |
| 56 | w | 32 | PSU | N1-C2-N3 | 4.42 | 120.13 | 115.13 |
| 34 | a | 516 | PSU | C4-N3-C2 | -4.42 | 119.98 | 126.34 |
| 56 | w | 55 | PSU | C4-N3-C2 | -4.39 | 120.02 | 126.34 |
| 56 | w | 54 | 5MU | N3-C2-N1 | 4.38 | 120.70 | 114.89 |
| 8 | A | 1917 | PSU | C4-N3-C2 | -4.38 | 120.03 | 126.34 |
| 55 | v | 55 | PSU | N1-C2-N3 | 4.33 | 120.03 | 115.13 |
| 34 | a | 516 | PSU | N1-C2-N3 | 4.26 | 119.96 | 115.13 |
| 56 | w | 54 | 5MU | C5M-C5-C4 | 4.23 | 123.42 | 118.77 |
| 8 | A | 2552 | OMU | N3-C2-N1 | 4.22 | 120.49 | 114.89 |
| 34 | a | 1498 | UR3 | C4-N3-C2 | -4.19 | 120.62 | 124.56 |
| 56 | w | 54 | 5MU | C5M-C5-C6 | -4.14 | 117.32 | 122.85 |
| 55 | v | 54 | 5MU | N3-C2-N1 | 4.12 | 120.36 | 114.89 |
| 55 | v | 54 | 5MU | C5M-C5-C4 | 4.11 | 123.30 | 118.77 |
| 8 | A | 745 | 1MG | C5-C6-N1 | 4.10 | 120.06 | 113.90 |
| 55 | v | 54 | 5MU | C5M-C5-C6 | -4.09 | 117.39 | 122.85 |
| 8 | A | 1915 | 3TD | C4-N3-C2 | -3.92 | 120.35 | 124.61 |
| 8 | A | 1618 | 6MZ | C9-N6-C6 | -3.81 | 119.59 | 122.87 |
| 55 | v | 8 | 4SU | N3-C2-N1 | 3.77 | 119.89 | 114.89 |
| 56 | w | 8 | 4SU | N3-C2-N1 | 3.66 | 119.75 | 114.89 |
| 8 | A | 1939 | 5MU | C5M-C5-C6 | -3.65 | 117.98 | 122.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 8 | A | 747 | 5MC | C5-C6-N1 | -3.64 | 119.59 | 123.34 |
| 8 | A | 2030 | 6MZ | C1'-N9-C4 | -3.62 | 120.28 | 126.64 |
| 56 | w | 37 | MIA | N3-C2-N1 | -3.61 | 120.34 | 126.98 |
| 56 | w | 55 | PSU | O2-C2-N1 | -3.60 | 118.82 | 122.79 |
| 34 | a | 966 | 2MG | C5-C6-N1 | 3.57 | 120.25 | 113.95 |
| 34 | a | 1516 | 2MG | C5-C6-N1 | 3.56 | 120.24 | 113.95 |
| 55 | v | 8 | 4SU | C5-C4-S4 | -3.56 | 119.88 | 124.47 |
| 8 | A | 2251 | OMG | C5-C6-N1 | 3.54 | 120.20 | 113.95 |
| 34 | a | 1207 | 2MG | C5-C6-N1 | 3.51 | 120.16 | 113.95 |
| 8 | A | 1835 | 2MG | C5-C6-N1 | 3.50 | 120.12 | 113.95 |
| 56 | w | 8 | 4SU | C5-C4-S4 | -3.48 | 119.98 | 124.47 |
| 8 | A | 2445 | 2MG | C5-C6-N1 | 3.43 | 120.02 | 113.95 |
| 8 | A | 1962 | 5MC | C5-C6-N1 | -3.43 | 119.81 | 123.34 |
| 56 | w | 37 | MIA | C2-N3-C4 | 3.35 | 119.95 | 115.32 |
| 34 | a | 967 | 5MC | C5-C6-N1 | -3.34 | 119.91 | 123.34 |
| 34 | a | 1407 | 5MC | C5-C6-N1 | -3.27 | 119.98 | 123.34 |
| 34 | a | 527 | G7M | C2-N1-C6 | -3.26 | 119.09 | 125.10 |
| 8 | A | 1939 | 5MU | O2-C2-N1 | -3.25 | 118.47 | 122.79 |
| 56 | w | 55 | PSU | C6-C5-C4 | 3.25 | 120.47 | 118.20 |
| 8 | A | 2552 | OMU | C5-C4-N3 | 3.23 | 119.67 | 114.84 |
| 55 | v | 20 | H2U | N3-C2-N1 | 3.23 | 120.07 | 116.65 |
