



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 24, 2017 – 07:40 AM EDT

PDB ID : 5LZB
EMDB ID: : EMD-4122
Title : Structure of SelB-Sec-tRNA^{Sec} bound to the 70S ribosome in the initial binding state (IB)
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : unknown
Resolution : 5.30 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.

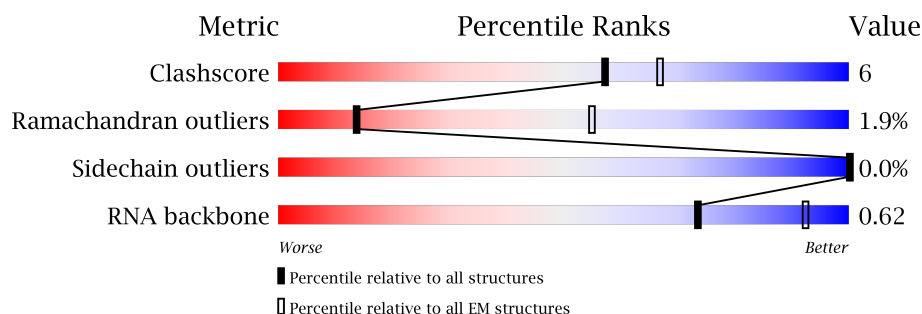
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance

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

The reported resolution of this entry is 5.30 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.



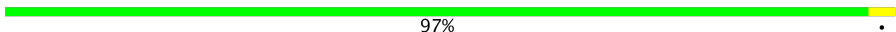

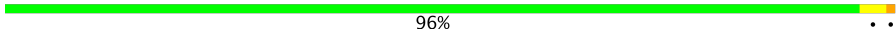
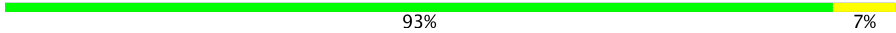
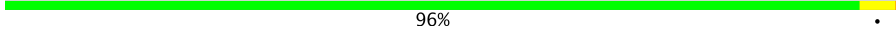
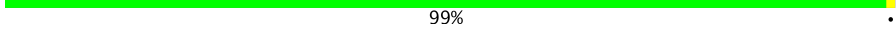
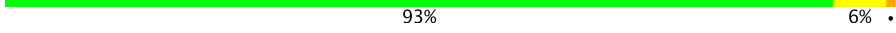
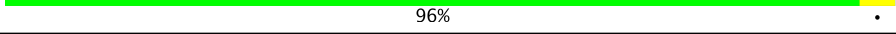
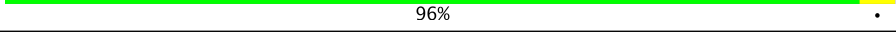

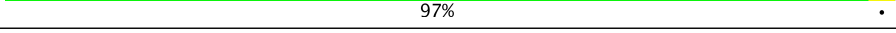
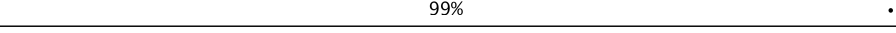
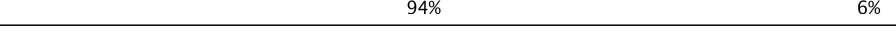
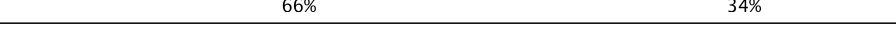
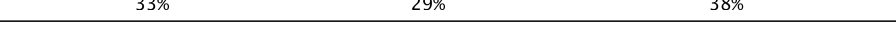

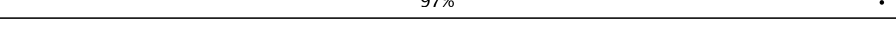
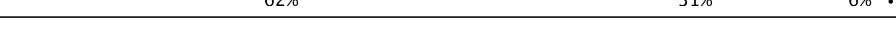


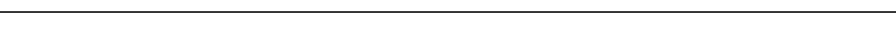




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |
| RNA backbone | 3398 | 335 |

