



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Feb 14, 2017 – 02:23 PM EST

PDB ID : 5T6R
EMDB ID: : EMD-8368
Title : Nmd3 is a structural mimic of eIF5A, and activates the cpGTPase Lsg1 during
60S ribosome biogenesis: 60S-Nmd3 Complex
Authors : Malyutin, A.G.; Musalgaonkar, S.; Patchett, S.; Frank, J.; Johnson, A.W.
Deposited on : 2016-09-01
Resolution : 4.50 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

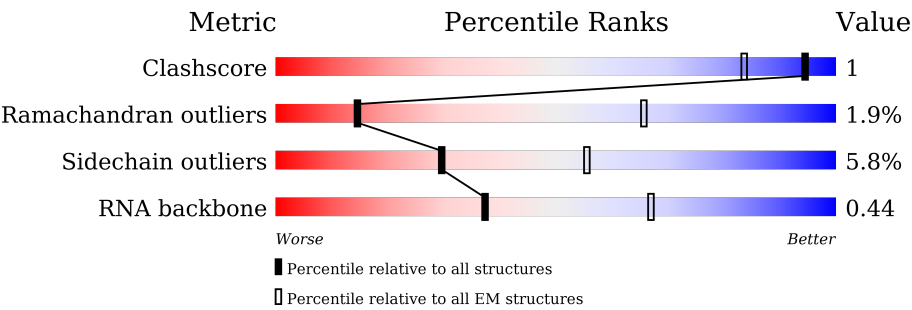
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 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.










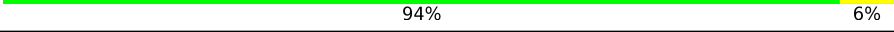
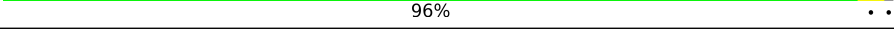
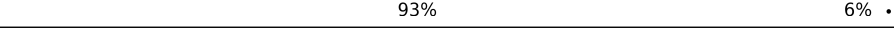
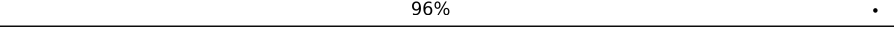
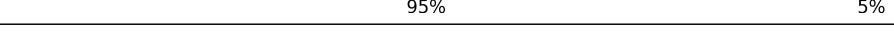
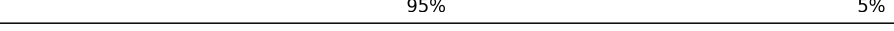


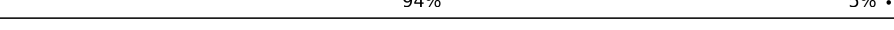


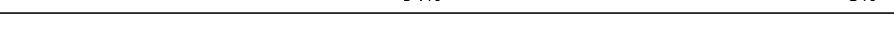
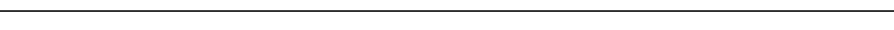

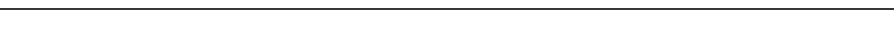
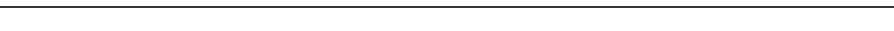


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |
| RNA backbone | 3027 | 244 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 | A | 3396 | <div><div>69%</div><div>23%</div><div>6%</div><div></div></div> |
| 2 | B | 121 | <div><div>81%</div><div>18%</div><div></div><div></div></div> |
| 3 | C | 158 | <div><div>75%</div><div>24%</div><div></div><div></div></div> |
| 4 | D | 254 | <div><div>95%</div><div></div><div></div><div></div></div> |
| 5 | E | 387 | <div><div>94%</div><div>6%</div><div></div><div></div></div> |
| 6 | F | 362 | <div><div>91%</div><div>9%</div><div></div><div></div></div> |
| 7 | G | 297 | <div><div>89%</div><div>10%</div><div></div><div></div></div> |
| 8 | H | 176 | <div><div>84%</div><div>5%</div><div>11%</div><div></div></div> |





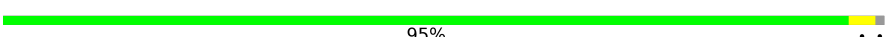

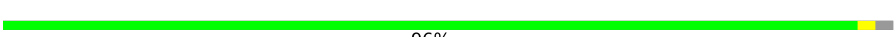



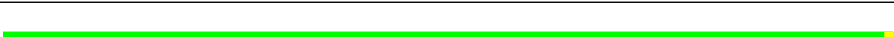

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 9 | I | 244 |  85% 6% 9% |
| 10 | J | 256 |  82% 9% 9% |
| 11 | K | 191 |  91% 8% . |
| 12 | L | 221 |  87% 9% 5% |
| 13 | M | 174 |  87% 9% . . |
| 14 | N | 199 |  88% 9% . |
| 15 | O | 138 |  92% 7% . |
| 16 | a | 204 |  94% 6% |
| 17 | b | 199 |  96% . . |
| 18 | c | 184 |  93% 6% . |
| 19 | d | 186 |  96% . . |
| 20 | e | 189 |  95% 5% . |
| 21 | f | 172 |  95% 5% |
| 22 | g | 160 |  91% 9% . |
| 23 | h | 121 |  80% . 17% |
| 24 | i | 137 |  94% 5% . |
| 25 | j | 155 |  61% . 37% |
| 26 | k | 142 |  79% 6% 15% |
| 27 | l | 127 |  94% 5% . . |
| 28 | m | 136 |  93% 7% . |
| 29 | n | 149 |  92% 7% . . |
| 30 | o | 59 |  88% 8% . . |
| 31 | p | 105 |  90% . 8% |
| 32 | q | 113 |  90% 6% . |
| 33 | r | 130 |  90% 8% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 34 | s | 107 |  46% 53% |
| 35 | t | 121 |  89% 7% |
| 36 | u | 120 |  91% 8% |
| 37 | v | 100 |  91% 8% |
| 38 | w | 88 |  95% |
| 39 | x | 78 |  92% 6% |
| 40 | y | 51 |  96% |
| 41 | z | 128 |  37% 59% |
| 42 | Q | 106 |  88% 11% |
| 43 | R | 92 |  96% |
| 44 | S | 210 |  99% |
| 45 | V | 917 |  19% 6% 73% |

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 126616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1 | A | 3204 | Total | C | N | O | P | 0 | 0 |
| | | | 68535 | 30613 | 12358 | 22360 | 3204 | | |

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 2 | B | 121 | Total | C | N | O | P | 0 | 0 |
| | | | 2579 | 1152 | 461 | 845 | 121 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 3 | C | 158 | Total | C | N | O | P | 0 | 0 |
| | | | 3353 | 1500 | 586 | 1109 | 158 | | |

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | D | 252 | Total | C | N | O | S | 0 | 0 |
| | | | 1914 | 1191 | 388 | 334 | 1 | | |

- Molecule 5 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | E | 386 | Total | C | N | O | S | 0 | 0 |
| | | | 3075 | 1950 | 584 | 533 | 8 | | |

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | F | 361 | Total | C | N | O | S | 0 | 0 |
| | | | 2748 | 1729 | 522 | 494 | 3 | | |

- Molecule 7 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | G | 296 | Total | C | N | O | S | 0 | 0 |
| | | | 2375 | 1501 | 414 | 458 | 2 | | |

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | H | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1239 | 800 | 222 | 216 | 1 | | |

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9 | I | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1784 | 1151 | 324 | 308 | 1 | | |

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10 | J | 233 | Total | C | N | O | S | 0 | 0 |
| | | | 1804 | 1151 | 323 | 327 | 3 | | |

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | K | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1518 | 963 | 274 | 277 | 4 | | |

- Molecule 12 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12 | L | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1705 | 1083 | 322 | 294 | 6 | | |

- Molecule 13 is a protein called 60S ribosomal protein L11-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | M | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1353 | 847 | 253 | 249 | 4 | | |

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 14 | N | 193 | Total | C | N | O | 0 | 0 |
| | | | 1543 | 962 | 315 | 266 | | |

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | O | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 675 | 199 | 177 | 2 | | |

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16 | a | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1720 | 1077 | 361 | 281 | 1 | | |

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17 | b | 197 | Total | C | N | O | S | 0 | 0 |
| | | | 1555 | 1003 | 289 | 262 | 1 | | |

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 18 | c | 183 | Total | C | N | O | 0 | 0 |
| | | | 1420 | 882 | 281 | 257 | | |

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | d | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1441 | 908 | 290 | 241 | 2 | | |

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 20 | e | 188 | Total | C | N | O | 0 | 0 |
| | | | 1521 | 935 | 326 | 260 | | |

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | f | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1445 | 930 | 267 | 244 | 4 | | |

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | g | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1276 | 805 | 246 | 221 | 4 | | |

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | h | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 796 | 516 | 131 | 149 | | | |

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | i | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1003 | 628 | 189 | 179 | 7 | | |

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | j | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 699 | 443 | 137 | 118 | 1 | | |

- Molecule 26 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | k | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 620 | 169 | 173 | 2 | | |

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | l | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 993 | 625 | 192 | 176 | | | |

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 28 | m | 135 | Total | C | N | O | 0 | 0 |
| | | | 1092 | 710 | 202 | 180 | | |

- Molecule 29 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | n | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1173 | 749 | 231 | 190 | 3 | | |

- Molecule 30 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 30 | o | 58 | Total | C | N | O | 0 | 0 |
| | | | 462 | 289 | 100 | 73 | | |

- Molecule 31 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | p | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 743 | 479 | 124 | 139 | 1 | | |

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | q | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 876 | 556 | 167 | 152 | 1 | | |

- Molecule 33 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | r | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1020 | 647 | 205 | 167 | 1 | | |

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 34 | s | 50 | Total | C | N | O | 0 | 0 |
| | | | 406 | 258 | 77 | 71 | | |

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | t | 112 | Total | C | N | O | S | 0 | 0 |
| | | | 880 | 545 | 179 | 152 | 4 | | |

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | u | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 969 | 615 | 186 | 167 | 1 | | |

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | v | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 771 | 481 | 156 | 132 | 2 | | |

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | w | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 681 | 414 | 148 | 114 | 5 | | |

- Molecule 39 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 39 | x | 77 | Total | C | N | O | 0 | 0 |
| | | | 612 | 391 | 115 | 106 | | |

- Molecule 40 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40 | y | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | |

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41 | z | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 417 | 259 | 86 | 67 | 5 | | |

- Molecule 42 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | Q | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | |

- Molecule 43 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | R | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 694 | 429 | 138 | 121 | 6 | | |

- Molecule 44 is a protein called Ribosomal Protein uL1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 44 | S | 210 | Total | C | N | O | | 0 | 0 |
| | | | 1050 | 630 | 210 | 210 | | | |

- Molecule 45 is a protein called Maltose binding protein, 60S ribosomal export protein Nmd3 fusion.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45 | V | 251 | Total | C | N | O | S | 0 | 0 |
| | | | 1975 | 1263 | 333 | 372 | 7 | | |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|----------------|
| V | -396 | ILE | THR | conflict | UNP A0A0F8NYV9 |
| V | -15 | HIS | - | linker | UNP A0A0F8NYV9 |
| V | -14 | HIS | - | linker | UNP A0A0F8NYV9 |
| V | -13 | HIS | - | linker | UNP A0A0F8NYV9 |
| V | -12 | HIS | - | linker | UNP A0A0F8NYV9 |
| V | -11 | HIS | - | linker | UNP A0A0F8NYV9 |
| V | -10 | HIS | - | linker | UNP A0A0F8NYV9 |
| V | -9 | HIS | - | linker | UNP A0A0F8NYV9 |
| V | -8 | HIS | - | linker | UNP A0A0F8NYV9 |
| V | -7 | HIS | - | linker | UNP A0A0F8NYV9 |
| V | -6 | HIS | - | linker | UNP A0A0F8NYV9 |
| V | -5 | GLU | - | linker | UNP A0A0F8NYV9 |
| V | -4 | ASN | - | linker | UNP A0A0F8NYV9 |
| V | -3 | LEU | - | linker | UNP A0A0F8NYV9 |
| V | -2 | TYR | - | linker | UNP A0A0F8NYV9 |
| V | -1 | PHE | - | linker | UNP A0A0F8NYV9 |
| V | 0 | GLN | - | linker | UNP A0A0F8NYV9 |
| V | 1 | GLY | - | linker | UNP A0A0F8NYV9 |

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 46 | A | 84 | Total 84 | Mg 84 | 0 |
| 46 | C | 1 | Total 1 | Mg 1 | 0 |
| 46 | i | 1 | Total 1 | Mg 1 | 0 |

- Molecule 47 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|--------|---------|
| 47 | A | 3 | Total 3 | K 3 | 0 |

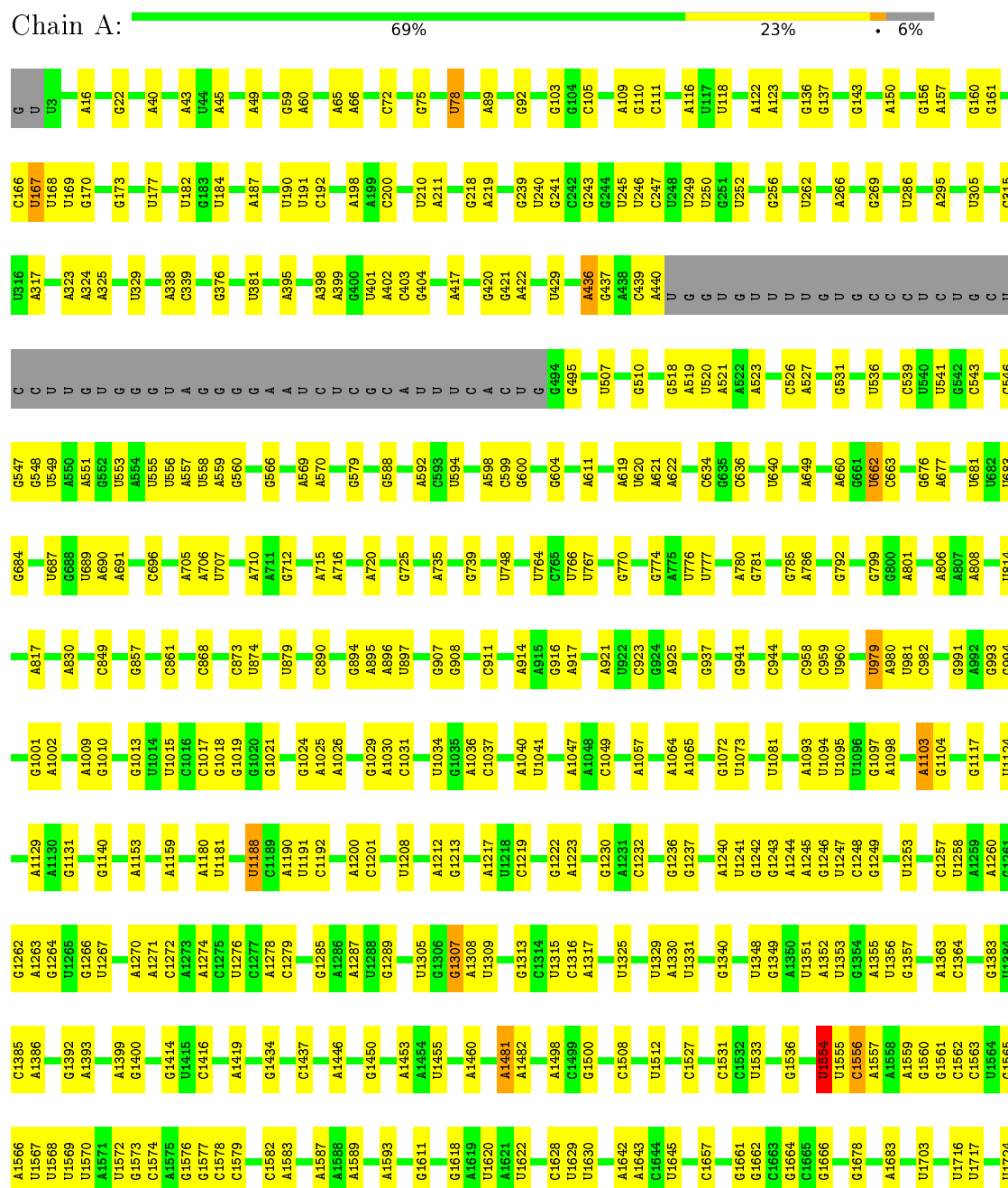
- Molecule 48 is water.