| 56 | w | 46 | G7M | C2-N1-C6 | -3.21 | 119.18 | 125.10 |
| 57 | y | 101 | FME | CA-N-CN | 3.21 | 127.75 | 122.82 |
| 8 | A | 2503 | 2MA | N3-C2-N1 | -3.19 | 119.90 | 125.73 |
| 8 | A | 1939 | 5MU | C5M-C5-C4 | 3.18 | 122.27 | 118.77 |
| 57 | y | 101 | FME | C-CA-N | 3.11 | 115.35 | 109.73 |
| 8 | A | 2251 | OMG | C2-N1-C6 | -3.07 | 119.44 | 125.10 |
| 8 | A | 2069 | G7M | C2-N1-C6 | -2.99 | 119.59 | 125.10 |
| 34 | a | 1498 | UR3 | C1'-N1-C2 | 2.92 | 121.92 | 116.99 |
| 8 | A | 1917 | PSU | O2-C2-N1 | -2.84 | 119.66 | 122.79 |
| 55 | v | 20 | H2U | C5-C6-N1 | 2.83 | 120.95 | 111.61 |
| 34 | a | 1498 | UR3 | C6-N1-C2 | -2.83 | 119.25 | 121.79 |
| 8 | A | 1939 | 5MU | O4-C4-N3 | -2.77 | 114.81 | 120.12 |
| 8 | A | 2251 | OMG | C8-N7-C5 | 2.75 | 108.23 | 102.99 |
| 8 | A | 745 | 1MG | C8-N7-C5 | 2.72 | 108.17 | 102.99 |
| 8 | A | 2580 | PSU | O2-C2-N1 | -2.72 | 119.80 | 122.79 |
| 8 | A | 2504 | PSU | O2-C2-N1 | -2.70 | 119.81 | 122.79 |
| 8 | A | 955 | PSU | O2-C2-N1 | -2.70 | 119.82 | 122.79 |
| 56 | w | 55 | PSU | C6-N1-C2 | -2.68 | 119.94 | 122.68 |
| 34 | a | 516 | PSU | O2-C2-N1 | -2.68 | 119.84 | 122.79 |
| 55 | v | 20 | H2U | C5-C4-N3 | 2.67 | 119.65 | 116.65 |
| 34 | a | 1516 | 2MG | C8-N7-C5 | 2.66 | 108.06 | 102.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | a | 966 | 2MG | C8-N7-C5 | 2.60 | 107.94 | 102.99 |
| 8 | A | 1835 | 2MG | C8-N7-C5 | 2.60 | 107.93 | 102.99 |
| 34 | a | 1207 | 2MG | C8-N7-C5 | 2.59 | 107.92 | 102.99 |
| 8 | A | 2580 | PSU | O4'-C1'-C2' | 2.57 | 108.78 | 105.14 |
| 8 | A | 2445 | 2MG | C8-N7-C5 | 2.57 | 107.88 | 102.99 |
| 55 | v | 54 | 5MU | O4-C4-N3 | -2.55 | 115.24 | 120.12 |
| 56 | w | 54 | 5MU | O4-C4-N3 | -2.52 | 115.28 | 120.12 |
| 8 | A | 745 | 1MG | O6-C6-C5 | -2.51 | 119.75 | 124.19 |
| 8 | A | 2552 | OMU | O4-C4-C5 | -2.51 | 120.75 | 125.16 |
| 8 | A | 2604 | PSU | O2-C2-N1 | -2.50 | 120.03 | 122.79 |
| 55 | v | 20 | H2U | O2-C2-N1 | -2.47 | 120.00 | 123.11 |
| 8 | A | 1962 | 5MC | CM5-C5-C6 | -2.47 | 119.55 | 122.85 |
| 8 | A | 2457 | PSU | O2-C2-N1 | -2.46 | 120.08 | 122.79 |
| 8 | A | 746 | PSU | O2-C2-N1 | -2.46 | 120.08 | 122.79 |
| 8 | A | 1911 | PSU | O2-C2-N1 | -2.45 | 120.09 | 122.79 |
| 34 | a | 516 | PSU | C6-N1-C2 | -2.42 | 120.21 | 122.68 |
| 56 | w | 37 | MIA | C16-C14-C15 | -2.41 | 109.27 | 114.60 |
| 56 | w | 37 | MIA | S10-C2-N1 | 2.40 | 124.31 | 116.01 |
| 8 | A | 2069 | G7M | O3'-C3'-C2' | 2.39 | 119.57 | 111.82 |
| 34 | a | 966 | 2MG | CM2-N2-C2 | -2.39 | 118.59 | 123.86 |