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 | 1539 | 75% 22% . |
| 2 | b | 218 | 96% . |
| 3 | c | 206 | 97% . |
| 4 | d | 205 | 97% . |
| 5 | e | 157 | 95% 5% |
| 6 | f | 100 | 95% 5% |
| 7 | g | 151 | 97% . |
| 8 | h | 129 | 98% . |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 9 | i | 127 |  97% . |
| 10 | j | 98 |  92% 7% . |
| 11 | k | 116 |  96% .. |
| 12 | l | 123 |  93% 7% |
| 13 | m | 114 |  96% .. |
| 14 | n | 100 |  99% . |
| 15 | o | 88 |  93% 6% . |
| 16 | p | 82 |  96% . |
| 17 | q | 80 |  96% . |
| 18 | r | 65 |  92% 8% |
| 19 | s | 79 |  97% . |
| 20 | t | 85 |  99% . |
| 21 | u | 65 |  94% 6% |
| 22 | v | 77 |  66% 34% |
| 23 | x | 48 |  33% 29% 38% |
| 24 | y | 95 |  44% 39% 17% |
| 25 | z | 614 |  97% . |
| 26 | A | 2903 |  62% 31% 6% . |
| 27 | B | 120 |  64% 29% 5% . |
| 28 | C | 271 |  82% 17% |
| 29 | D | 209 |  78% 22% |
| 30 | E | 201 |  87% 13% |
| 31 | F | 177 |  81% 18% . |
| 32 | G | 176 |  74% 23% . |
| 33 | I | 141 |  78% 21% .. |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 34 | H | 149 |  83% 15% . |
| 35 | J | 142 |  82% 17% . |
| 36 | K | 122 |  78% 21% . |
| 37 | L | 143 |  78% 22% . |
| 38 | M | 136 |  81% 18% . |
| 39 | N | 120 |  82% 18% |
| 40 | O | 116 |  83% 17% |
| 41 | P | 114 |  81% 19% |
| 42 | Q | 117 |  85% 15% |
| 43 | R | 103 |  80% 20% |
| 44 | S | 110 |  87% 11% . |
| 45 | T | 93 |  75% 24% . |
| 46 | U | 102 |  67% 31% . |
| 47 | V | 94 |  86% 14% |
| 48 | W | 75 |  83% 17% |
| 49 | X | 77 |  91% 9% |
| 50 | Y | 63 |  83% 16% . |
| 51 | Z | 58 |  76% 24% |
| 52 | 0 | 56 |  84% 16% |
| 53 | 1 | 50 |  76% 24% |
| 54 | 2 | 46 |  87% 13% |
| 55 | 3 | 64 |  86% 13% . |
| 56 | 4 | 38 |  82% 16% . |
| 57 | 6 | 66 |  73% 21% 6% |
| 58 | w | 3 |  100% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 1 | G7M | a | 527 | X | - | - | - |
| 26 | G7M | A | 2069 | X | - | - | - |

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 152991 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 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1 | a | 1539 | Total | C | N | O | P | 0 | 0 |
| | | | 33029 | 14738 | 6052 | 10700 | 1539 | | |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | b | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1705 | 1081 | 305 | 312 | 7 | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3 | c | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1625 | 1028 | 305 | 289 | 3 | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | e | 157 | Total | C | N | O | S | 0 | 0 |
| | | | 1157 | 719 | 218 | 214 | 6 | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | f | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 818 | 515 | 148 | 149 | 6 | | |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | g | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1182 | 735 | 227 | 216 | 4 | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | h | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | i | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | j | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 787 | 493 | 150 | 143 | 1 | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | k | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 870 | 535 | 173 | 159 | 3 | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | l | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | m | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 884 | 546 | 178 | 157 | 3 | | |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | n | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 794 | 495 | 164 | 132 | 3 | | |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | o | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | p | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | q | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 649 | 411 | 121 | 114 | 3 | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 18 | r | 65 | Total | C | N | O | 0 | 0 |
| | | | 505 | 317 | 96 | 92 | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | s | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 638 | 408 | 120 | 108 | 2 | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | t | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 21 | u | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 496 | 307 | 100 | 88 | 1 | | |

- Molecule 22 is a RNA chain called fMet-tRNA^{fMet}.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|---|
| 22 | v | 77 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1642 | 733 | 297 | 534 | 77 | 1 | | |

- Molecule 23 is a RNA chain called SECIS mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23 | x | 48 | Total | C | N | O | P | 0 | 0 |
| | | | 1025 | 457 | 183 | 337 | 48 | | |

- Molecule 24 is a RNA chain called Sec-tRNA^{Sec}.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 24 | y | 95 | Total | C | N | O | P | 0 | 0 |
| | | | 2031 | 907 | 357 | 672 | 95 | | |

- Molecule 25 is a protein called Selenocysteine-specific elongation factor.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25 | z | 614 | Total | C | N | O | S | 1 | 0 |
| | | | 4863 | 3049 | 904 | 893 | 17 | | |