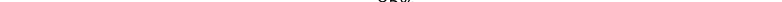
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 48 | A | 10 | Total 10 | O 10 | 0 |
| 48 | c | 1 | Total 1 | O 1 | 0 |
| 48 | e | 1 | Total 1 | O 1 | 0 |

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 25S Ribosomal RNA

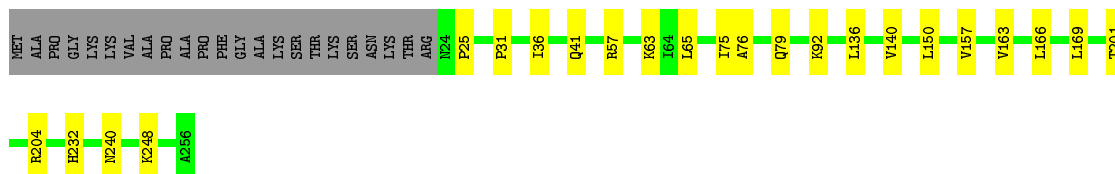


- Chain I:  85% 6% 9%



- Molecule 10: 60S ribosomal protein L8-A

Chain J: 82% 9% 9%



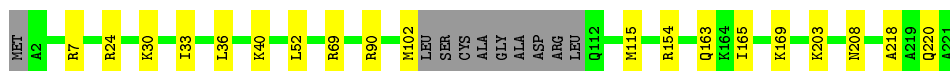
- Molecule 11: 60S ribosomal protein L9-A

Chain K: 91% 8% .



- Molecule 12: 60S ribosomal protein L10

Chain L: 87% 9% 5%



- Molecule 13: 60S ribosomal protein L11-A

Chain M: 87% 9% . .



- Molecule 14: 60S ribosomal protein L13-A

Chain N: 88% 9% .



- Molecule 15: 60S ribosomal protein L14-A

Chain O: 92% 7% .



- Molecule 16: 60S ribosomal protein L15-A

Chain a: 94% 6%



- Molecule 17: 60S ribosomal protein L16-A

Chain b: 96% ..



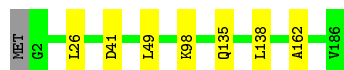
- Molecule 18: 60S ribosomal protein L17-A

Chain c: 93% 6% .



- Molecule 19: 60S ribosomal protein L18-A

Chain d: 96% ..



- Molecule 20: 60S ribosomal protein L19-A

Chain e: 95% 5% .



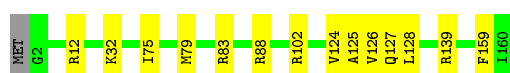
- Molecule 21: 60S ribosomal protein L20-A

Chain f: 95% 5%



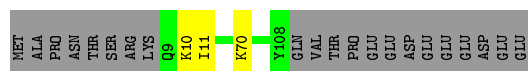
- Molecule 22: 60S ribosomal protein L21-A

Chain g: 91% 9% .



- Molecule 23: 60S ribosomal protein L22-A

Chain h: 80% 17%



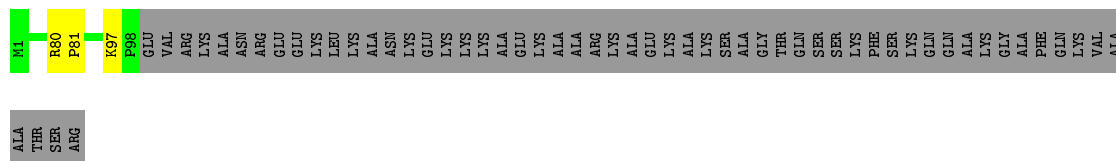
- Molecule 24: 60S ribosomal protein L23-A

Chain i:  94% 5% .




- Molecule 25: 60S ribosomal protein L24-A

Chain j:  61% . 37%



- Molecule 26: 60S ribosomal protein L25

Chain k:  79% 6% 15%



- Molecule 27: 60S ribosomal protein L26-A

Chain l:  94% 5% ..




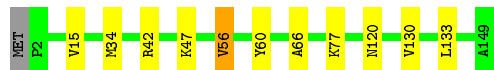
- Molecule 28: 60S ribosomal protein L27-A

Chain m:  93% 7% .




- Molecule 29: 60S ribosomal protein L28

Chain n:  92% 7% ..




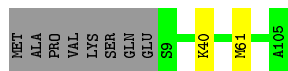
- Molecule 30: 60S ribosomal protein L29

Chain o:  88% 8% . .




- Molecule 31: 60S ribosomal protein L30

Chain p:  90% 8%




- Molecule 32: 60S ribosomal protein L31-A

Chain q:  90% 6%



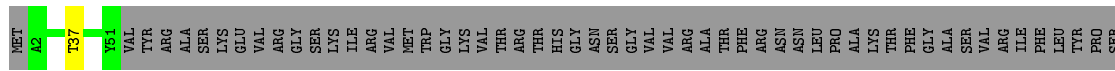
- Molecule 33: 60S ribosomal protein L32

Chain r:  90% 8%




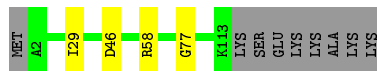
- Molecule 34: 60S ribosomal protein L33-A

Chain s:  46% 53%




- Molecule 35: 60S ribosomal protein L34-A

Chain t:  89% 7%



- Molecule 36: 60S ribosomal protein L35-A

Chain u:  91% 8%



- Molecule 37: 60S ribosomal protein L36-A

Chain v:  91% 8%



- Molecule 38: 60S ribosomal protein L37-A

Chain w:  95% ..



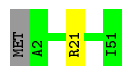
- Molecule 39: 60S ribosomal protein L38

Chain x:  92% 6% .



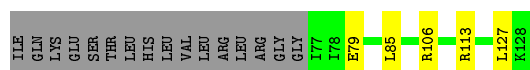
- Molecule 40: 60S ribosomal protein L39

Chain y:  96% ..




- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain z:  37% . 59%



- Molecule 42: 60S ribosomal protein L42-A

Chain Q:  88% 11% .



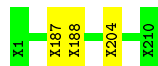
- Molecule 43: 60S ribosomal protein L43-A

Chain R:  96% ..

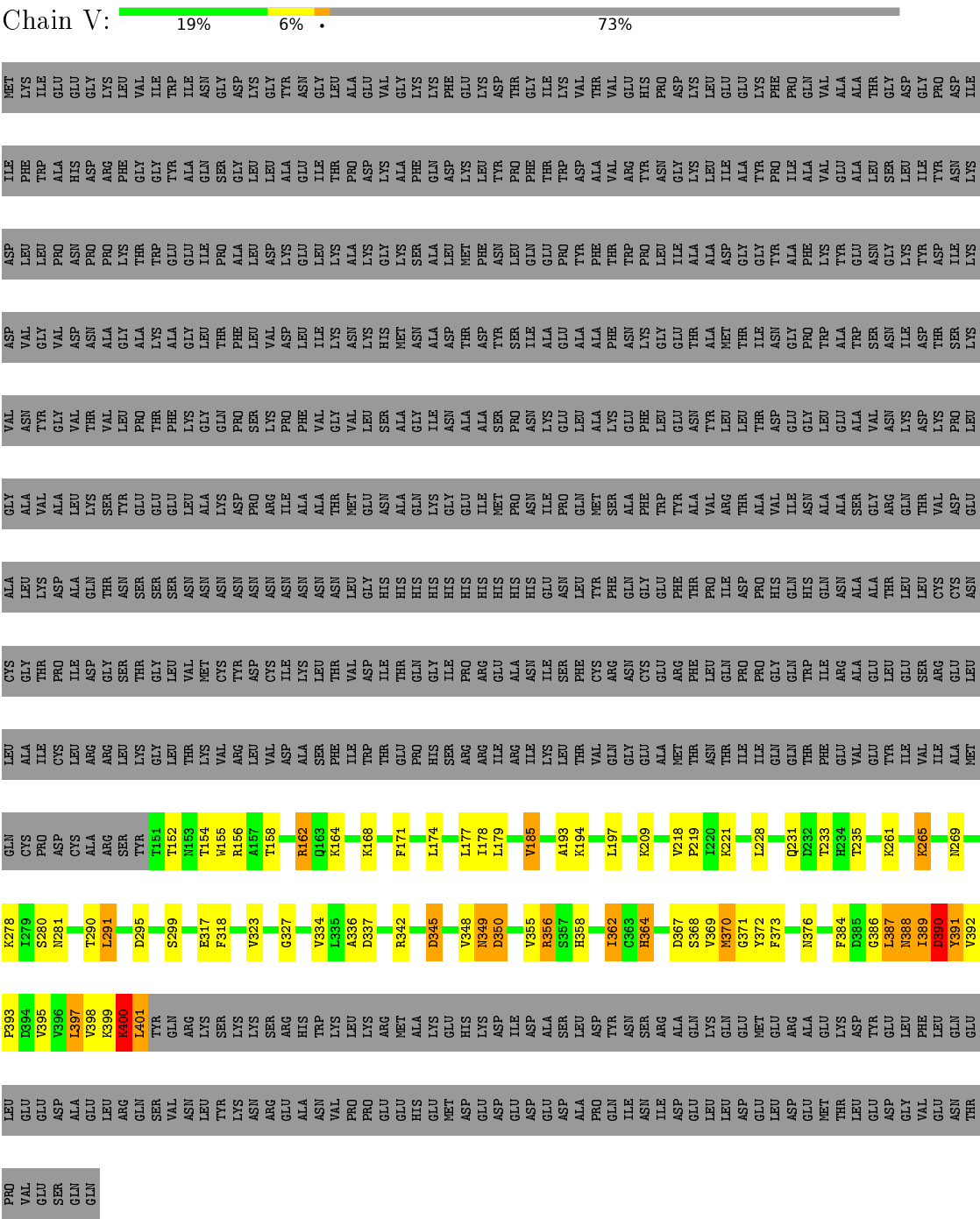


- Molecule 44: Ribosomal Protein uL1

Chain S:  99% .