| 8 | A | 1917 | PSU | C6-N1-C2 | -2.38 | 120.25 | 122.68 |
| 34 | a | 966 | 2MG | O6-C6-C5 | -2.38 | 119.72 | 124.37 |
| 8 | A | 2552 | OMU | C1'-N1-C2 | 2.38 | 121.87 | 117.57 |
| 56 | w | 54 | 5MU | O2-C2-N1 | -2.38 | 119.63 | 122.79 |
| 56 | w | 32 | PSU | O2-C2-N1 | -2.37 | 120.18 | 122.79 |
| 8 | A | 2580 | PSU | C6-C5-C4 | 2.35 | 119.84 | 118.20 |
| 8 | A | 2251 | OMG | O6-C6-C5 | -2.34 | 119.81 | 124.37 |
| 8 | A | 2580 | PSU | C6-N1-C2 | -2.33 | 120.30 | 122.68 |
| 8 | A | 1835 | 2MG | O6-C6-C5 | -2.31 | 119.85 | 124.37 |
| 8 | A | 2445 | 2MG | CM2-N2-C2 | -2.28 | 118.83 | 123.86 |
| 8 | A | 2504 | PSU | C6-N1-C2 | -2.26 | 120.38 | 122.68 |
| 34 | a | 1402 | 4OC | C6-C5-C4 | 2.25 | 119.72 | 116.96 |
| 8 | A | 747 | 5MC | CM5-C5-C6 | -2.25 | 119.85 | 122.85 |
| 34 | a | 1516 | 2MG | O6-C6-C5 | -2.24 | 119.99 | 124.37 |
| 8 | A | 1618 | 6MZ | C1'-N9-C4 | -2.24 | 122.71 | 126.64 |
| 8 | A | 1911 | PSU | C6-N1-C2 | -2.22 | 120.41 | 122.68 |
| 55 | v | 55 | PSU | O2-C2-N1 | -2.21 | 120.36 | 122.79 |
| 8 | A | 955 | PSU | C6-N1-C2 | -2.19 | 120.44 | 122.68 |
| 56 | w | 37 | MIA | C12-N6-C6 | -2.19 | 119.30 | 122.55 |
| 8 | A | 2457 | PSU | C6-C5-C4 | 2.18 | 119.72 | 118.20 |
| 8 | A | 2605 | PSU | O2-C2-N1 | -2.18 | 120.39 | 122.79 |
| 34 | a | 1207 | 2MG | O6-C6-C5 | -2.18 | 120.12 | 124.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 56 | w | 32 | PSU | C6-N1-C2 | -2.17 | 120.47 | 122.68 |
| 34 | a | 1407 | 5MC | CM5-C5-C6 | -2.16 | 119.96 | 122.85 |
| 8 | A | 2445 | 2MG | O6-C6-C5 | -2.16 | 120.16 | 124.37 |
| 8 | A | 1835 | 2MG | CM2-N2-C2 | -2.12 | 119.18 | 123.86 |
| 55 | v | 54 | 5MU | O2-C2-N1 | -2.11 | 119.98 | 122.79 |
| 34 | a | 1516 | 2MG | CM2-N2-C2 | -2.11 | 119.21 | 123.86 |
| 56 | w | 39 | PSU | C6-N1-C2 | -2.10 | 120.53 | 122.68 |
| 55 | v | 55 | PSU | C6-N1-C2 | -2.10 | 120.54 | 122.68 |
| 8 | A | 1939 | 5MU | C6-C5-C4 | 2.06 | 119.75 | 118.03 |
| 34 | a | 516 | PSU | O4'-C1'-C2' | 2.05 | 108.04 | 105.14 |
| 34 | a | 967 | 5MC | CM5-C5-C6 | -2.05 | 120.11 | 122.85 |
| 8 | A | 955 | PSU | C6-C5-C4 | 2.04 | 119.63 | 118.20 |
| 8 | A | 746 | PSU | C6-N1-C2 | -2.03 | 120.61 | 122.68 |
| 8 | A | 2503 | 2MA | C1'-N9-C4 | -2.02 | 123.08 | 126.64 |
| 8 | A | 1917 | PSU | O4'-C1'-C2' | 2.02 | 107.99 | 105.14 |
| 8 | A | 2604 | PSU | C6-N1-C2 | -2.01 | 120.63 | 122.68 |
| 8 | A | 2605 | PSU | C6-C5-C4 | 2.01 | 119.60 | 118.20 |
| 8 | A | 2457 | PSU | O4'-C1'-C2' | 2.01 | 107.97 | 105.14 |

There are no chirality outliers.