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 26 | A | 2903 | Total | C | N | O | P | 0 | 0 |
| | | | 62335 | 27815 | 11467 | 20150 | 2903 | | |

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 27 | B | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2570 | 1144 | 468 | 838 | 120 | | |

- Molecule 28 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28 | C | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2083 | 1288 | 423 | 365 | 7 | | |

- Molecule 29 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | D | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | |

- Molecule 30 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | E | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 31 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | F | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1411 | 899 | 249 | 257 | 6 | | |

- Molecule 32 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | G | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 33 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | I | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | |

- Molecule 34 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | H | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | |

- Molecule 35 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | J | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 36 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | K | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 939 | 587 | 180 | 166 | 6 | | |

- Molecule 37 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | L | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | |

- Molecule 38 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | M | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | |

- Molecule 39 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | N | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 961 | 593 | 196 | 167 | 5 | | |

- Molecule 40 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 40 | O | 116 | Total | C | N | O | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | |

- Molecule 41 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | P | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 42 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 42 | Q | 117 | Total | C | N | O | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | |

- Molecule 43 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | R | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 44 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | S | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 45 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | T | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 739 | 466 | 139 | 132 | 2 | | |

- Molecule 46 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 46 | U | 102 | Total | C | N | O | 0 | 0 |
| | | | 780 | 492 | 146 | 142 | | |

- Molecule 47 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47 | V | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 48 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | W | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 575 | 356 | 116 | 102 | 1 | | |

- Molecule 49 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49 | X | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50 | Y | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | |

- Molecule 51 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51 | Z | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

- Molecule 52 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 52 | 0 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

- Molecule 53 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 53 | 1 | 50 | Total | C | N | O | 0 | 0 |
| | | | 410 | 263 | 75 | 72 | | |

- Molecule 54 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54 | 2 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

- Molecule 55 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 55 | 3 | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 56 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 56 | 4 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

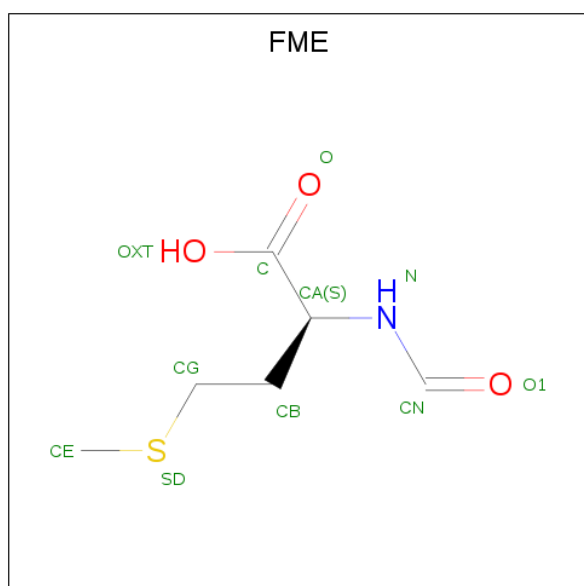
- Molecule 57 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 57 | 6 | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 523 | 323 | 99 | 95 | 6 | | |

- Molecule 58 is a RNA chain called CCA 3' end of E-site tRNA^{Sec} (low occupancy).

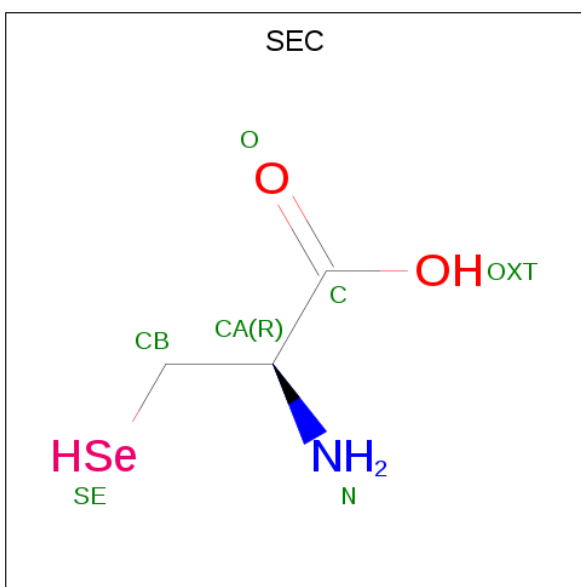
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 58 | w | 3 | Total | C | N | O | P | 0 | 0 |
| | | | 62 | 28 | 11 | 20 | 3 | | |