- Molecule 45: Maltose binding protein, 60S ribosomal export protein Nmd3 fusion



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 65650 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI TECNAI F30 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 31000 | Depositor |
| Image detector | Not provided | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | A | 0.24 | 1/76717 (0.0%) | 0.69 | 8/119611 (0.0%) |
| 10 | J | 0.37 | 0/1836 | 0.54 | 0/2481 |
| 11 | K | 0.36 | 0/1539 | 0.57 | 0/2073 |
| 12 | L | 0.38 | 0/1741 | 0.61 | 0/2335 |
| 13 | M | 0.38 | 0/1374 | 0.64 | 0/1842 |
| 14 | N | 0.39 | 0/1568 | 0.65 | 0/2106 |
| 15 | O | 0.36 | 0/1068 | 0.59 | 0/1438 |
| 16 | a | 0.38 | 0/1757 | 0.68 | 0/2354 |
| 17 | b | 0.37 | 0/1585 | 0.55 | 0/2128 |
| 18 | c | 0.36 | 0/1443 | 0.62 | 0/1944 |
| 19 | d | 0.37 | 0/1465 | 0.65 | 0/1965 |
| 2 | B | 0.24 | 0/2883 | 0.67 | 0/4491 |
| 20 | e | 0.36 | 0/1538 | 0.62 | 0/2050 |
| 21 | f | 0.36 | 0/1481 | 0.59 | 0/1990 |
| 22 | g | 0.36 | 0/1300 | 0.58 | 0/1743 |
| 23 | h | 0.39 | 0/812 | 0.51 | 0/1099 |
| 24 | i | 0.36 | 0/1018 | 0.59 | 0/1369 |
| 25 | j | 0.38 | 0/712 | 0.58 | 0/958 |
| 26 | k | 0.35 | 0/979 | 0.55 | 0/1321 |
| 27 | l | 0.36 | 0/1004 | 0.60 | 0/1341 |
| 28 | m | 0.37 | 0/1118 | 0.54 | 0/1497 |
| 29 | n | 0.35 | 0/1204 | 0.62 | 0/1612 |
| 3 | C | 0.23 | 0/3746 | 0.68 | 1/5832 (0.0%) |
| 30 | o | 0.37 | 0/473 | 0.61 | 0/629 |
| 31 | p | 0.36 | 0/751 | 0.50 | 0/1008 |
| 32 | q | 0.35 | 0/890 | 0.60 | 0/1196 |
| 33 | r | 0.36 | 0/1041 | 0.60 | 0/1394 |
| 34 | s | 0.36 | 0/414 | 0.58 | 0/556 |
| 35 | t | 0.35 | 0/890 | 0.63 | 0/1189 |
| 36 | u | 0.37 | 0/978 | 0.60 | 0/1301 |
| 37 | v | 0.40 | 0/778 | 0.60 | 0/1034 |
| 38 | w | 0.39 | 0/696 | 0.66 | 0/923 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 39 | x | 0.35 | 0/618 | 0.56 | 0/826 |
| 4 | D | 0.35 | 0/1948 | 0.63 | 0/2617 |
| 40 | y | 0.39 | 0/443 | 0.64 | 0/588 |
| 41 | z | 0.38 | 0/423 | 0.61 | 0/562 |
| 42 | Q | 0.37 | 0/860 | 0.60 | 0/1136 |
| 43 | R | 0.37 | 0/701 | 0.65 | 0/934 |
| 45 | V | 0.39 | 0/2015 | 0.75 | 3/2738 (0.1%) |
| 5 | E | 0.36 | 0/3146 | 0.62 | 0/4228 |
| 6 | F | 0.37 | 0/2800 | 0.58 | 0/3790 |
| 7 | G | 0.38 | 0/2425 | 0.60 | 1/3271 (0.0%) |
| 8 | H | 0.37 | 0/1260 | 0.56 | 0/1694 |
| 9 | I | 0.38 | 0/1821 | 0.57 | 0/2451 |
| All | All | 0.30 | 1/135259 (0.0%) | 0.66 | 13/199645 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 30 | o | 0 | 1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1 | A | 2595 | A | C5-C6 | 5.44 | 1.46 | 1.41 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 45 | V | 386 | GLY | C-N-CA | 14.40 | 157.70 | 121.70 |
| 45 | V | 386 | GLY | O-C-N | -13.14 | 101.67 | 122.70 |
| 45 | V | 386 | GLY | CA-C-N | 9.55 | 138.20 | 117.20 |
| 1 | A | 2249 | G | C2'-C3'-O3' | 7.62 | 126.26 | 109.50 |
| 1 | A | 1307 | G | C2'-C3'-O3' | 7.11 | 125.14 | 109.50 |
| 1 | A | 1554 | U | O4'-C1'-N1 | 5.87 | 112.89 | 108.20 |
| 1 | A | 3003 | G | C2'-C3'-O3' | 5.69 | 122.80 | 113.70 |
| 1 | A | 2434 | U | N1-C1'-C2' | 5.55 | 121.22 | 114.00 |
| 1 | A | 78 | U | N3-C4-O4 | -5.33 | 115.67 | 119.40 |
| 3 | C | 82 | U | C2'-C3'-O3' | 5.18 | 122.00 | 113.70 |
| 1 | A | 979 | U | C2'-C3'-O3' | 5.17 | 121.97 | 113.70 |
| 1 | A | 78 | U | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 7 | G | 131 | LEU | CA-CB-CG | 5.03 | 126.87 | 115.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 30 | o | 20 | GLY | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 68535 | 0 | 34437 | 205 | 0 |
| 2 | B | 2579 | 0 | 1304 | 1 | 0 |
| 3 | C | 3353 | 0 | 1695 | 0 | 0 |
| 4 | D | 1914 | 0 | 1981 | 3 | 0 |
| 5 | E | 3075 | 0 | 3142 | 4 | 0 |
| 6 | F | 2748 | 0 | 2859 | 1 | 0 |
| 7 | G | 2375 | 0 | 2325 | 2 | 0 |
| 8 | H | 1239 | 0 | 1326 | 0 | 0 |
| 9 | I | 1784 | 0 | 1862 | 5 | 0 |
| 10 | J | 1804 | 0 | 1877 | 2 | 0 |
| 11 | K | 1518 | 0 | 1587 | 3 | 0 |
| 12 | L | 1705 | 0 | 1736 | 11 | 0 |
| 13 | M | 1353 | 0 | 1383 | 0 | 0 |
| 14 | N | 1543 | 0 | 1608 | 2 | 0 |
| 15 | O | 1053 | 0 | 1149 | 0 | 0 |
| 16 | a | 1720 | 0 | 1779 | 0 | 0 |
| 17 | b | 1555 | 0 | 1659 | 0 | 0 |
| 18 | c | 1420 | 0 | 1437 | 0 | 0 |
| 19 | d | 1441 | 0 | 1543 | 0 | 0 |
| 20 | e | 1521 | 0 | 1617 | 0 | 0 |
| 21 | f | 1445 | 0 | 1487 | 0 | 0 |
| 22 | g | 1276 | 0 | 1323 | 0 | 0 |
| 23 | h | 796 | 0 | 812 | 0 | 0 |
| 24 | i | 1003 | 0 | 1048 | 0 | 0 |
| 25 | j | 699 | 0 | 640 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 26 | k | 964 | 0 | 1025 | 0 | 0 |
| 27 | l | 993 | 0 | 1081 | 0 | 0 |
| 28 | m | 1092 | 0 | 1155 | 0 | 0 |
| 29 | n | 1173 | 0 | 1215 | 0 | 0 |
| 30 | o | 462 | 0 | 491 | 0 | 0 |
| 31 | p | 743 | 0 | 797 | 0 | 0 |
| 32 | q | 876 | 0 | 912 | 0 | 0 |
| 33 | r | 1020 | 0 | 1090 | 0 | 0 |
| 34 | s | 406 | 0 | 416 | 0 | 0 |
| 35 | t | 880 | 0 | 945 | 0 | 0 |
| 36 | u | 969 | 0 | 1078 | 0 | 0 |
| 37 | v | 771 | 0 | 849 | 0 | 0 |
| 38 | w | 681 | 0 | 687 | 0 | 0 |
| 39 | x | 612 | 0 | 682 | 0 | 0 |
| 40 | y | 436 | 0 | 475 | 0 | 0 |
| 41 | z | 417 | 0 | 459 | 0 | 0 |
| 42 | Q | 847 | 0 | 918 | 0 | 0 |
| 43 | R | 694 | 0 | 738 | 0 | 0 |
| 44 | S | 1050 | 0 | 247 | 2 | 0 |
| 45 | V | 1975 | 0 | 1984 | 70 | 0 |
| 46 | A | 84 | 0 | 0 | 0 | 0 |
| 46 | C | 1 | 0 | 0 | 0 | 0 |
| 46 | i | 1 | 0 | 0 | 0 | 0 |
| 47 | A | 3 | 0 | 0 | 0 | 0 |
| 48 | A | 10 | 0 | 0 | 2 | 0 |
| 48 | c | 1 | 0 | 0 | 0 | 0 |
| 48 | e | 1 | 0 | 0 | 0 | 0 |
| All | All | 126616 | 0 | 90860 | 286 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (286) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:2434:U:O4 | 1:A:2595:A:N1 | 1.60 | 1.33 |
| 12:L:102:MET:CG | 45:V:152:THR:HA | 1.58 | 1.32 |
| 12:L:102:MET:HG3 | 45:V:152:THR:CA | 1.63 | 1.28 |
| 45:V:388:ASN:O | 45:V:390:ASP:N | 1.73 | 1.21 |
| 1:A:2410:U:O4 | 1:A:2801:A:N1 | 1.87 | 1.06 |
| 1:A:2461:A:C4 | 1:A:2485:A:C2 | 2.45 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2490:C:C2 | 1:A:2491:A:N6 | 2.28 | 1.02 |
| 1:A:1453:A:H61 | 1:A:1840:U:H3 | 1.07 | 1.02 |
| 1:A:2469:G:C6 | 1:A:2470:C:N4 | 2.32 | 0.97 |
| 1:A:2449:A:N1 | 1:A:2498:U:O2 | 1.97 | 0.97 |
| 1:A:2482:U:O4 | 1:A:2486:A:N6 | 1.98 | 0.96 |
| 1:A:2434:U:O4 | 1:A:2595:A:C2 | 2.19 | 0.95 |
| 1:A:2440:G:N2 | 1:A:2508:U:O2 | 2.00 | 0.95 |
| 1:A:78:U:H3 | 1:A:325:A:H61 | 1.08 | 0.95 |
| 1:A:2463:G:N2 | 1:A:2493:U:N3 | 2.15 | 0.95 |
| 1:A:2448:G:O6 | 1:A:2498:U:C2 | 2.20 | 0.94 |
| 1:A:2490:C:O2 | 1:A:2491:A:N7 | 2.01 | 0.94 |
| 1:A:2922:G:O6 | 45:V:235:THR:OG1 | 1.85 | 0.94 |
| 1:A:2636:A:H61 | 1:A:2641:U:H3 | 1.05 | 0.94 |
| 1:A:2448:G:C2 | 1:A:2499:U:O2 | 2.21 | 0.93 |
| 1:A:1190:A:H61 | 1:A:1315:U:H3 | 1.15 | 0.93 |
| 45:V:389:ILE:HG22 | 45:V:389:ILE:O | 1.67 | 0.92 |
| 1:A:2461:A:C5 | 1:A:2485:A:C2 | 2.58 | 0.92 |
| 1:A:2448:G:O6 | 1:A:2498:U:O2 | 1.91 | 0.89 |
| 45:V:337:ASP:OD2 | 45:V:356:ARG:HG3 | 1.70 | 0.89 |
| 1:A:3077:A:N6 | 48:A:3501:HOH:O | 2.04 | 0.89 |
| 1:A:1554:U:H3 | 1:A:1559:A:H61 | 1.14 | 0.89 |
| 12:L:102:MET:HG3 | 45:V:152:THR:HA | 0.87 | 0.87 |
| 1:A:2450:G:N1 | 1:A:2497:U:N3 | 2.21 | 0.87 |
| 1:A:2450:G:H1 | 1:A:2497:U:H3 | 1.23 | 0.85 |
| 1:A:2658:G:N2 | 1:A:2713:U:O2 | 2.08 | 0.85 |
| 1:A:2507:C:H6 | 1:A:2507:C:H5'' | 1.43 | 0.83 |
| 1:A:2463:G:N2 | 1:A:2493:U:C4 | 2.47 | 0.82 |
| 1:A:2636:A:N6 | 1:A:2641:U:H3 | 1.79 | 0.80 |
| 12:L:102:MET:CB | 45:V:152:THR:HA | 2.10 | 0.80 |
| 45:V:367:ASP:CG | 45:V:400:LYS:NZ | 2.35 | 0.79 |
| 1:A:2449:A:C2 | 1:A:2498:U:O2 | 2.36 | 0.79 |
| 1:A:2636:A:N1 | 1:A:2641:U:O4 | 2.16 | 0.79 |
| 45:V:367:ASP:CG | 45:V:400:LYS:HZ2 | 1.85 | 0.78 |
| 45:V:372:TYR:CE1 | 45:V:398:VAL:HG21 | 2.20 | 0.77 |
| 1:A:78:U:O4 | 1:A:324:A:N1 | 2.18 | 0.77 |
| 45:V:372:TYR:CE1 | 45:V:398:VAL:CG2 | 2.68 | 0.77 |
| 1:A:2445:A:N3 | 1:A:2502:A:C2 | 2.53 | 0.77 |
| 1:A:2469:G:C5 | 1:A:2470:C:N4 | 2.52 | 0.77 |
| 1:A:1554:U:H3 | 1:A:1559:A:N6 | 1.82 | 0.76 |
| 1:A:2876:C:H4' | 45:V:233:THR:HB | 1.67 | 0.76 |
| 1:A:1190:A:N1 | 1:A:1315:U:O4 | 2.19 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1453:A:N6 | 1:A:1840:U:H3 | 1.84 | 0.75 |
| 1:A:2448:G:N1 | 1:A:2499:U:C2 | 2.54 | 0.75 |
| 1:A:2449:A:C6 | 1:A:2498:U:O2 | 2.39 | 0.75 |
| 1:A:2469:G:N1 | 1:A:2470:C:N4 | 2.33 | 0.75 |
| 1:A:2249:G:C8 | 1:A:2272:G:C8 | 2.74 | 0.75 |
| 1:A:2437:G:C6 | 1:A:2438:A:C6 | 2.73 | 0.75 |
| 1:A:1481:A:O2' | 1:A:1858:A:H1' | 1.87 | 0.75 |
| 45:V:367:ASP:OD2 | 45:V:400:LYS:NZ | 2.19 | 0.75 |
| 1:A:2439:A:C2 | 1:A:2440:G:C5 | 2.75 | 0.74 |
| 1:A:2451:G:H21 | 1:A:2495:C:N4 | 1.85 | 0.74 |
| 1:A:2463:G:N2 | 1:A:2493:U:H3 | 1.83 | 0.74 |
| 1:A:2493:U:C4 | 1:A:2494:A:C4 | 2.75 | 0.74 |
| 1:A:1188:U:O4 | 1:A:1317:A:N1 | 2.21 | 0.74 |
| 1:A:2410:U:O4 | 1:A:2801:A:C2 | 2.40 | 0.74 |
| 1:A:2490:C:H1' | 1:A:2491:A:N7 | 2.03 | 0.74 |
| 1:A:78:U:H3 | 1:A:325:A:N6 | 1.84 | 0.74 |
| 1:A:2488:A:OP2 | 1:A:2490:C:N4 | 2.21 | 0.73 |
| 1:A:2253:G:O6 | 1:A:2263:C:N4 | 2.22 | 0.73 |
| 1:A:3064:U:O4 | 48:A:3501:HOH:O | 2.07 | 0.73 |
| 1:A:2463:G:C2 | 1:A:2493:U:O4 | 2.43 | 0.72 |
| 45:V:368:SER:O | 45:V:401:LEU:C | 2.28 | 0.71 |
| 45:V:372:TYR:HE1 | 45:V:398:VAL:CG2 | 2.03 | 0.71 |
| 1:A:1190:A:N6 | 1:A:1315:U:H3 | 1.86 | 0.71 |
| 1:A:1453:A:N1 | 1:A:1840:U:O4 | 2.25 | 0.70 |
| 1:A:2461:A:C5 | 1:A:2485:A:N1 | 2.60 | 0.69 |
| 1:A:2410:U:H3 | 1:A:2801:A:H61 | 1.39 | 0.69 |
| 1:A:2470:C:H1' | 1:A:2489:C:O4' | 1.92 | 0.68 |
| 1:A:2482:U:C4 | 1:A:2486:A:N6 | 2.59 | 0.68 |
| 45:V:323:VAL:HG13 | 45:V:336:ALA:HB1 | 1.76 | 0.68 |
| 1:A:2447:A:N1 | 1:A:2499:U:O4 | 2.27 | 0.68 |
| 1:A:2447:A:C2 | 1:A:2500:A:C2 | 2.82 | 0.68 |
| 1:A:2469:G:C2 | 1:A:2470:C:N4 | 2.62 | 0.67 |
| 1:A:2440:G:C2 | 1:A:2508:U:O2 | 2.47 | 0.66 |
| 1:A:78:U:O4 | 1:A:325:A:N1 | 2.28 | 0.66 |
| 1:A:2450:G:N2 | 1:A:2497:U:C2 | 2.62 | 0.66 |
| 45:V:261:LYS:O | 45:V:265:LYS:HG3 | 1.96 | 0.66 |
| 45:V:401:LEU:HD13 | 45:V:401:LEU:O | 1.96 | 0.66 |
| 1:A:2624:G:OP1 | 45:V:162:ARG:HD3 | 1.96 | 0.66 |
| 45:V:389:ILE:CG2 | 45:V:389:ILE:O | 2.40 | 0.66 |
| 45:V:350:ASP:OD2 | 45:V:350:ASP:N | 2.27 | 0.65 |
| 45:V:401:LEU:HD22 | 45:V:401:LEU:O | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2490:C:N3 | 1:A:2491:A:N6 | 2.42 | 0.65 |
| 45:V:231:GLN:O | 45:V:231:GLN:HG3 | 1.97 | 0.64 |
| 12:L:102:MET:HG3 | 45:V:152:THR:N | 2.12 | 0.64 |
| 1:A:2437:G:C6 | 1:A:2438:A:C5 | 2.86 | 0.64 |
| 1:A:2448:G:N1 | 1:A:2499:U:O2 | 2.30 | 0.63 |
| 1:A:2249:G:N7 | 1:A:2272:G:C4 | 2.67 | 0.63 |
| 1:A:2469:G:H2' | 1:A:2470:C:C6 | 2.35 | 0.62 |
| 45:V:373:PHE:HD1 | 45:V:395:VAL:HG22 | 1.64 | 0.62 |
| 45:V:342:ARG:HB2 | 45:V:345:ASP:HB2 | 1.80 | 0.62 |
| 45:V:369:VAL:HG12 | 45:V:400:LYS:HA | 1.81 | 0.62 |
| 5:E:67:PHE:CE1 | 9:I:88:ARG:HB2 | 111.24 | 0.62 |
| 1:A:2493:U:C5 | 1:A:2494:A:C8 | 2.89 | 0.61 |
| 45:V:362:ILE:HG13 | 45:V:362:ILE:O | 2.00 | 0.61 |
| 45:V:392:VAL:HG13 | 45:V:393:PRO:HD2 | 1.82 | 0.61 |
| 1:A:2452:G:N2 | 1:A:2462:A:C8 | 2.68 | 0.60 |
| 45:V:348:VAL:O | 45:V:349:ASN:CB | 2.49 | 0.60 |
| 1:A:2469:G:H2' | 1:A:2470:C:C5 | 2.36 | 0.60 |
| 1:A:2445:A:C2 | 1:A:2502:A:N1 | 2.69 | 0.60 |
| 1:A:2463:G:N2 | 1:A:2464:U:C2 | 2.70 | 0.60 |
| 1:A:2461:A:C4 | 1:A:2485:A:H2 | 2.17 | 0.59 |
| 1:A:640:U:OP1 | 14:N:21:ARG:NH2 | 43.38 | 0.59 |
| 1:A:2439:A:C2 | 1:A:2440:G:C4 | 2.91 | 0.59 |
| 1:A:2656:A:N1 | 1:A:2713:U:O4 | 2.36 | 0.59 |
| 1:A:2450:G:N1 | 1:A:2497:U:C4 | 2.70 | 0.59 |
| 1:A:78:U:H3 | 1:A:324:A:N6 | 2.01 | 0.59 |
| 1:A:2449:A:N1 | 1:A:2498:U:C2 | 2.71 | 0.59 |
| 45:V:387:LEU:HD13 | 45:V:392:VAL:HG22 | 1.85 | 0.59 |
| 1:A:167:U:O2 | 1:A:256:G:N2 | 2.36 | 0.58 |
| 45:V:291:LEU:HD11 | 45:V:358:HIS:CB | 2.34 | 0.58 |
| 1:A:2492:C:H2' | 1:A:2493:U:C5 | 2.38 | 0.58 |