All (52) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 55 | v | 20 | H2U | O4'-C4'-C5'-O5' |
| 55 | v | 55 | PSU | O4'-C1'-C5-C4 |
| 55 | v | 55 | PSU | O4'-C1'-C5-C6 |
| 8 | A | 746 | PSU | C2'-C1'-C5-C4 |
| 8 | A | 1915 | 3TD | C2'-C1'-C5-C4 |
| 8 | A | 1915 | 3TD | O4'-C1'-C5-C4 |
| 8 | A | 1915 | 3TD | O4'-C1'-C5-C6 |
| 8 | A | 2251 | OMG | C1'-C2'-O2'-CM2 |
| 8 | A | 2445 | 2MG | C3'-C4'-C5'-O5' |
| 8 | A | 2498 | OMC | O4'-C4'-C5'-O5' |
| 8 | A | 2552 | OMU | O4'-C1'-N1-C2 |
| 8 | A | 2552 | OMU | O4'-C1'-N1-C6 |
| 8 | A | 2552 | OMU | C1'-C2'-O2'-CM2 |
| 34 | a | 1498 | UR3 | O4'-C1'-N1-C2 |
| 56 | w | 32 | PSU | O4'-C1'-C5-C4 |
| 56 | w | 32 | PSU | C2'-C1'-C5-C6 |
| 56 | w | 32 | PSU | O4'-C1'-C5-C6 |
| 56 | w | 37 | MIA | C12-C13-C14-C15 |
| 56 | w | 37 | MIA | C12-C13-C14-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 56 | w | 39 | PSU | C2'-C1'-C5-C4 |
| 56 | w | 39 | PSU | O4'-C1'-C5-C4 |
| 56 | w | 39 | PSU | O4'-C1'-C5-C6 |
| 57 | y | 101 | FME | CB-CA-N-CN |
| 57 | y | 101 | FME | N-CA-CB-CG |
| 57 | y | 101 | FME | C-CA-CB-CG |
| 34 | a | 1498 | UR3 | O4'-C1'-N1-C6 |
| 8 | A | 1939 | 5MU | O4'-C4'-C5'-O5' |
| 8 | A | 2030 | 6MZ | O4'-C4'-C5'-O5' |
| 8 | A | 2030 | 6MZ | C3'-C4'-C5'-O5' |
| 8 | A | 2503 | 2MA | O4'-C4'-C5'-O5' |
| 8 | A | 2503 | 2MA | C3'-C4'-C5'-O5' |