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



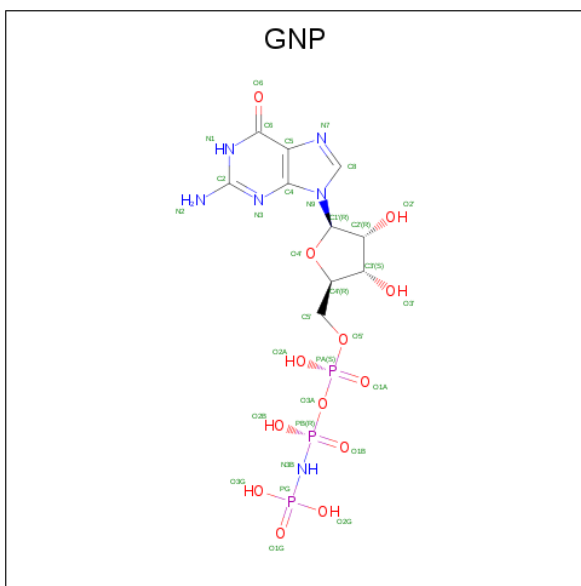
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 59 | v | 1 | Total | C | N | O | S | 0 |
| | | | 10 | 6 | 1 | 2 | 1 | |

- Molecule 60 is SELENOCYSTEINE (three-letter code: SEC) (formula: C₃H₇NO₂Se).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 60 | y | 1 | Total 6 | C 3 | N 1 | O 1 | Se 1 | 0 |

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{13}\text{P}_3$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 61 | z | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 6 | 13 | 3 | |

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 62 | z | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 63 | 4 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 63 | 6 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

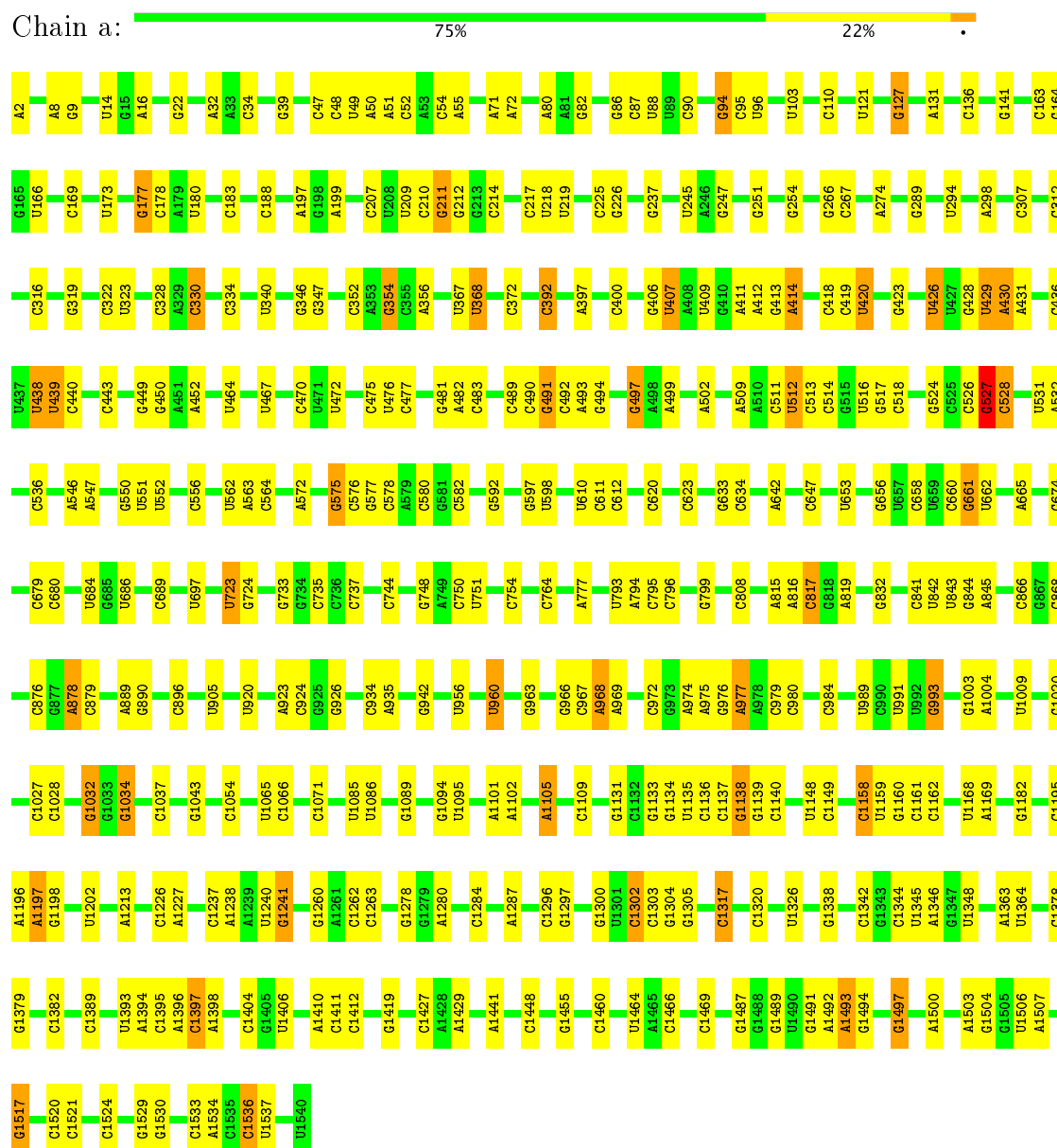
- Molecule 64 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|---|---------|
| 64 | z | 2 | Total | O | 0 |
| | | | 2 | 2 | |