| 1:A:324:A:C6 | 1:A:325:A:N6 | 2.72 | 0.58 |
| 1:A:2445:A:C4 | 1:A:2502:A:N1 | 2.72 | 0.58 |
| 1:A:2451:G:N2 | 1:A:2495:C:N4 | 2.50 | 0.58 |
| 45:V:392:VAL:CG1 | 45:V:393:PRO:HD2 | 2.34 | 0.57 |
| 1:A:1661:G:H2' | 1:A:1662:G:C8 | 2.39 | 0.57 |
| 1:A:2507:C:H6 | 1:A:2507:C:C5' | 2.13 | 0.57 |
| 1:A:2445:A:C2 | 1:A:2502:A:C2 | 2.92 | 0.57 |
| 1:A:2253:G:C2 | 1:A:2264:U:C2 | 2.93 | 0.56 |
| 1:A:2482:U:H3 | 1:A:2486:A:H61 | 1.52 | 0.56 |
| 1:A:2446:U:H2' | 1:A:2447:A:C8 | 2.40 | 0.56 |
| 1:A:2448:G:C6 | 1:A:2499:U:C2 | 2.94 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2437:G:C5 | 1:A:2438:A:C5 | 2.94 | 0.56 |
| 1:A:2448:G:N2 | 1:A:2499:U:O2 | 2.39 | 0.56 |
| 1:A:103:G:OP1 | 14:N:70:ARG:NH2 | 2.39 | 0.56 |
| 45:V:162:ARG:NH2 | 45:V:193:ALA:HB3 | 2.21 | 0.55 |
| 1:A:2437:G:O6 | 1:A:2438:A:C6 | 2.59 | 0.55 |
| 1:A:2445:A:N3 | 1:A:2502:A:N1 | 2.55 | 0.55 |
| 1:A:2457:G:N2 | 1:A:2486:A:C2 | 2.74 | 0.55 |
| 45:V:318:PHE:CE2 | 45:V:342:ARG:HG2 | 2.41 | 0.55 |
| 45:V:388:ASN:HB3 | 45:V:391:TYR:HB2 | 1.88 | 0.55 |
| 1:A:2490:C:O2 | 1:A:2491:A:C5 | 2.59 | 0.54 |
| 1:A:324:A:N6 | 1:A:325:A:N6 | 2.55 | 0.54 |
| 45:V:372:TYR:HE1 | 45:V:398:VAL:HG21 | 1.62 | 0.54 |
| 1:A:1820:U:O2 | 1:A:1820:U:O4' | 2.25 | 0.54 |
| 1:A:2469:G:C4 | 1:A:2470:C:N4 | 2.75 | 0.54 |
| 1:A:2499:U:C4 | 1:A:2500:A:C5 | 2.96 | 0.54 |
| 1:A:2469:G:C2 | 1:A:2470:C:C4 | 2.96 | 0.54 |
| 1:A:662:U:H2' | 1:A:663:C:C6 | 2.43 | 0.54 |
| 1:A:2249:G:H2' | 1:A:2250:G:H8 | 1.73 | 0.53 |
| 1:A:160:G:N2 | 1:A:262:U:O2 | 2.41 | 0.53 |
| 1:A:2271:A:N7 | 1:A:2272:G:C6 | 2.76 | 0.53 |
| 1:A:78:U:N3 | 1:A:324:A:N6 | 2.57 | 0.53 |
| 12:L:102:MET:CG | 45:V:152:THR:CA | 2.43 | 0.53 |
| 1:A:1556:C:O4' | 1:A:1556:C:O2 | 2.25 | 0.53 |
| 1:A:2493:U:H3' | 1:A:2494:A:O4' | 2.09 | 0.53 |
| 45:V:261:LYS:NZ | 45:V:265:LYS:HD3 | 2.23 | 0.53 |
| 45:V:401:LEU:HD22 | 45:V:401:LEU:C | 2.29 | 0.53 |
| 1:A:2499:U:O4 | 1:A:2500:A:C6 | 2.62 | 0.53 |
| 1:A:2507:C:C6 | 1:A:2507:C:H5'' | 2.34 | 0.53 |
| 2:B:121:U:O4' | 2:B:121:U:O2 | 2.27 | 0.53 |
| 45:V:348:VAL:O | 45:V:349:ASN:HB3 | 2.09 | 0.53 |
| 1:A:2456:A:H2' | 1:A:2457:G:O4' | 2.09 | 0.53 |
| 1:A:2445:A:C2 | 1:A:2502:A:C6 | 2.97 | 0.53 |
| 1:A:3217:C:O2 | 1:A:3217:C:C2' | 2.57 | 0.52 |
| 1:A:2449:A:C6 | 1:A:2498:U:C2 | 2.98 | 0.52 |
| 1:A:2490:C:C1' | 1:A:2491:A:N7 | 2.72 | 0.52 |
| 1:A:2410:U:C4 | 1:A:2801:A:N1 | 2.72 | 0.52 |
| 1:A:2470:C:C4 | 1:A:2471:U:O4 | 2.62 | 0.52 |
| 1:A:3153:U:O2 | 1:A:3153:U:O4' | 2.28 | 0.52 |
| 1:A:2438:A:H2' | 1:A:2439:A:H8 | 1.76 | 0.51 |
| 12:L:102:MET:HB2 | 45:V:152:THR:HA | 1.91 | 0.51 |
| 1:A:2624:G:OP1 | 45:V:162:ARG:CD | 2.58 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2507:C:C6 | 1:A:2507:C:C5' | 2.93 | 0.50 |
| 1:A:2438:A:H2' | 1:A:2439:A:C8 | 2.47 | 0.50 |
| 1:A:2440:G:N2 | 1:A:2508:U:C2 | 2.78 | 0.50 |
| 1:A:1573:G:H2' | 1:A:1573:G:N3 | 2.27 | 0.50 |
| 11:K:22:SER:OG | 11:K:23:ARG:N | 2.42 | 0.50 |
| 1:A:2463:G:C2 | 1:A:2493:U:C4 | 2.97 | 0.50 |
| 5:E:67:PHE:CE2 | 9:I:88:ARG:HD3 | 108.85 | 0.50 |
| 1:A:2470:C:O4' | 1:A:2489:C:H1' | 2.12 | 0.50 |
| 1:A:3354:U:O2 | 1:A:3354:U:O4' | 2.29 | 0.50 |
| 5:E:67:PHE:CD2 | 9:I:88:ARG:HD3 | 108.41 | 0.50 |
| 1:A:2481:G:H2' | 1:A:2482:U:C4 | 2.48 | 0.49 |
| 1:A:2270:A:N6 | 1:A:2271:A:C6 | 2.81 | 0.49 |
| 1:A:2481:G:H2' | 1:A:2482:U:C5 | 2.48 | 0.49 |
| 7:G:148:ILE:HG13 | 7:G:159:VAL:HG11 | 1.95 | 0.49 |
| 1:A:2505:U:H1' | 1:A:2506:U:N3 | 2.28 | 0.48 |
| 1:A:2463:G:N2 | 1:A:2493:U:O4 | 2.45 | 0.48 |
| 1:A:324:A:C6 | 1:A:325:A:C6 | 3.02 | 0.48 |
| 12:L:102:MET:O | 45:V:154:THR:CG2 | 2.62 | 0.48 |
| 45:V:355:VAL:HG21 | 45:V:395:VAL:O | 2.12 | 0.48 |
| 1:A:2448:G:C6 | 1:A:2499:U:N3 | 2.82 | 0.48 |
| 1:A:2461:A:N9 | 1:A:2485:A:H2 | 2.11 | 0.48 |
| 1:A:2469:G:C4 | 1:A:2470:C:C5 | 3.02 | 0.47 |
| 1:A:2267:C:H2' | 1:A:2268:U:C6 | 2.49 | 0.47 |
| 1:A:2505:U:H1' | 1:A:2506:U:H3 | 1.79 | 0.47 |
| 1:A:2506:U:C3' | 1:A:2506:U:C6 | 2.97 | 0.47 |
| 1:A:2439:A:N1 | 1:A:2440:G:C6 | 2.82 | 0.47 |
| 7:G:30:TYR:HB3 | 7:G:38:THR:HG22 | 10.94 | 0.47 |
| 5:E:67:PHE:CZ | 9:I:88:ARG:HB2 | 111.02 | 0.47 |
| 45:V:174:LEU:O | 45:V:178:ILE:HG22 | 2.15 | 0.47 |
| 1:A:2249:G:C4 | 1:A:2250:G:C8 | 3.03 | 0.47 |
| 12:L:102:MET:C | 45:V:154:THR:HG23 | 2.36 | 0.46 |
| 45:V:218:VAL:HG22 | 45:V:219:PRO:HD2 | 1.96 | 0.46 |
| 45:V:387:LEU:HD13 | 45:V:392:VAL:CG2 | 2.46 | 0.46 |
| 1:A:2493:U:C4 | 1:A:2494:A:C5 | 3.03 | 0.46 |
| 1:A:3018:C:H2' | 1:A:3019:U:C6 | 2.50 | 0.46 |
| 45:V:399:LYS:O | 45:V:400:LYS:O | 2.33 | 0.46 |
| 44:S:187:UNK:O | 44:S:188:UNK:CB | 2.63 | 0.46 |
| 1:A:2476:C:H2' | 1:A:2477:G:H4' | 1.98 | 0.45 |
| 1:A:1103:A:N6 | 1:A:1363:A:O2' | 2.49 | 0.45 |
| 1:A:2467:G:H8 | 1:A:2467:G:O5' | 1.99 | 0.45 |
| 1:A:2253:G:N1 | 1:A:2264:U:C4 | 2.84 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:V:162:ARG:HH22 | 45:V:193:ALA:HB3 | 1.82 | 0.45 |
| 1:A:2506:U:H3' | 1:A:2507:C:H5'' | 1.98 | 0.45 |
| 45:V:323:VAL:CG1 | 45:V:336:ALA:HB1 | 2.46 | 0.45 |
| 1:A:2236:G:O2' | 45:V:269:ASN:HB2 | 2.17 | 0.45 |
| 1:A:2437:G:H2' | 1:A:2438:A:C8 | 2.52 | 0.45 |
| 45:V:364:HIS:CB | 45:V:367:ASP:OD2 | 2.64 | 0.45 |
| 1:A:2249:G:C5 | 1:A:2250:G:N7 | 2.85 | 0.44 |
| 1:A:2689:A:N3 | 1:A:2689:A:H2' | 2.32 | 0.44 |
| 45:V:280:SER:OG | 45:V:281:ASN:N | 2.49 | 0.44 |
| 1:A:2253:G:C6 | 1:A:2264:U:C4 | 3.05 | 0.44 |
| 1:A:2493:U:O4 | 1:A:2494:A:C5 | 2.70 | 0.44 |
| 11:K:41:ILE:HD11 | 11:K:67:ALA:HB1 | 1.99 | 0.44 |
| 1:A:2270:A:C5 | 1:A:2271:A:C5 | 3.06 | 0.44 |
| 1:A:2270:A:C6 | 1:A:2271:A:C6 | 3.05 | 0.44 |
| 1:A:2452:G:O2' | 1:A:2462:A:OP2 | 2.31 | 0.44 |
| 1:A:2180:G:H2' | 1:A:2181:C:C6 | 2.52 | 0.44 |
| 1:A:2922:G:C6 | 45:V:235:THR:OG1 | 2.55 | 0.44 |
| 45:V:261:LYS:HZ1 | 45:V:265:LYS:HD3 | 1.81 | 0.44 |
| 1:A:2439:A:C8 | 1:A:2439:A:O5' | 2.71 | 0.44 |
| 4:D:112:ILE:HG23 | 4:D:133:TYR:HB2 | 1.99 | 0.44 |
| 1:A:2461:A:N9 | 1:A:2485:A:C2 | 2.81 | 0.43 |
| 1:A:3214:U:O4' | 1:A:3214:U:O2 | 2.33 | 0.43 |
| 1:A:2838:A:N6 | 1:A:2850:G:O2' | 2.50 | 0.43 |
| 6:F:181:VAL:HG11 | 6:F:224:GLY:HA3 | 2.00 | 0.43 |
| 1:A:1913:A:N3 | 1:A:2120:A:H2' | 2.32 | 0.43 |
| 9:I:98:LYS:HB3 | 9:I:99:PRO:HD3 | 2.01 | 0.43 |
| 1:A:2506:U:H6 | 1:A:2506:U:H3' | 1.84 | 0.43 |
| 1:A:3277:U:O2 | 1:A:3277:U:O4' | 2.34 | 0.43 |
| 1:A:706:A:H2' | 1:A:707:U:O4' | 2.17 | 0.43 |
| 45:V:291:LEU:HD23 | 45:V:334:VAL:HG11 | 1.51 | 0.43 |
| 1:A:2439:A:N1 | 1:A:2440:G:C5 | 2.87 | 0.43 |
| 1:A:2606:G:N3 | 1:A:2606:G:H2' | 2.34 | 0.43 |
| 1:A:2469:G:O6 | 1:A:2474:G:N1 | 2.51 | 0.42 |
| 1:A:2459:A:N1 | 1:A:2487:U:C2 | 2.87 | 0.42 |
| 12:L:36:LEU:HD11 | 12:L:69:ARG:HD3 | 2.00 | 0.42 |
| 45:V:371:GLY:HA3 | 45:V:397:LEU:HA | 2.01 | 0.42 |
| 45:V:155:TRP:CZ3 | 45:V:158:THR:OG1 | 2.72 | 0.42 |
| 1:A:2270:A:N6 | 1:A:2271:A:N1 | 2.68 | 0.42 |
| 1:A:2470:C:N4 | 1:A:2474:G:H22 | 2.18 | 0.42 |
| 45:V:290:THR:O | 45:V:291:LEU:C | 2.57 | 0.42 |
| 1:A:2439:A:H8 | 1:A:2439:A:O5' | 2.03 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2446:U:H2' | 1:A:2447:A:H8 | 1.84 | 0.42 |
| 1:A:2493:U:H2' | 1:A:2494:A:O4' | 2.19 | 0.42 |
| 1:A:1554:U:O4 | 1:A:1559:A:N1 | 2.52 | 0.42 |
| 1:A:2499:U:C5 | 1:A:2500:A:N7 | 2.88 | 0.42 |
| 10:J:140:VAL:HG22 | 10:J:166:LEU:HD21 | 2.01 | 0.42 |
| 1:A:2213:A:H2' | 1:A:2214:A:C8 | 2.55 | 0.42 |
| 1:A:2437:G:C5 | 1:A:2438:A:N7 | 2.89 | 0.41 |
| 1:A:2461:A:N7 | 1:A:2485:A:N1 | 2.67 | 0.41 |
| 10:J:75:ILE:O | 10:J:76:ALA:HB3 | 2.20 | 0.41 |
| 1:A:78:U:C4 | 1:A:325:A:N1 | 2.88 | 0.41 |
| 1:A:436:A:H2' | 1:A:437:G:O4' | 2.20 | 0.41 |
| 45:V:384:PHE:O | 45:V:387:LEU:HB2 | 2.20 | 0.41 |
| 1:A:1188:U:C4 | 1:A:1317:A:N1 | 2.89 | 0.41 |
| 1:A:3017:A:C6 | 1:A:3018:C:C4 | 3.08 | 0.41 |
| 1:A:2424:A:N1 | 4:D:230:VAL:HG11 | 2.36 | 0.41 |
| 12:L:102:MET:C | 45:V:154:THR:CG2 | 2.89 | 0.41 |
| 45:V:355:VAL:HG22 | 45:V:356:ARG:O | 2.20 | 0.41 |
| 1:A:2410:U:H3 | 1:A:2801:A:N6 | 2.11 | 0.41 |
| 1:A:2456:A:O2' | 1:A:2457:G:C4' | 2.69 | 0.41 |
| 1:A:1793:C:C4 | 4:D:179:LEU:HD11 | 2.55 | 0.41 |
| 11:K:112:ILE:HD13 | 11:K:161:LEU:HD12 | 2.03 | 0.41 |
| 45:V:265:LYS:HE3 | 45:V:265:LYS:HB3 | 1.72 | 0.41 |
| 45:V:291:LEU:HD11 | 45:V:358:HIS:HB2 | 2.01 | 0.41 |
| 1:A:2493:U:C3' | 1:A:2494:A:O4' | 2.69 | 0.41 |
| 45:V:367:ASP:CB | 45:V:400:LYS:NZ | 2.84 | 0.41 |
| 1:A:2249:G:C8 | 1:A:2272:G:N7 | 2.90 | 0.40 |
| 1:A:2191:U:H2' | 1:A:2192:C:O4' | 2.21 | 0.40 |
| 1:A:2490:C:OP1 | 44:S:204:UNK:O | 2.38 | 0.40 |
| 1:A:2469:G:C4 | 1:A:2470:C:C4 | 3.10 | 0.40 |
| 1:A:2485:A:O5' | 1:A:2485:A:H8 | 2.05 | 0.40 |
| 1:A:2594:C:C5 | 1:A:2595:A:C2 | 3.09 | 0.40 |
| 1:A:527:A:N6 | 1:A:566:G:C6 | 2.90 | 0.40 |
| 45:V:218:VAL:HG22 | 45:V:219:PRO:CD | 2.52 | 0.40 |
| 45:V:317:GLU:HA | 45:V:370:MET:HE3 | 2.04 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4 | D | 250/254 (98%) | 228 (91%) | 20 (8%) | 2 (1%) | 24 | 70 |
| 5 | E | 384/387 (99%) | 343 (89%) | 34 (9%) | 7 (2%) | 11 | 55 |
| 6 | F | 359/362 (99%) | 311 (87%) | 32 (9%) | 16 (4%) | 3 | 33 |
| 7 | G | 294/297 (99%) | 267 (91%) | 19 (6%) | 8 (3%) | 6 | 47 |
| 8 | H | 152/176 (86%) | 137 (90%) | 12 (8%) | 3 (2%) | 9 | 53 |
| 9 | I | 220/244 (90%) | 203 (92%) | 14 (6%) | 3 (1%) | 14 | 59 |
| 10 | J | 231/256 (90%) | 202 (87%) | 24 (10%) | 5 (2%) | 8 | 51 |
| 11 | K | 189/191 (99%) | 173 (92%) | 16 (8%) | 0 | 100 | 100 |
| 12 | L | 207/221 (94%) | 187 (90%) | 17 (8%) | 3 (1%) | 14 | 59 |
| 13 | M | 167/174 (96%) | 145 (87%) | 15 (9%) | 7 (4%) | 3 | 35 |
| 14 | N | 191/199 (96%) | 170 (89%) | 19 (10%) | 2 (1%) | 19 | 65 |
| 15 | O | 134/138 (97%) | 125 (93%) | 5 (4%) | 4 (3%) | 5 | 44 |
| 16 | a | 201/204 (98%) | 189 (94%) | 9 (4%) | 3 (2%) | 13 | 58 |
| 17 | b | 195/199 (98%) | 187 (96%) | 7 (4%) | 1 (0%) | 34 | 77 |
| 18 | c | 181/184 (98%) | 161 (89%) | 20 (11%) | 0 | 100 | 100 |
| 19 | d | 183/186 (98%) | 169 (92%) | 11 (6%) | 3 (2%) | 12 | 57 |
| 20 | e | 186/189 (98%) | 175 (94%) | 7 (4%) | 4 (2%) | 8 | 51 |
| 21 | f | 170/172 (99%) | 158 (93%) | 10 (6%) | 2 (1%) | 16 | 62 |
| 22 | g | 157/160 (98%) | 142 (90%) | 12 (8%) | 3 (2%) | 10 | 54 |
| 23 | h | 98/121 (81%) | 84 (86%) | 13 (13%) | 1 (1%) | 19 | 65 |
| 24 | i | 134/137 (98%) | 126 (94%) | 7 (5%) | 1 (1%) | 26 | 71 |
| 25 | j | 96/155 (62%) | 83 (86%) | 10 (10%) | 3 (3%) | 5 | 44 |
| 26 | k | 119/142 (84%) | 111 (93%) | 7 (6%) | 1 (1%) | 24 | 70 |
| 27 | l | 124/127 (98%) | 115 (93%) | 7 (6%) | 2 (2%) | 12 | 57 |
| 28 | m | 133/136 (98%) | 113 (85%) | 18 (14%) | 2 (2%) | 13 | 58 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 29 | n | 146/149 (98%) | 125 (86%) | 16 (11%) | 5 (3%) | 5 | 42 |
| 30 | o | 56/59 (95%) | 48 (86%) | 5 (9%) | 3 (5%) | 2 | 30 |
| 31 | p | 95/105 (90%) | 89 (94%) | 6 (6%) | 0 | 100 | 100 |
| 32 | q | 107/113 (95%) | 98 (92%) | 7 (6%) | 2 (2%) | 10 | 54 |
| 33 | r | 125/130 (96%) | 115 (92%) | 8 (6%) | 2 (2%) | 12 | 57 |
| 34 | s | 48/107 (45%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 35 | t | 110/121 (91%) | 105 (96%) | 3 (3%) | 2 (2%) | 11 | 55 |
| 36 | u | 117/120 (98%) | 108 (92%) | 6 (5%) | 3 (3%) | 7 | 47 |
| 37 | v | 97/100 (97%) | 88 (91%) | 7 (7%) | 2 (2%) | 9 | 52 |
| 38 | w | 85/88 (97%) | 76 (89%) | 9 (11%) | 0 | 100 | 100 |
| 39 | x | 75/78 (96%) | 68 (91%) | 4 (5%) | 3 (4%) | 4 | 37 |
| 40 | y | 48/51 (94%) | 44 (92%) | 4 (8%) | 0 | 100 | 100 |
| 41 | z | 50/128 (39%) | 48 (96%) | 1 (2%) | 1 (2%) | 9 | 53 |
| 42 | Q | 103/106 (97%) | 88 (85%) | 11 (11%) | 4 (4%) | 4 | 37 |
| 43 | R | 89/92 (97%) | 84 (94%) | 5 (6%) | 0 | 100 | 100 |
| 45 | V | 249/917 (27%) | 222 (89%) | 20 (8%) | 7 (3%) | 6 | 46 |
| All | All | 6355/7475 (85%) | 5756 (91%) | 479 (8%) | 120 (2%) | 14 | 54 |