| 8 | A | 2498 | OMC | C3'-C4'-C5'-O5' |
| 8 | A | 2445 | 2MG | O4'-C4'-C5'-O5' |
| 8 | A | 1939 | 5MU | C3'-C4'-C5'-O5' |
| 55 | v | 20 | H2U | C4'-C5'-O5'-P |
| 8 | A | 1835 | 2MG | O4'-C4'-C5'-O5' |
| 8 | A | 2504 | PSU | O4'-C4'-C5'-O5' |
| 34 | a | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 57 | y | 101 | FME | CA-CB-CG-SD |
| 57 | y | 101 | FME | CB-CG-SD-CE |
| 8 | A | 1835 | 2MG | C3'-C4'-C5'-O5' |
| 34 | a | 527 | G7M | C4'-C5'-O5'-P |
| 56 | w | 55 | PSU | O4'-C1'-C5-C4 |
| 8 | A | 746 | PSU | O4'-C1'-C5-C6 |
| 8 | A | 1917 | PSU | C4'-C5'-O5'-P |
| 8 | A | 2504 | PSU | C3'-C4'-C5'-O5' |
| 55 | v | 20 | H2U | C2'-C1'-N1-C6 |
| 8 | A | 1962 | 5MC | C2'-C1'-N1-C6 |
| 8 | A | 2069 | G7M | O4'-C4'-C5'-O5' |
| 34 | a | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 8 | A | 1962 | 5MC | O4'-C1'-N1-C6 |
| 34 | a | 1519 | MA6 | C4'-C5'-O5'-P |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 371 ligands modelled in this entry, 367 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 62 | AM2 | a | 1685 | - | 40,40,40 | 1.67 | 7 (17%) | 53,60,60 | 1.08 | 5 (9%) |
| 62 | AM2 | a | 1689 | - | 40,40,40 | 1.64 | 8 (20%) | 53,60,60 | 1.09 | 4 (7%) |
| 62 | AM2 | a | 1682 | - | 40,40,40 | 1.61 | 9 (22%) | 53,60,60 | 1.05 | 3 (5%) |