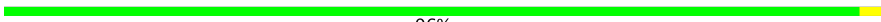
3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA



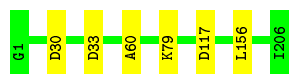
- Molecule 2: 30S ribosomal protein S2

Chain b:  96% .



- Molecule 3: 30S ribosomal protein S3

Chain c:  97% .



- Molecule 4: 30S ribosomal protein S4

Chain d:  97% .



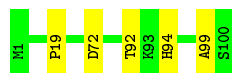
- Molecule 5: 30S ribosomal protein S5

Chain e:  95% 5%



- Molecule 6: 30S ribosomal protein S6

Chain f:  95% 5%



- Molecule 7: 30S ribosomal protein S7

Chain g:  97% .



- Molecule 8: 30S ribosomal protein S8

Chain h:  98% .



- Molecule 9: 30S ribosomal protein S9

Chain i:  97% .



- Molecule 10: 30S ribosomal protein S10

Chain j: 92% 7% .



- Molecule 11: 30S ribosomal protein S11

Chain k: 96% . .



- Molecule 12: 30S ribosomal protein S12

Chain l: 93% 7%



- Molecule 13: 30S ribosomal protein S13

Chain m: 96% . .



- Molecule 14: 30S ribosomal protein S14

Chain n: 99% .



- Molecule 15: 30S ribosomal protein S15

Chain o: 93% 6% .



- Molecule 16: 30S ribosomal protein S16

Chain p: 96% .



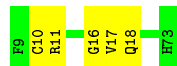
- Molecule 17: 30S ribosomal protein S17

Chain q:  96% .



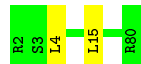
- Molecule 18: 30S ribosomal protein S18

Chain r:  92% 8%



- Molecule 19: 30S ribosomal protein S19

Chain s:  97% .



- Molecule 20: 30S ribosomal protein S20

Chain t:  99% .



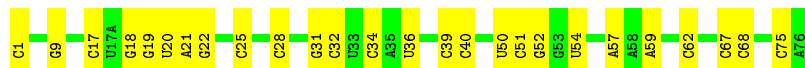
- Molecule 21: 30S ribosomal protein S21