All (120) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 292 | SER |
| 9 | I | 178 | ILE |
| 10 | J | 31 | PRO |
| 10 | J | 157 | VAL |
| 14 | N | 47 | ALA |
| 16 | a | 94 | TYR |
| 20 | e | 131 | ALA |
| 22 | g | 124 | VAL |
| 25 | j | 81 | PRO |
| 42 | Q | 30 | ALA |
| 45 | V | 185 | VAL |
| 45 | V | 389 | ILE |
| 45 | V | 400 | LYS |
| 4 | D | 144 | ASN |
| 5 | E | 347 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 348 | ARG |
| 5 | E | 351 | LEU |
| 6 | F | 130 | ALA |
| 6 | F | 131 | VAL |
| 6 | F | 182 | LEU |
| 6 | F | 293 | SER |
| 7 | G | 87 | GLY |
| 8 | H | 98 | VAL |
| 9 | I | 159 | GLN |
| 10 | J | 36 | ILE |
| 10 | J | 79 | GLN |
| 13 | M | 10 | ARG |
| 13 | M | 95 | ASN |
| 15 | O | 8 | LYS |
| 19 | d | 41 | ASP |
| 25 | j | 97 | LYS |
| 27 | l | 84 | LYS |
| 29 | n | 77 | LYS |
| 45 | V | 390 | ASP |
| 5 | E | 187 | SER |
| 6 | F | 140 | HIS |
| 6 | F | 173 | GLY |
| 6 | F | 233 | LEU |
| 6 | F | 268 | ALA |
| 6 | F | 269 | SER |
| 7 | G | 258 | LYS |
| 7 | G | 259 | LYS |
| 7 | G | 260 | PHE |
| 8 | H | 5 | LYS |
| 10 | J | 25 | PRO |
| 12 | L | 24 | ARG |
| 13 | M | 114 | ILE |
| 15 | O | 9 | ALA |
| 15 | O | 29 | ALA |
| 17 | b | 187 | GLU |
| 19 | d | 98 | LYS |
| 21 | f | 24 | LEU |
| 22 | g | 159 | PHE |
| 26 | k | 50 | ALA |
| 28 | m | 17 | ARG |
| 29 | n | 66 | ALA |
| 30 | o | 25 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | r | 40 | SER |
| 35 | t | 46 | ASP |
| 36 | u | 84 | LYS |
| 39 | x | 18 | ALA |
| 39 | x | 33 | LYS |
| 42 | Q | 34 | SER |
| 45 | V | 194 | LYS |
| 6 | F | 338 | LYS |
| 7 | G | 21 | ARG |
| 12 | L | 218 | ALA |
| 13 | M | 8 | PRO |
| 13 | M | 9 | MET |
| 13 | M | 117 | ASP |
| 14 | N | 166 | ALA |
| 19 | d | 162 | ALA |
| 20 | e | 53 | LYS |
| 20 | e | 178 | ALA |
| 21 | f | 167 | ARG |
| 28 | m | 59 | ALA |
| 32 | q | 82 | GLU |
| 33 | r | 12 | LYS |
| 37 | v | 3 | VAL |
| 39 | x | 34 | ALA |
| 41 | z | 79 | GLU |
| 42 | Q | 17 | CYS |
| 42 | Q | 60 | LYS |
| 45 | V | 349 | ASN |
| 5 | E | 155 | ALA |
| 6 | F | 82 | THR |
| 6 | F | 232 | SER |
| 6 | F | 311 | HIS |
| 7 | G | 251 | PRO |
| 7 | G | 253 | PHE |
| 12 | L | 220 | GLN |
| 13 | M | 108 | GLU |
| 23 | h | 11 | ILE |
| 27 | l | 126 | LEU |
| 30 | o | 29 | TYR |
| 36 | u | 39 | PRO |
| 36 | u | 75 | TYR |
| 4 | D | 125 | ALA |
| 6 | F | 189 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 125 | VAL |
| 16 | a | 81 | TYR |
| 16 | a | 184 | LYS |
| 20 | e | 129 | GLY |
| 22 | g | 125 | ALA |
| 29 | n | 15 | VAL |
| 29 | n | 47 | LYS |
| 32 | q | 7 | VAL |
| 24 | i | 3 | GLY |
| 29 | n | 56 | VAL |
| 45 | V | 327 | GLY |
| 5 | E | 317 | ILE |
| 35 | t | 77 | GLY |
| 37 | v | 21 | THR |
| 6 | F | 317 | PRO |
| 15 | O | 6 | ILE |
| 25 | j | 80 | ARG |
| 30 | o | 21 | ILE |
| 9 | I | 191 | VAL |
| 5 | E | 90 | VAL |
| 8 | H | 6 | ALA |

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4 | D | 193/196 (98%) | 187 (97%) | 6 (3%) | 47 | 78 |
| 5 | E | 318/323 (98%) | 304 (96%) | 14 (4%) | 35 | 71 |
| 6 | F | 288/289 (100%) | 275 (96%) | 13 (4%) | 34 | 70 |
| 7 | G | 244/245 (100%) | 224 (92%) | 20 (8%) | 14 | 51 |
| 8 | H | 134/153 (88%) | 128 (96%) | 6 (4%) | 34 | 70 |
| 9 | I | 186/205 (91%) | 176 (95%) | 10 (5%) | 27 | 66 |
| 10 | J | 187/208 (90%) | 173 (92%) | 14 (8%) | 17 | 56 |
| 11 | K | 171/171 (100%) | 158 (92%) | 13 (8%) | 16 | 55 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 12 | L | 177/187 (95%) | 164 (93%) | 13 (7%) | 17 | 57 |
| 13 | M | 147/150 (98%) | 136 (92%) | 11 (8%) | 17 | 56 |
| 14 | N | 154/159 (97%) | 141 (92%) | 13 (8%) | 14 | 51 |
| 15 | O | 107/109 (98%) | 102 (95%) | 5 (5%) | 32 | 69 |
| 16 | a | 175/176 (99%) | 166 (95%) | 9 (5%) | 29 | 67 |
| 17 | b | 160/162 (99%) | 155 (97%) | 5 (3%) | 47 | 78 |
| 18 | c | 140/146 (96%) | 129 (92%) | 11 (8%) | 15 | 53 |
| 19 | d | 150/151 (99%) | 146 (97%) | 4 (3%) | 52 | 80 |
| 20 | e | 153/154 (99%) | 148 (97%) | 5 (3%) | 45 | 77 |
| 21 | f | 156/156 (100%) | 149 (96%) | 7 (4%) | 34 | 70 |
| 22 | g | 136/137 (99%) | 125 (92%) | 11 (8%) | 15 | 52 |
| 23 | h | 87/107 (81%) | 85 (98%) | 2 (2%) | 58 | 83 |
| 24 | i | 104/105 (99%) | 98 (94%) | 6 (6%) | 25 | 64 |
| 25 | j | 57/129 (44%) | 57 (100%) | 0 | 100 | 100 |
| 26 | k | 104/118 (88%) | 96 (92%) | 8 (8%) | 16 | 55 |
| 27 | l | 109/110 (99%) | 103 (94%) | 6 (6%) | 27 | 66 |
| 28 | m | 115/116 (99%) | 108 (94%) | 7 (6%) | 23 | 62 |
| 29 | n | 118/119 (99%) | 111 (94%) | 7 (6%) | 24 | 63 |
| 30 | o | 46/47 (98%) | 43 (94%) | 3 (6%) | 21 | 60 |
| 31 | p | 81/88 (92%) | 79 (98%) | 2 (2%) | 55 | 82 |
| 32 | q | 92/97 (95%) | 87 (95%) | 5 (5%) | 27 | 66 |
| 33 | r | 109/111 (98%) | 101 (93%) | 8 (7%) | 17 | 57 |
| 34 | s | 43/91 (47%) | 42 (98%) | 1 (2%) | 58 | 83 |
| 35 | t | 95/103 (92%) | 93 (98%) | 2 (2%) | 61 | 85 |
| 36 | u | 104/105 (99%) | 97 (93%) | 7 (7%) | 20 | 59 |
| 37 | v | 81/82 (99%) | 75 (93%) | 6 (7%) | 17 | 56 |
| 38 | w | 70/71 (99%) | 67 (96%) | 3 (4%) | 35 | 71 |
| 39 | x | 68/69 (99%) | 66 (97%) | 2 (3%) | 50 | 79 |
| 40 | y | 45/46 (98%) | 44 (98%) | 1 (2%) | 60 | 84 |
| 41 | z | 47/116 (40%) | 43 (92%) | 4 (8%) | 13 | 50 |
| 42 | Q | 90/91 (99%) | 82 (91%) | 8 (9%) | 12 | 47 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 43 | R | 71/72 (99%) | 68 (96%) | 3 (4%) | 36 72 |
| 45 | V | 224/791 (28%) | 193 (86%) | 31 (14%) | 4 29 |
| All | All | 5336/6261 (85%) | 5024 (94%) | 312 (6%) | 29 64 |