| 62 | AM2 | a | 1684 | - | 40,40,40 | 1.62 | 8 (20%) | 53,60,60 | 1.10 | 3 (5%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 62 | AM2 | a | 1685 | - | - | 4/12/84/84 | 0/4/4/4 |
| 62 | AM2 | a | 1689 | - | - | 3/12/84/84 | 0/4/4/4 |
| 62 | AM2 | a | 1682 | - | - | 1/12/84/84 | 0/4/4/4 |
| 62 | AM2 | a | 1684 | - | - | 4/12/84/84 | 0/4/4/4 |

All (32) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 62 | a | 1685 | AM2 | OA4-CA1 | 4.60 | 1.53 | 1.41 |
| 62 | a | 1689 | AM2 | OA4-CA1 | 4.58 | 1.53 | 1.41 |
| 62 | a | 1684 | AM2 | OA4-CA1 | 4.49 | 1.53 | 1.41 |
| 62 | a | 1682 | AM2 | OA4-CA1 | 4.32 | 1.52 | 1.41 |
| 62 | a | 1685 | AM2 | OA4-CA5 | 3.77 | 1.49 | 1.44 |
| 62 | a | 1685 | AM2 | OA5-CA8 | 3.76 | 1.51 | 1.41 |
| 62 | a | 1689 | AM2 | OA4-CA5 | 3.73 | 1.49 | 1.44 |
| 62 | a | 1685 | AM2 | OB1-CB1 | 3.69 | 1.51 | 1.41 |
| 62 | a | 1684 | AM2 | OA4-CA5 | 3.62 | 1.49 | 1.44 |
| 62 | a | 1689 | AM2 | OA5-CA8 | 3.52 | 1.50 | 1.41 |
| 62 | a | 1684 | AM2 | OA5-CA8 | 3.49 | 1.50 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 62 | a | 1689 | AM2 | OB1-CB1 | 3.49 | 1.50 | 1.41 |
| 62 | a | 1684 | AM2 | OB1-CB1 | 3.48 | 1.50 | 1.41 |
| 62 | a | 1682 | AM2 | OB1-CB1 | 3.43 | 1.50 | 1.41 |
| 62 | a | 1685 | AM2 | OA5-CA4 | 3.41 | 1.52 | 1.44 |
| 62 | a | 1682 | AM2 | OA5-CA8 | 3.34 | 1.50 | 1.41 |
| 62 | a | 1682 | AM2 | OA4-CA5 | 3.15 | 1.48 | 1.44 |