All (312) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 17 | THR |
| 4 | D | 116 | VAL |
| 4 | D | 122 | ASP |
| 4 | D | 207 | VAL |
| 4 | D | 227 | ARG |
| 4 | D | 230 | VAL |
| 5 | E | 10 | ARG |
| 5 | E | 19 | ARG |
| 5 | E | 25 | ILE |
| 5 | E | 85 | VAL |
| 5 | E | 159 | ARG |
| 5 | E | 169 | THR |
| 5 | E | 188 | ILE |
| 5 | E | 232 | ARG |
| 5 | E | 246 | LEU |
| 5 | E | 252 | ILE |
| 5 | E | 296 | THR |
| 5 | E | 332 | ARG |
| 5 | E | 339 | ARG |
| 5 | E | 364 | LYS |
| 6 | F | 52 | VAL |
| 6 | F | 67 | THR |
| 6 | F | 73 | ARG |
| 6 | F | 74 | ILE |
| 6 | F | 99 | MET |
| 6 | F | 112 | LYS |
| 6 | F | 114 | ASN |
| 6 | F | 150 | LEU |
| 6 | F | 154 | THR |
| 6 | F | 179 | LEU |
| 6 | F | 246 | ARG |
| 6 | F | 307 | GLN |
| 6 | F | 361 | HIS |
| 7 | G | 13 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 15 | ARG |
| 7 | G | 18 | THR |
| 7 | G | 22 | ARG |
| 7 | G | 23 | ARG |
| 7 | G | 24 | ARG |
| 7 | G | 41 | LYS |
| 7 | G | 75 | LEU |
| 7 | G | 92 | LEU |
| 7 | G | 95 | TRP |
| 7 | G | 105 | ILE |
| 7 | G | 115 | LEU |
| 7 | G | 131 | LEU |
| 7 | G | 151 | GLN |
| 7 | G | 193 | GLU |
| 7 | G | 211 | LEU |
| 7 | G | 259 | LYS |
| 7 | G | 264 | GLN |
| 7 | G | 273 | ARG |
| 7 | G | 279 | LYS |
| 8 | H | 34 | LEU |
| 8 | H | 46 | ARG |
| 8 | H | 64 | LEU |
| 8 | H | 65 | ILE |
| 8 | H | 134 | ARG |
| 8 | H | 137 | ASP |
| 9 | I | 24 | GLU |
| 9 | I | 82 | LYS |
| 9 | I | 88 | ARG |
| 9 | I | 92 | ILE |
| 9 | I | 124 | LEU |
| 9 | I | 125 | GLU |
| 9 | I | 145 | ARG |
| 9 | I | 179 | LEU |
| 9 | I | 218 | ARG |
| 9 | I | 239 | LEU |
| 10 | J | 41 | GLN |
| 10 | J | 57 | ARG |
| 10 | J | 63 | LYS |
| 10 | J | 65 | LEU |
| 10 | J | 92 | LYS |
| 10 | J | 136 | LEU |
| 10 | J | 150 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 163 | VAL |
| 10 | J | 169 | LEU |
| 10 | J | 201 | THR |
| 10 | J | 204 | ARG |
| 10 | J | 232 | HIS |
| 10 | J | 240 | ASN |
| 10 | J | 248 | LYS |
| 11 | K | 5 | GLN |
| 11 | K | 23 | ARG |
| 11 | K | 41 | ILE |
| 11 | K | 49 | ASN |
| 11 | K | 52 | LEU |
| 11 | K | 69 | ARG |
| 11 | K | 118 | LEU |
| 11 | K | 120 | ASP |
| 11 | K | 135 | GLU |
| 11 | K | 139 | ASN |
| 11 | K | 164 | ILE |
| 11 | K | 166 | ARG |
| 11 | K | 177 | ASP |
| 12 | L | 7 | ARG |
| 12 | L | 30 | LYS |
| 12 | L | 33 | ILE |
| 12 | L | 40 | LYS |
| 12 | L | 52 | LEU |
| 12 | L | 90 | ARG |
| 12 | L | 115 | MET |
| 12 | L | 154 | ARG |
| 12 | L | 163 | GLN |
| 12 | L | 165 | ILE |
| 12 | L | 169 | LYS |
| 12 | L | 203 | LYS |
| 12 | L | 208 | ASN |
| 13 | M | 10 | ARG |
| 13 | M | 11 | ASP |
| 13 | M | 12 | LEU |
| 13 | M | 13 | LYS |
| 13 | M | 40 | LEU |
| 13 | M | 80 | LEU |
| 13 | M | 81 | GLU |
| 13 | M | 94 | ARG |
| 13 | M | 107 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | M | 130 | VAL |
| 13 | M | 140 | ARG |
| 14 | N | 24 | VAL |
| 14 | N | 36 | ARG |
| 14 | N | 49 | ARG |
| 14 | N | 67 | ARG |
| 14 | N | 85 | LEU |
| 14 | N | 101 | ARG |
| 14 | N | 104 | ARG |
| 14 | N | 124 | ILE |
| 14 | N | 131 | LYS |
| 14 | N | 136 | GLU |
| 14 | N | 168 | ARG |
| 14 | N | 176 | GLU |
| 14 | N | 190 | LYS |
| 15 | O | 12 | TRP |
| 15 | O | 20 | VAL |
| 15 | O | 28 | SER |
| 15 | O | 72 | LEU |
| 15 | O | 108 | ARG |
| 16 | a | 22 | LEU |
| 16 | a | 27 | VAL |
| 16 | a | 50 | ARG |
| 16 | a | 133 | ILE |
| 16 | a | 138 | GLN |
| 16 | a | 174 | ILE |
| 16 | a | 180 | PHE |
| 16 | a | 183 | THR |
| 16 | a | 201 | ARG |
| 17 | b | 34 | VAL |
| 17 | b | 78 | ARG |
| 17 | b | 124 | LEU |
| 17 | b | 125 | ARG |
| 17 | b | 155 | LYS |
| 18 | c | 24 | VAL |
| 18 | c | 49 | GLU |
| 18 | c | 52 | LEU |
| 18 | c | 53 | ASP |
| 18 | c | 96 | GLN |
| 18 | c | 120 | ASN |
| 18 | c | 125 | GLN |
| 18 | c | 126 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | c | 127 | ARG |
| 18 | c | 168 | LEU |
| 18 | c | 180 | LYS |
| 19 | d | 26 | LEU |
| 19 | d | 49 | LEU |
| 19 | d | 135 | GLN |
| 19 | d | 138 | LEU |
| 20 | e | 17 | VAL |
| 20 | e | 25 | ASP |
| 20 | e | 74 | ARG |
| 20 | e | 103 | ARG |
| 20 | e | 138 | LEU |
| 21 | f | 12 | ARG |
| 21 | f | 45 | LEU |
| 21 | f | 61 | ILE |
| 21 | f | 71 | LYS |
| 21 | f | 115 | ARG |
| 21 | f | 137 | ARG |
| 21 | f | 172 | TYR |
| 22 | g | 12 | ARG |
| 22 | g | 32 | LYS |
| 22 | g | 75 | ILE |
| 22 | g | 79 | MET |
| 22 | g | 83 | ARG |
| 22 | g | 88 | ARG |
| 22 | g | 102 | ARG |
| 22 | g | 126 | VAL |
| 22 | g | 127 | GLN |
| 22 | g | 128 | LEU |
| 22 | g | 139 | ARG |
| 23 | h | 10 | LYS |
| 23 | h | 70 | LYS |
| 24 | i | 32 | ARG |
| 24 | i | 33 | ASN |
| 24 | i | 34 | LEU |
| 24 | i | 40 | LYS |
| 24 | i | 83 | LYS |
| 24 | i | 132 | ASN |
| 26 | k | 34 | LEU |
| 26 | k | 63 | ILE |
| 26 | k | 70 | GLU |
| 26 | k | 125 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | k | 129 | ASP |
| 26 | k | 133 | LEU |
| 26 | k | 135 | ILE |
| 26 | k | 142 | ILE |
| 27 | l | 13 | ARG |
| 27 | l | 37 | LYS |
| 27 | l | 50 | ILE |
| 27 | l | 56 | VAL |
| 27 | l | 74 | TYR |
| 27 | l | 126 | LEU |
| 28 | m | 3 | LYS |
| 28 | m | 14 | VAL |
| 28 | m | 24 | VAL |
| 28 | m | 34 | LYS |
| 28 | m | 120 | GLU |
| 28 | m | 121 | ARG |
| 28 | m | 126 | LYS |
| 29 | n | 34 | MET |
| 29 | n | 42 | ARG |
| 29 | n | 56 | VAL |
| 29 | n | 60 | TYR |
| 29 | n | 120 | ASN |
| 29 | n | 130 | VAL |
| 29 | n | 133 | LEU |
| 30 | o | 22 | LYS |
| 30 | o | 25 | LYS |
| 30 | o | 59 | LYS |
| 31 | p | 40 | LYS |
| 31 | p | 61 | MET |
| 32 | q | 16 | LEU |
| 32 | q | 50 | ARG |
| 32 | q | 55 | LEU |
| 32 | q | 79 | ARG |
| 32 | q | 86 | LYS |
| 33 | r | 19 | ARG |
| 33 | r | 27 | ARG |
| 33 | r | 33 | ARG |
| 33 | r | 44 | ARG |
| 33 | r | 47 | ARG |
| 33 | r | 87 | MET |
| 33 | r | 125 | ARG |
| 33 | r | 128 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | s | 37 | THR |
| 35 | t | 29 | ILE |
| 35 | t | 58 | ARG |
| 36 | u | 20 | GLN |
| 36 | u | 21 | LEU |
| 36 | u | 49 | LYS |
| 36 | u | 71 | LYS |
| 36 | u | 107 | LYS |
| 36 | u | 115 | LYS |
| 36 | u | 119 | LYS |
| 37 | v | 26 | ILE |
| 37 | v | 45 | ARG |
| 37 | v | 57 | LEU |
| 37 | v | 58 | ILE |
| 37 | v | 75 | LYS |
| 37 | v | 76 | ARG |
| 38 | w | 17 | THR |
| 38 | w | 24 | ARG |
| 38 | w | 25 | ARG |
| 39 | x | 67 | GLN |
| 39 | x | 77 | ARG |
| 40 | y | 21 | ARG |
| 41 | z | 85 | LEU |
| 41 | z | 106 | ARG |
| 41 | z | 113 | ARG |
| 41 | z | 127 | LEU |
| 42 | Q | 35 | LEU |
| 42 | Q | 38 | GLN |
| 42 | Q | 45 | ARG |
| 42 | Q | 71 | ARG |
| 42 | Q | 78 | LYS |
| 42 | Q | 83 | LEU |
| 42 | Q | 99 | GLN |
| 42 | Q | 100 | LYS |
| 43 | R | 45 | LYS |
| 43 | R | 49 | ARG |
| 43 | R | 60 | CYS |
| 45 | V | 156 | ARG |
| 45 | V | 162 | ARG |
| 45 | V | 164 | LYS |
| 45 | V | 168 | LYS |
| 45 | V | 171 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | V | 177 | LEU |
| 45 | V | 179 | LEU |
| 45 | V | 185 | VAL |
| 45 | V | 197 | LEU |
| 45 | V | 209 | LYS |
| 45 | V | 221 | LYS |
| 45 | V | 228 | LEU |
| 45 | V | 265 | LYS |
| 45 | V | 278 | LYS |
| 45 | V | 291 | LEU |
| 45 | V | 295 | ASP |
| 45 | V | 299 | SER |
| 45 | V | 345 | ASP |
| 45 | V | 350 | ASP |
| 45 | V | 356 | ARG |
| 45 | V | 362 | ILE |
| 45 | V | 364 | HIS |
| 45 | V | 370 | MET |
| 45 | V | 376 | ASN |
| 45 | V | 387 | LEU |
| 45 | V | 388 | ASN |
| 45 | V | 390 | ASP |
| 45 | V | 391 | TYR |
| 45 | V | 397 | LEU |
| 45 | V | 400 | LYS |
| 45 | V | 401 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 48 | GLN |
| 6 | F | 114 | ASN |
| 6 | F | 221 | ASN |
| 8 | H | 167 | ASN |
| 9 | I | 225 | GLN |
| 11 | K | 8 | GLN |
| 12 | L | 12 | GLN |
| 12 | L | 14 | ASN |
| 16 | a | 87 | GLN |
| 16 | a | 182 | ASN |
| 19 | d | 73 | GLN |
| 29 | n | 74 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | q | 87 | ASN |
| 33 | r | 104 | ASN |
| 42 | Q | 82 | GLN |
| 45 | V | 160 | GLN |
| 45 | V | 163 | GLN |
| 45 | V | 231 | GLN |
| 45 | V | 388 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 3201/3396 (94%) | 770 (24%) | 77 (2%) |
| 2 | B | 120/121 (99%) | 22 (18%) | 2 (1%) |
| 3 | C | 157/158 (99%) | 38 (24%) | 3 (1%) |
| All | All | 3478/3675 (94%) | 830 (23%) | 82 (2%) |

All (830) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 16 | A |
| 1 | A | 22 | G |
| 1 | A | 40 | A |
| 1 | A | 43 | A |
| 1 | A | 45 | A |
| 1 | A | 49 | A |
| 1 | A | 59 | G |
| 1 | A | 60 | A |
| 1 | A | 65 | A |
| 1 | A | 66 | A |
| 1 | A | 72 | C |
| 1 | A | 75 | G |
| 1 | A | 89 | A |
| 1 | A | 92 | G |
| 1 | A | 105 | C |
| 1 | A | 109 | A |
| 1 | A | 110 | G |
| 1 | A | 111 | C |
| 1 | A | 116 | A |
| 1 | A | 118 | U |
| 1 | A | 122 | A |
| 1 | A | 123 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 136 | G |
| 1 | A | 137 | G |
| 1 | A | 143 | G |
| 1 | A | 150 | A |
| 1 | A | 156 | G |
| 1 | A | 157 | A |
| 1 | A | 161 | G |
| 1 | A | 166 | C |
| 1 | A | 167 | U |
| 1 | A | 168 | U |
| 1 | A | 170 | G |
| 1 | A | 173 | G |
| 1 | A | 177 | U |
| 1 | A | 182 | U |
| 1 | A | 184 | U |
| 1 | A | 187 | A |
| 1 | A | 190 | U |
| 1 | A | 191 | U |
| 1 | A | 192 | C |
| 1 | A | 198 | A |
| 1 | A | 200 | C |
| 1 | A | 210 | U |
| 1 | A | 211 | A |
| 1 | A | 218 | G |
| 1 | A | 219 | A |
| 1 | A | 240 | U |
| 1 | A | 241 | G |
| 1 | A | 243 | G |
| 1 | A | 245 | U |
| 1 | A | 246 | U |
| 1 | A | 247 | C |
| 1 | A | 249 | U |
| 1 | A | 250 | U |
| 1 | A | 252 | U |
| 1 | A | 266 | A |
| 1 | A | 269 | G |
| 1 | A | 286 | U |
| 1 | A | 295 | A |
| 1 | A | 305 | U |
| 1 | A | 315 | C |
| 1 | A | 317 | A |
| 1 | A | 323 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 329 | U |
| 1 | A | 338 | A |
| 1 | A | 339 | C |
| 1 | A | 376 | G |
| 1 | A | 381 | U |
| 1 | A | 395 | A |
| 1 | A | 398 | A |
| 1 | A | 399 | A |
| 1 | A | 401 | U |
| 1 | A | 402 | A |
| 1 | A | 403 | C |
| 1 | A | 404 | G |
| 1 | A | 417 | A |
| 1 | A | 420 | G |
| 1 | A | 421 | G |
| 1 | A | 422 | A |
| 1 | A | 429 | U |
| 1 | A | 436 | A |
| 1 | A | 439 | C |
| 1 | A | 440 | A |
| 1 | A | 495 | G |
| 1 | A | 507 | U |
| 1 | A | 510 | G |
| 1 | A | 518 | G |
| 1 | A | 519 | A |
| 1 | A | 520 | U |
| 1 | A | 521 | A |
| 1 | A | 523 | A |
| 1 | A | 526 | C |
| 1 | A | 531 | G |
| 1 | A | 536 | U |
| 1 | A | 539 | C |
| 1 | A | 541 | U |
| 1 | A | 543 | C |
| 1 | A | 546 | C |
| 1 | A | 547 | G |
| 1 | A | 548 | G |
| 1 | A | 549 | U |
| 1 | A | 551 | A |
| 1 | A | 553 | U |
| 1 | A | 555 | U |
| 1 | A | 556 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 557 | A |
| 1 | A | 559 | A |
| 1 | A | 560 | G |
| 1 | A | 569 | A |
| 1 | A | 570 | A |
| 1 | A | 579 | G |
| 1 | A | 592 | A |
| 1 | A | 598 | A |
| 1 | A | 600 | G |
| 1 | A | 604 | G |
| 1 | A | 611 | A |
| 1 | A | 619 | A |
| 1 | A | 620 | U |
| 1 | A | 621 | A |
| 1 | A | 622 | A |
| 1 | A | 634 | C |
| 1 | A | 636 | C |
| 1 | A | 649 | A |
| 1 | A | 660 | A |
| 1 | A | 662 | U |
| 1 | A | 676 | G |
| 1 | A | 677 | A |
| 1 | A | 681 | U |
| 1 | A | 683 | U |
| 1 | A | 684 | G |
| 1 | A | 687 | U |
| 1 | A | 689 | U |
| 1 | A | 690 | A |
| 1 | A | 691 | A |
| 1 | A | 696 | C |
| 1 | A | 705 | A |
| 1 | A | 710 | A |
| 1 | A | 712 | G |
| 1 | A | 715 | A |
| 1 | A | 716 | A |
| 1 | A | 720 | A |
| 1 | A | 725 | G |
| 1 | A | 735 | A |
| 1 | A | 739 | G |
| 1 | A | 748 | U |
| 1 | A | 764 | U |
| 1 | A | 766 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 767 | U |
| 1 | A | 774 | G |
| 1 | A | 776 | U |
| 1 | A | 777 | U |
| 1 | A | 780 | A |
| 1 | A | 781 | G |
| 1 | A | 785 | G |
| 1 | A | 786 | A |
| 1 | A | 792 | G |
| 1 | A | 799 | G |
| 1 | A | 801 | A |
| 1 | A | 806 | A |
| 1 | A | 808 | A |
| 1 | A | 814 | U |
| 1 | A | 817 | A |
| 1 | A | 830 | A |
| 1 | A | 849 | C |
| 1 | A | 857 | G |
| 1 | A | 861 | C |
| 1 | A | 868 | C |
| 1 | A | 874 | U |
| 1 | A | 879 | U |
| 1 | A | 890 | C |
| 1 | A | 894 | G |
| 1 | A | 895 | A |
| 1 | A | 896 | A |
| 1 | A | 897 | U |
| 1 | A | 907 | G |
| 1 | A | 908 | G |
| 1 | A | 911 | C |
| 1 | A | 914 | A |
| 1 | A | 916 | G |
| 1 | A | 917 | A |
| 1 | A | 921 | A |
| 1 | A | 923 | C |
| 1 | A | 925 | A |
| 1 | A | 937 | G |
| 1 | A | 941 | G |
| 1 | A | 944 | C |
| 1 | A | 958 | C |
| 1 | A | 959 | C |
| 1 | A | 960 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 979 | U |
| 1 | A | 980 | A |
| 1 | A | 981 | U |
| 1 | A | 982 | C |
| 1 | A | 991 | G |
| 1 | A | 994 | G |
| 1 | A | 1001 | G |
| 1 | A | 1002 | A |
| 1 | A | 1009 | A |
| 1 | A | 1010 | G |
| 1 | A | 1013 | G |
| 1 | A | 1015 | U |
| 1 | A | 1017 | C |
| 1 | A | 1018 | G |
| 1 | A | 1019 | G |
| 1 | A | 1021 | G |
| 1 | A | 1024 | G |
| 1 | A | 1025 | A |
| 1 | A | 1026 | A |
| 1 | A | 1029 | G |
| 1 | A | 1030 | A |
| 1 | A | 1031 | C |
| 1 | A | 1034 | U |
| 1 | A | 1036 | A |
| 1 | A | 1037 | C |
| 1 | A | 1040 | A |
| 1 | A | 1041 | U |
| 1 | A | 1047 | A |
| 1 | A | 1049 | C |
| 1 | A | 1057 | A |
| 1 | A | 1064 | A |
| 1 | A | 1065 | A |
| 1 | A | 1072 | G |
| 1 | A | 1073 | U |
| 1 | A | 1081 | U |
| 1 | A | 1093 | A |
| 1 | A | 1094 | U |
| 1 | A | 1095 | U |
| 1 | A | 1098 | A |
| 1 | A | 1103 | A |
| 1 | A | 1104 | G |
| 1 | A | 1117 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1124 | U |
| 1 | A | 1129 | A |
| 1 | A | 1131 | G |
| 1 | A | 1140 | G |
| 1 | A | 1153 | A |
| 1 | A | 1159 | A |
| 1 | A | 1180 | A |
| 1 | A | 1181 | U |
| 1 | A | 1188 | U |
| 1 | A | 1191 | U |
| 1 | A | 1192 | C |
| 1 | A | 1200 | A |
| 1 | A | 1201 | C |
| 1 | A | 1208 | U |
| 1 | A | 1212 | A |
| 1 | A | 1213 | G |
| 1 | A | 1217 | A |
| 1 | A | 1219 | C |
| 1 | A | 1222 | G |
| 1 | A | 1223 | A |
| 1 | A | 1230 | G |
| 1 | A | 1232 | C |
| 1 | A | 1236 | G |
| 1 | A | 1237 | G |
| 1 | A | 1240 | A |
| 1 | A | 1241 | U |
| 1 | A | 1242 | G |
| 1 | A | 1243 | G |
| 1 | A | 1244 | A |
| 1 | A | 1245 | A |
| 1 | A | 1246 | G |
| 1 | A | 1247 | U |
| 1 | A | 1248 | C |
| 1 | A | 1249 | G |
| 1 | A | 1253 | U |
| 1 | A | 1257 | C |
| 1 | A | 1258 | U |
| 1 | A | 1260 | A |
| 1 | A | 1262 | G |
| 1 | A | 1263 | A |
| 1 | A | 1264 | G |
| 1 | A | 1266 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1267 | U |
| 1 | A | 1270 | A |
| 1 | A | 1271 | A |
| 1 | A | 1272 | C |
| 1 | A | 1274 | A |
| 1 | A | 1276 | U |
| 1 | A | 1278 | A |
| 1 | A | 1279 | C |
| 1 | A | 1285 | G |
| 1 | A | 1287 | A |
| 1 | A | 1289 | G |
| 1 | A | 1305 | U |
| 1 | A | 1307 | G |
| 1 | A | 1308 | A |
| 1 | A | 1309 | U |
| 1 | A | 1313 | G |
| 1 | A | 1316 | C |
| 1 | A | 1325 | U |
| 1 | A | 1329 | U |
| 1 | A | 1330 | A |
| 1 | A | 1331 | U |
| 1 | A | 1340 | G |
| 1 | A | 1348 | U |
| 1 | A | 1349 | G |
| 1 | A | 1351 | U |
| 1 | A | 1352 | A |
| 1 | A | 1353 | U |
| 1 | A | 1356 | U |
| 1 | A | 1357 | G |
| 1 | A | 1364 | C |
| 1 | A | 1383 | G |
| 1 | A | 1385 | C |
| 1 | A | 1386 | A |
| 1 | A | 1392 | G |
| 1 | A | 1393 | A |
| 1 | A | 1399 | A |
| 1 | A | 1400 | G |
| 1 | A | 1414 | G |
| 1 | A | 1416 | C |
| 1 | A | 1419 | A |
| 1 | A | 1434 | G |
| 1 | A | 1437 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1446 | A |
| 1 | A | 1450 | G |
| 1 | A | 1455 | U |
| 1 | A | 1460 | A |
| 1 | A | 1481 | A |
| 1 | A | 1482 | A |
| 1 | A | 1498 | A |
| 1 | A | 1500 | G |
| 1 | A | 1508 | C |
| 1 | A | 1512 | U |
| 1 | A | 1527 | C |
| 1 | A | 1531 | C |
| 1 | A | 1533 | U |
| 1 | A | 1536 | G |
| 1 | A | 1555 | U |
| 1 | A | 1556 | C |
| 1 | A | 1557 | A |
| 1 | A | 1560 | G |
| 1 | A | 1561 | G |
| 1 | A | 1562 | C |
| 1 | A | 1563 | C |
| 1 | A | 1565 | G |
| 1 | A | 1566 | A |
| 1 | A | 1567 | U |
| 1 | A | 1568 | U |
| 1 | A | 1569 | U |
| 1 | A | 1570 | U |
| 1 | A | 1572 | U |
| 1 | A | 1574 | C |
| 1 | A | 1576 | G |
| 1 | A | 1577 | G |
| 1 | A | 1578 | C |
| 1 | A | 1579 | C |
| 1 | A | 1582 | C |
| 1 | A | 1583 | A |
| 1 | A | 1587 | A |
| 1 | A | 1589 | A |
| 1 | A | 1593 | A |
| 1 | A | 1611 | G |
| 1 | A | 1618 | G |
| 1 | A | 1620 | U |
| 1 | A | 1622 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1628 | C |
| 1 | A | 1629 | U |
| 1 | A | 1630 | U |
| 1 | A | 1642 | A |
| 1 | A | 1643 | A |
| 1 | A | 1645 | U |
| 1 | A | 1657 | C |
| 1 | A | 1664 | G |
| 1 | A | 1666 | G |
| 1 | A | 1678 | G |
| 1 | A | 1683 | A |
| 1 | A | 1703 | U |
| 1 | A | 1716 | U |
| 1 | A | 1717 | U |
| 1 | A | 1724 | U |
| 1 | A | 1725 | C |
| 1 | A | 1741 | A |
| 1 | A | 1742 | U |
| 1 | A | 1749 | A |
| 1 | A | 1750 | A |
| 1 | A | 1751 | G |
| 1 | A | 1760 | A |
| 1 | A | 1761 | C |
| 1 | A | 1762 | C |
| 1 | A | 1765 | U |
| 1 | A | 1766 | G |
| 1 | A | 1770 | G |
| 1 | A | 1775 | G |
| 1 | A | 1779 | C |
| 1 | A | 1780 | G |
| 1 | A | 1797 | A |
| 1 | A | 1798 | A |
| 1 | A | 1808 | G |
| 1 | A | 1812 | G |
| 1 | A | 1813 | A |
| 1 | A | 1814 | A |
| 1 | A | 1815 | U |
| 1 | A | 1816 | A |
| 1 | A | 1817 | G |
| 1 | A | 1820 | U |
| 1 | A | 1821 | U |
| 1 | A | 1839 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1840 | U |
| 1 | A | 1841 | A |
| 1 | A | 1842 | A |
| 1 | A | 1847 | A |
| 1 | A | 1849 | C |
| 1 | A | 1850 | A |
| 1 | A | 1855 | U |
| 1 | A | 1866 | C |
| 1 | A | 1880 | U |
| 1 | A | 1886 | A |
| 1 | A | 1893 | A |
| 1 | A | 1906 | G |
| 1 | A | 1908 | A |
| 1 | A | 1910 | A |
| 1 | A | 1936 | A |
| 1 | A | 1951 | C |
| 1 | A | 1952 | G |
| 1 | A | 1953 | G |
| 1 | A | 1954 | G |
| 1 | A | 2095 | G |
| 1 | A | 2099 | A |
| 1 | A | 2101 | C |
| 1 | A | 2102 | U |
| 1 | A | 2111 | G |
| 1 | A | 2112 | U |
| 1 | A | 2113 | A |
| 1 | A | 2114 | C |
| 1 | A | 2115 | G |
| 1 | A | 2120 | A |
| 1 | A | 2121 | G |
| 1 | A | 2122 | G |
| 1 | A | 2131 | A |
| 1 | A | 2134 | G |
| 1 | A | 2140 | U |
| 1 | A | 2158 | A |
| 1 | A | 2169 | G |
| 1 | A | 2180 | G |
| 1 | A | 2185 | G |
| 1 | A | 2192 | C |
| 1 | A | 2193 | U |
| 1 | A | 2198 | A |
| 1 | A | 2204 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2205 | U |
| 1 | A | 2210 | G |
| 1 | A | 2211 | U |
| 1 | A | 2228 | A |
| 1 | A | 2239 | G |
| 1 | A | 2244 | A |
| 1 | A | 2245 | C |
| 1 | A | 2246 | G |
| 1 | A | 2250 | G |
| 1 | A | 2252 | A |
| 1 | A | 2253 | G |
| 1 | A | 2255 | A |
| 1 | A | 2256 | A |
| 1 | A | 2257 | C |
| 1 | A | 2258 | U |
| 1 | A | 2270 | A |
| 1 | A | 2273 | G |
| 1 | A | 2274 | U |
| 1 | A | 2276 | G |
| 1 | A | 2279 | A |
| 1 | A | 2281 | A |
| 1 | A | 2282 | U |
| 1 | A | 2285 | C |
| 1 | A | 2288 | G |
| 1 | A | 2298 | U |
| 1 | A | 2307 | G |
| 1 | A | 2308 | C |
| 1 | A | 2310 | U |
| 1 | A | 2313 | A |
| 1 | A | 2314 | U |
| 1 | A | 2315 | G |
| 1 | A | 2327 | U |
| 1 | A | 2334 | U |
| 1 | A | 2335 | G |
| 1 | A | 2336 | U |
| 1 | A | 2337 | C |
| 1 | A | 2357 | A |
| 1 | A | 2372 | A |
| 1 | A | 2373 | A |
| 1 | A | 2374 | C |
| 1 | A | 2375 | G |
| 1 | A | 2385 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2388 | U |
| 1 | A | 2393 | G |
| 1 | A | 2397 | A |
| 1 | A | 2402 | A |
| 1 | A | 2403 | G |
| 1 | A | 2404 | A |
| 1 | A | 2411 | U |
| 1 | A | 2418 | G |
| 1 | A | 2419 | A |
| 1 | A | 2421 | U |
| 1 | A | 2422 | C |
| 1 | A | 2425 | G |
| 1 | A | 2437 | G |
| 1 | A | 2438 | A |
| 1 | A | 2440 | G |
| 1 | A | 2442 | G |
| 1 | A | 2443 | A |
| 1 | A | 2444 | C |
| 1 | A | 2445 | A |
| 1 | A | 2446 | U |
| 1 | A | 2448 | G |
| 1 | A | 2449 | A |
| 1 | A | 2450 | G |
| 1 | A | 2451 | G |
| 1 | A | 2452 | G |
| 1 | A | 2453 | U |
| 1 | A | 2454 | G |
| 1 | A | 2455 | U |
| 1 | A | 2456 | A |
| 1 | A | 2457 | G |
| 1 | A | 2458 | A |
| 1 | A | 2459 | A |
| 1 | A | 2461 | A |
| 1 | A | 2462 | A |
| 1 | A | 2463 | G |
| 1 | A | 2465 | G |
| 1 | A | 2472 | U |
| 1 | A | 2473 | C |
| 1 | A | 2474 | G |
| 1 | A | 2475 | G |
| 1 | A | 2477 | G |
| 1 | A | 2481 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2484 | A |
| 1 | A | 2487 | U |
| 1 | A | 2488 | A |
| 1 | A | 2491 | A |
| 1 | A | 2492 | C |
| 1 | A | 2494 | A |
| 1 | A | 2495 | C |
| 1 | A | 2496 | C |
| 1 | A | 2497 | U |
| 1 | A | 2498 | U |
| 1 | A | 2499 | U |
| 1 | A | 2501 | U |
| 1 | A | 2502 | A |
| 1 | A | 2503 | G |
| 1 | A | 2505 | U |
| 1 | A | 2506 | U |
| 1 | A | 2507 | C |
| 1 | A | 2508 | U |
| 1 | A | 2513 | U |
| 1 | A | 2514 | U |
| 1 | A | 2515 | A |
| 1 | A | 2522 | G |
| 1 | A | 2530 | G |
| 1 | A | 2531 | C |
| 1 | A | 2532 | U |
| 1 | A | 2533 | G |
| 1 | A | 2537 | U |
| 1 | A | 2538 | U |
| 1 | A | 2539 | C |
| 1 | A | 2540 | A |
| 1 | A | 2541 | U |
| 1 | A | 2542 | U |
| 1 | A | 2543 | U |
| 1 | A | 2544 | U |
| 1 | A | 2547 | A |
| 1 | A | 2548 | C |
| 1 | A | 2549 | G |
| 1 | A | 2550 | U |
| 1 | A | 2552 | C |
| 1 | A | 2554 | A |
| 1 | A | 2555 | G |
| 1 | A | 2558 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2561 | A |
| 1 | A | 2562 | A |
| 1 | A | 2565 | U |
| 1 | A | 2566 | C |
| 1 | A | 2568 | C |
| 1 | A | 2569 | A |
| 1 | A | 2570 | U |
| 1 | A | 2571 | U |
| 1 | A | 2572 | C |
| 1 | A | 2573 | G |
| 1 | A | 2575 | G |
| 1 | A | 2576 | G |
| 1 | A | 2582 | C |
| 1 | A | 2585 | G |
| 1 | A | 2586 | G |
| 1 | A | 2593 | A |
| 1 | A | 2594 | C |
| 1 | A | 2602 | G |
| 1 | A | 2606 | G |
| 1 | A | 2607 | G |
| 1 | A | 2614 | G |
| 1 | A | 2621 | G |
| 1 | A | 2626 | A |
| 1 | A | 2652 | U |
| 1 | A | 2655 | U |
| 1 | A | 2656 | A |
| 1 | A | 2657 | A |
| 1 | A | 2665 | U |
| 1 | A | 2674 | A |
| 1 | A | 2677 | G |
| 1 | A | 2681 | U |
| 1 | A | 2689 | A |
| 1 | A | 2691 | A |
| 1 | A | 2692 | A |
| 1 | A | 2694 | A |
| 1 | A | 2696 | A |
| 1 | A | 2703 | A |
| 1 | A | 2704 | A |
| 1 | A | 2713 | U |
| 1 | A | 2719 | U |
| 1 | A | 2726 | C |
| 1 | A | 2728 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2729 | U |
| 1 | A | 2737 | C |
| 1 | A | 2752 | U |
| 1 | A | 2753 | G |
| 1 | A | 2754 | G |
| 1 | A | 2762 | A |
| 1 | A | 2772 | C |
| 1 | A | 2777 | G |
| 1 | A | 2778 | G |
| 1 | A | 2800 | G |
| 1 | A | 2801 | A |
| 1 | A | 2803 | A |
| 1 | A | 2810 | C |
| 1 | A | 2814 | G |
| 1 | A | 2816 | G |
| 1 | A | 2817 | A |
| 1 | A | 2821 | C |
| 1 | A | 2841 | G |
| 1 | A | 2842 | U |
| 1 | A | 2843 | U |
| 1 | A | 2844 | C |
| 1 | A | 2845 | A |
| 1 | A | 2847 | A |
| 1 | A | 2849 | C |
| 1 | A | 2850 | G |
| 1 | A | 2861 | U |
| 1 | A | 2867 | C |
| 1 | A | 2871 | G |
| 1 | A | 2872 | A |
| 1 | A | 2887 | A |
| 1 | A | 2898 | G |
| 1 | A | 2899 | C |
| 1 | A | 2904 | U |
| 1 | A | 2907 | G |
| 1 | A | 2914 | G |
| 1 | A | 2921 | U |
| 1 | A | 2923 | U |
| 1 | A | 2935 | U |
| 1 | A | 2936 | A |
| 1 | A | 2938 | G |
| 1 | A | 2941 | A |
| 1 | A | 2942 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2947 | G |
| 1 | A | 2971 | A |
| 1 | A | 2975 | U |
| 1 | A | 2983 | C |
| 1 | A | 2996 | U |
| 1 | A | 2997 | G |
| 1 | A | 3004 | C |
| 1 | A | 3011 | A |
| 1 | A | 3012 | A |
| 1 | A | 3014 | U |
| 1 | A | 3028 | G |
| 1 | A | 3049 | A |
| 1 | A | 3056 | U |
| 1 | A | 3057 | U |
| 1 | A | 3058 | U |
| 1 | A | 3059 | G |
| 1 | A | 3078 | U |
| 1 | A | 3079 | U |
| 1 | A | 3086 | A |
| 1 | A | 3092 | C |
| 1 | A | 3102 | G |
| 1 | A | 3109 | G |
| 1 | A | 3110 | C |
| 1 | A | 3114 | A |
| 1 | A | 3115 | C |
| 1 | A | 3117 | C |
| 1 | A | 3122 | A |
| 1 | A | 3124 | G |
| 1 | A | 3128 | G |
| 1 | A | 3129 | A |
| 1 | A | 3130 | A |
| 1 | A | 3131 | U |
| 1 | A | 3142 | A |
| 1 | A | 3143 | C |
| 1 | A | 3153 | U |
| 1 | A | 3154 | C |
| 1 | A | 3155 | U |
| 1 | A | 3156 | U |
| 1 | A | 3157 | U |
| 1 | A | 3163 | A |
| 1 | A | 3164 | C |
| 1 | A | 3165 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 3170 | A |
| 1 | A | 3173 | G |
| 1 | A | 3174 | A |
| 1 | A | 3176 | G |
| 1 | A | 3179 | U |
| 1 | A | 3181 | C |
| 1 | A | 3187 | A |
| 1 | A | 3196 | U |
| 1 | A | 3197 | G |
| 1 | A | 3200 | G |
| 1 | A | 3202 | G |
| 1 | A | 3207 | U |
| 1 | A | 3208 | G |
| 1 | A | 3212 | C |
| 1 | A | 3213 | A |
| 1 | A | 3217 | C |
| 1 | A | 3218 | A |
| 1 | A | 3219 | G |
| 1 | A | 3228 | C |
| 1 | A | 3229 | G |
| 1 | A | 3232 | G |
| 1 | A | 3234 | A |
| 1 | A | 3243 | A |
| 1 | A | 3244 | A |
| 1 | A | 3245 | A |
| 1 | A | 3246 | G |
| 1 | A | 3247 | G |
| 1 | A | 3249 | C |
| 1 | A | 3259 | U |
| 1 | A | 3260 | G |
| 1 | A | 3261 | C |
| 1 | A | 3263 | G |
| 1 | A | 3270 | U |
| 1 | A | 3271 | G |
| 1 | A | 3275 | U |
| 1 | A | 3276 | G |
| 1 | A | 3279 | A |
| 1 | A | 3280 | U |
| 1 | A | 3283 | U |
| 1 | A | 3284 | G |
| 1 | A | 3286 | G |
| 1 | A | 3289 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 3294 | A |
| 1 | A | 3295 | A |
| 1 | A | 3304 | U |
| 1 | A | 3308 | C |
| 1 | A | 3313 | U |
| 1 | A | 3316 | A |
| 1 | A | 3317 | U |
| 1 | A | 3318 | G |
| 1 | A | 3319 | U |
| 1 | A | 3320 | A |
| 1 | A | 3324 | C |
| 1 | A | 3325 | G |
| 1 | A | 3342 | A |
| 1 | A | 3345 | G |
| 1 | A | 3349 | C |
| 1 | A | 3350 | C |
| 1 | A | 3351 | U |
| 1 | A | 3352 | U |
| 1 | A | 3353 | G |
| 1 | A | 3354 | U |
| 1 | A | 3355 | U |
| 1 | A | 3356 | G |
| 1 | A | 3357 | U |
| 1 | A | 3363 | U |
| 1 | A | 3366 | G |
| 1 | A | 3368 | U |
| 1 | A | 3369 | G |
| 1 | A | 3375 | A |
| 1 | A | 3378 | C |
| 1 | A | 3382 | U |
| 1 | A | 3383 | G |
| 1 | A | 3386 | G |
| 1 | A | 3390 | G |
| 1 | A | 3396 | U |
| 2 | B | 10 | C |
| 2 | B | 19 | C |
| 2 | B | 22 | A |
| 2 | B | 42 | A |
| 2 | B | 49 | G |
| 2 | B | 52 | G |
| 2 | B | 53 | U |
| 2 | B | 54 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 55 | A |
| 2 | B | 56 | A |
| 2 | B | 60 | G |
| 2 | B | 65 | G |
| 2 | B | 71 | G |
| 2 | B | 73 | C |
| 2 | B | 91 | G |
| 2 | B | 99 | G |
| 2 | B | 101 | G |
| 2 | B | 102 | A |
| 2 | B | 112 | G |
| 2 | B | 114 | U |
| 2 | B | 120 | C |
| 2 | B | 121 | U |
| 3 | C | 2 | A |
| 3 | C | 23 | U |
| 3 | C | 24 | G |
| 3 | C | 34 | U |
| 3 | C | 35 | C |
| 3 | C | 50 | C |
| 3 | C | 52 | A |
| 3 | C | 53 | A |
| 3 | C | 57 | C |
| 3 | C | 59 | A |
| 3 | C | 62 | C |
| 3 | C | 63 | G |
| 3 | C | 80 | A |
| 3 | C | 81 | U |
| 3 | C | 82 | U |
| 3 | C | 83 | C |
| 3 | C | 84 | C |
| 3 | C | 86 | U |
| 3 | C | 87 | G |
| 3 | C | 90 | U |
| 3 | C | 91 | C |
| 3 | C | 95 | G |
| 3 | C | 104 | A |
| 3 | C | 106 | C |
| 3 | C | 108 | C |
| 3 | C | 111 | A |
| 3 | C | 113 | U |
| 3 | C | 125 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 126 | A |
| 3 | C | 129 | C |
| 3 | C | 136 | G |
| 3 | C | 138 | A |
| 3 | C | 146 | U |
| 3 | C | 148 | G |
| 3 | C | 151 | C |
| 3 | C | 152 | G |
| 3 | C | 155 | A |
| 3 | C | 158 | U |