| 62 | a | 1689 | AM2 | OA5-CA4 | 3.14 | 1.52 | 1.44 |
| 62 | a | 1684 | AM2 | OA5-CA4 | 3.09 | 1.51 | 1.44 |
| 62 | a | 1682 | AM2 | OA5-CA4 | 2.92 | 1.51 | 1.44 |
| 62 | a | 1682 | AM2 | CB3-CB4 | -2.90 | 1.49 | 1.53 |
| 62 | a | 1684 | AM2 | CB3-CB4 | -2.79 | 1.50 | 1.53 |
| 62 | a | 1685 | AM2 | CB3-CB4 | -2.63 | 1.50 | 1.53 |
| 62 | a | 1689 | AM2 | CB3-CB4 | -2.58 | 1.50 | 1.53 |
| 62 | a | 1682 | AM2 | OA1-CA1 | -2.47 | 1.34 | 1.41 |
| 62 | a | 1684 | AM2 | OA1-CA1 | -2.37 | 1.35 | 1.41 |
| 62 | a | 1682 | AM2 | OA8-CA8 | -2.32 | 1.35 | 1.41 |
| 62 | a | 1689 | AM2 | OA1-CA1 | -2.31 | 1.35 | 1.41 |
| 62 | a | 1685 | AM2 | OA1-CA1 | -2.27 | 1.35 | 1.41 |
| 62 | a | 1689 | AM2 | OA8-CA8 | -2.15 | 1.35 | 1.41 |
| 62 | a | 1682 | AM2 | OA8-CB1 | -2.09 | 1.35 | 1.41 |
| 62 | a | 1684 | AM2 | OA8-CA8 | -2.01 | 1.36 | 1.41 |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 62 | a | 1684 | AM2 | CA9-NA7-CA7 | -3.48 | 109.32 | 114.38 |
| 62 | a | 1682 | AM2 | CA9-NA7-CA7 | -3.46 | 109.35 | 114.38 |
| 62 | a | 1684 | AM2 | CA1-OA1-CC1 | -3.28 | 109.83 | 117.96 |
| 62 | a | 1689 | AM2 | CA9-NA7-CA7 | -3.19 | 109.74 | 114.38 |
| 62 | a | 1689 | AM2 | CA1-OA1-CC1 | -3.08 | 110.35 | 117.96 |
| 62 | a | 1682 | AM2 | CA1-OA1-CC1 | -2.97 | 110.61 | 117.96 |
| 62 | a | 1685 | AM2 | CA1-OA1-CC1 | -2.96 | 110.64 | 117.96 |