All (82) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 65 | A |
| 1 | A | 169 | U |
| 1 | A | 239 | G |
| 1 | A | 518 | G |
| 1 | A | 547 | G |
| 1 | A | 558 | U |
| 1 | A | 588 | G |
| 1 | A | 594 | U |
| 1 | A | 599 | C |
| 1 | A | 619 | A |
| 1 | A | 770 | G |
| 1 | A | 873 | C |
| 1 | A | 896 | A |
| 1 | A | 916 | G |
| 1 | A | 959 | C |
| 1 | A | 960 | U |
| 1 | A | 979 | U |
| 1 | A | 993 | G |
| 1 | A | 1064 | A |
| 1 | A | 1097 | G |
| 1 | A | 1103 | A |
| 1 | A | 1263 | A |
| 1 | A | 1307 | G |
| 1 | A | 1329 | U |
| 1 | A | 1352 | A |
| 1 | A | 1355 | A |
| 1 | A | 1482 | A |
| 1 | A | 1554 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1556 | C |
| 1 | A | 1562 | C |
| 1 | A | 1576 | G |
| 1 | A | 1716 | U |
| 1 | A | 1778 | G |
| 1 | A | 1814 | A |
| 1 | A | 1815 | U |
| 1 | A | 1816 | A |
| 1 | A | 1820 | U |
| 1 | A | 1841 | A |
| 1 | A | 1846 | C |
| 1 | A | 1858 | A |
| 1 | A | 2101 | C |
| 1 | A | 2112 | U |
| 1 | A | 2144 | A |
| 1 | A | 2209 | U |
| 1 | A | 2249 | G |
| 1 | A | 2269 | U |
| 1 | A | 2281 | A |
| 1 | A | 2418 | G |
| 1 | A | 2434 | U |
| 1 | A | 2453 | U |
| 1 | A | 2495 | C |
| 1 | A | 2496 | C |
| 1 | A | 2501 | U |
| 1 | A | 2506 | U |
| 1 | A | 2513 | U |
| 1 | A | 2537 | U |
| 1 | A | 2541 | U |
| 1 | A | 2585 | G |
| 1 | A | 2593 | A |
| 1 | A | 2754 | G |
| 1 | A | 2801 | A |
| 1 | A | 2983 | C |
| 1 | A | 3003 | G |
| 1 | A | 3048 | A |
| 1 | A | 3055 | U |
| 1 | A | 3056 | U |
| 1 | A | 3057 | U |
| 1 | A | 3078 | U |
| 1 | A | 3195 | U |
| 1 | A | 3218 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 3228 | C |
| 1 | A | 3242 | G |
| 1 | A | 3269 | U |
| 1 | A | 3317 | U |
| 1 | A | 3350 | C |
| 1 | A | 3351 | U |
| 1 | A | 3353 | G |
| 2 | B | 52 | G |
| 2 | B | 111 | U |
| 3 | C | 80 | A |
| 3 | C | 82 | U |
| 3 | C | 85 | G |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 89 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.