| 62 | a | 1685 | AM2 | OA4-CA5-CA4 | 2.76 | 113.07 | 108.88 |
| 62 | a | 1682 | AM2 | CB1-OA8-CA8 | -2.68 | 109.64 | 114.42 |
| 62 | a | 1684 | AM2 | CB1-OA8-CA8 | -2.61 | 109.75 | 114.42 |
| 62 | a | 1685 | AM2 | CB1-OA8-CA8 | -2.55 | 109.86 | 114.42 |
| 62 | a | 1689 | AM2 | CB1-OA8-CA8 | -2.55 | 109.87 | 114.42 |
| 62 | a | 1685 | AM2 | CC5-CC4-CC3 | 2.34 | 113.57 | 110.04 |
| 62 | a | 1685 | AM2 | CC3-CC2-CC1 | 2.29 | 114.92 | 109.68 |
| 62 | a | 1689 | AM2 | OA4-CA5-CA4 | 2.29 | 112.35 | 108.88 |

There are no chirality outliers.

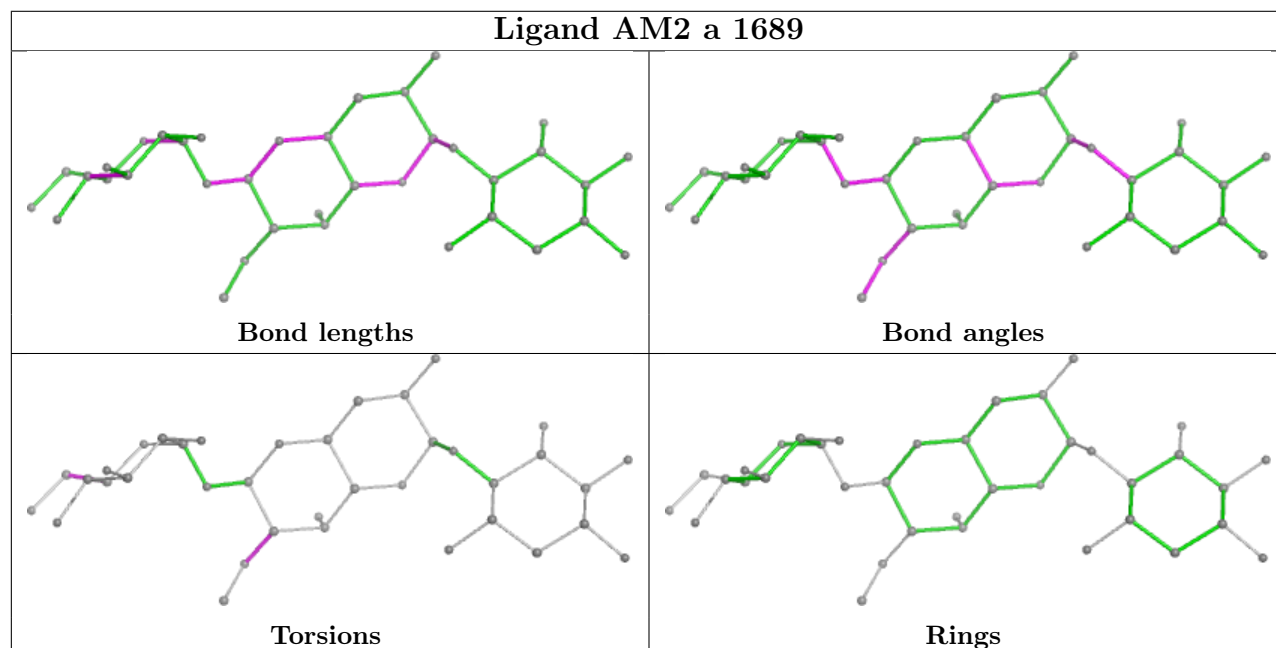
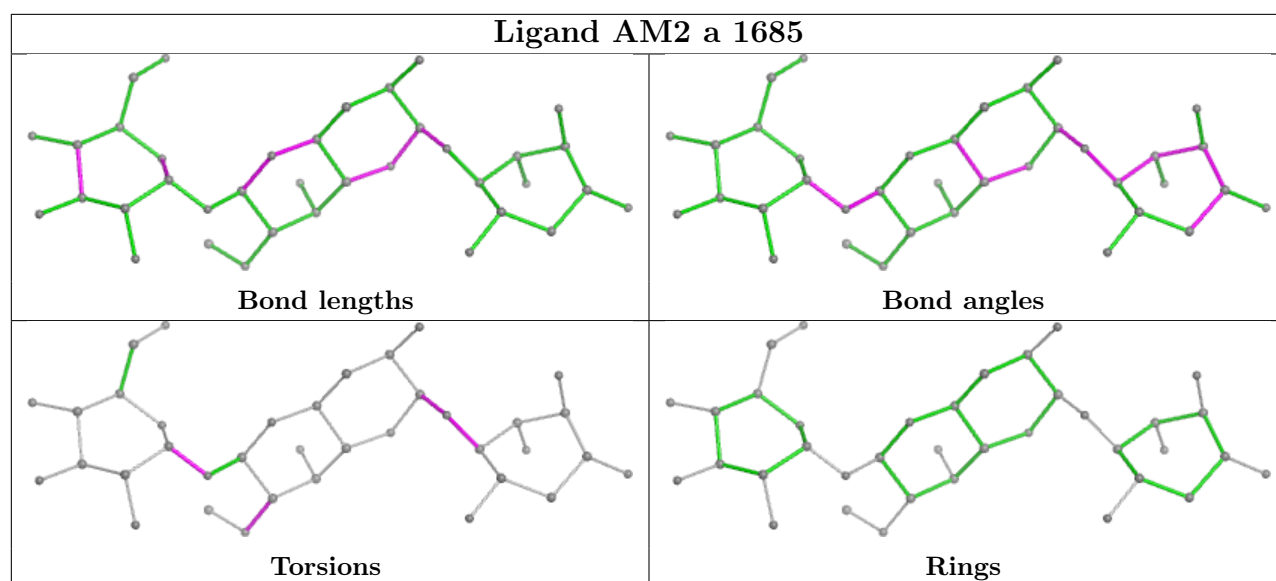
All (12) torsion outliers are listed below:

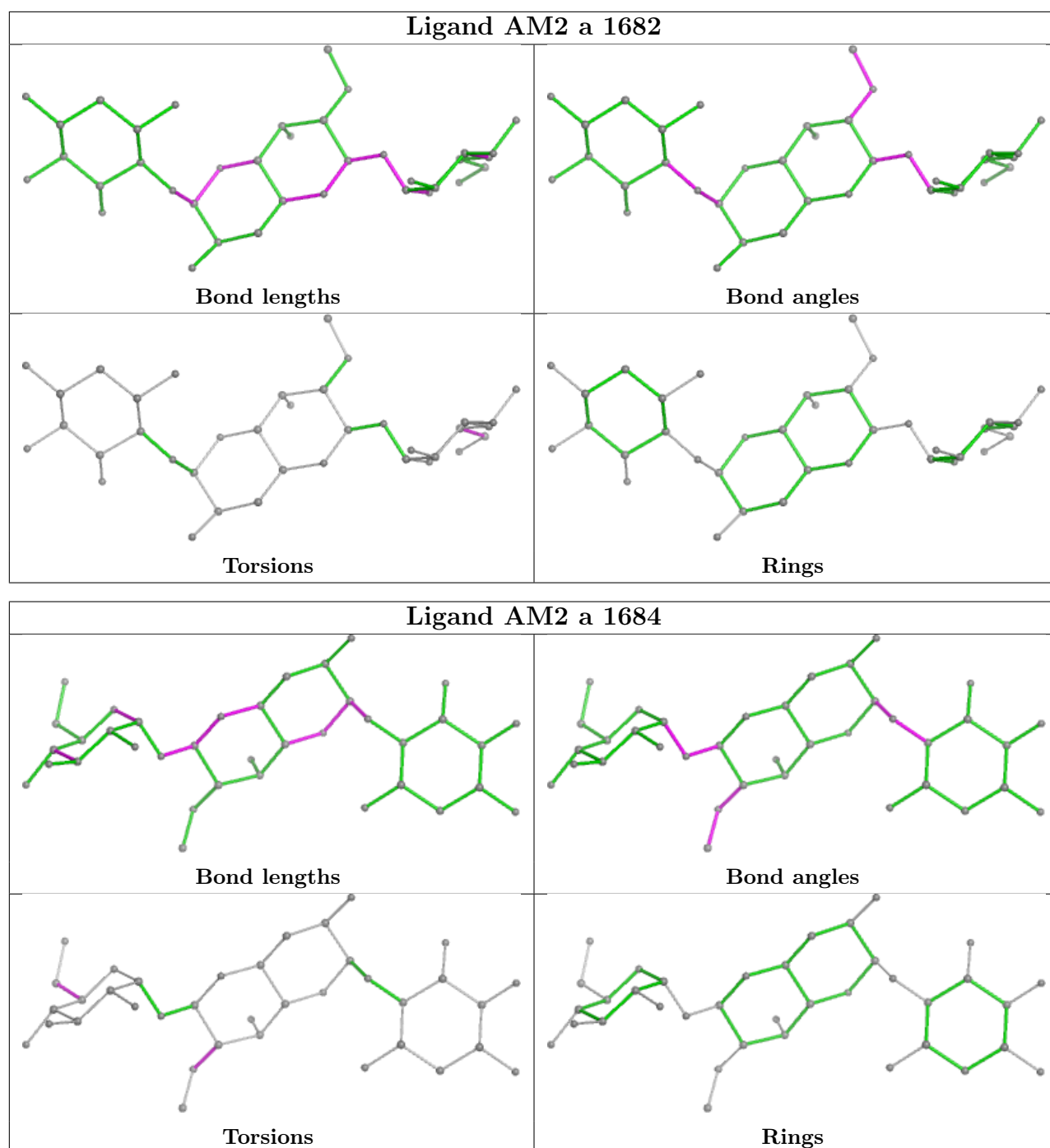
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 62 | a | 1684 | AM2 | CA6-CA7-NA7-CA9 |
| 62 | a | 1684 | AM2 | CA8-CA7-NA7-CA9 |
| 62 | a | 1685 | AM2 | CA8-CA7-NA7-CA9 |
| 62 | a | 1684 | AM2 | OB1-CB5-CB6-OB6 |
| 62 | a | 1684 | AM2 | CB4-CB5-CB6-OB6 |
| 62 | a | 1685 | AM2 | OB1-CB1-OA8-CA8 |
| 62 | a | 1685 | AM2 | CC2-CC1-OA1-CA1 |
| 62 | a | 1689 | AM2 | OB1-CB5-CB6-OB6 |
| 62 | a | 1682 | AM2 | OB1-CB5-CB6-OB6 |
| 62 | a | 1685 | AM2 | OA4-CA1-OA1-CC1 |
| 62 | a | 1689 | AM2 | CA6-CA7-NA7-CA9 |
| 62 | a | 1689 | AM2 | CA8-CA7-NA7-CA9 |

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.