Chain u:  94% 6%

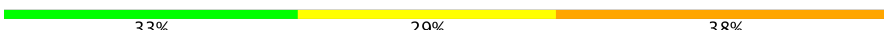


- Molecule 22: fMet-tRNA^{fMet}

Chain v:  66% 34%



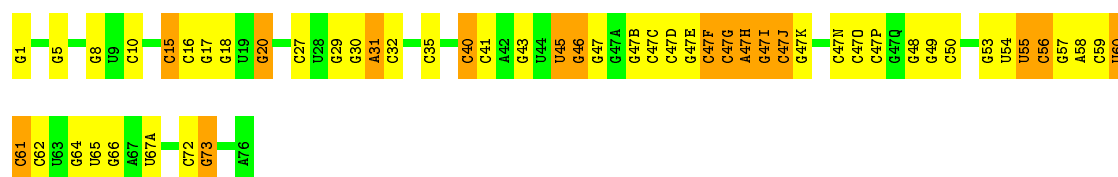
- Molecule 23: SECIS mRNA

Chain x:  33% 29% 38%



- Molecule 24: Sec-tRNA^{Sec}

Chain y:  44% 39% 17%



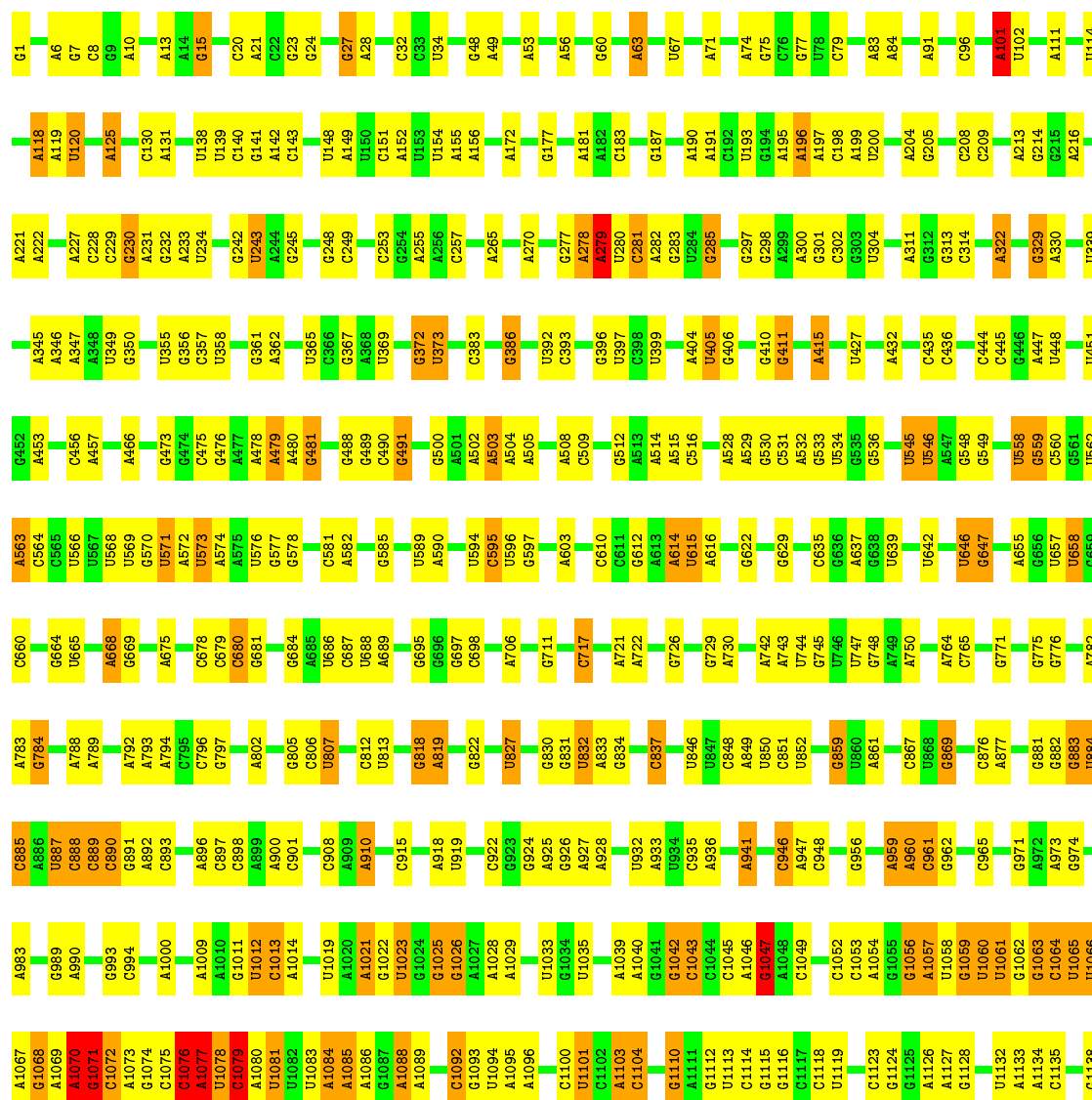
- Molecule 25: Selenocysteine-specific elongation factor

Chain z: 97%

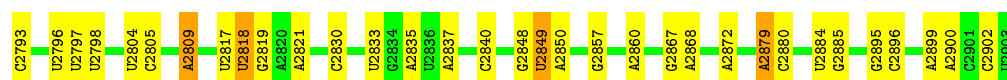


- Molecule 26: 23S ribosomal RNA

Chain A: 62% 31% 6%

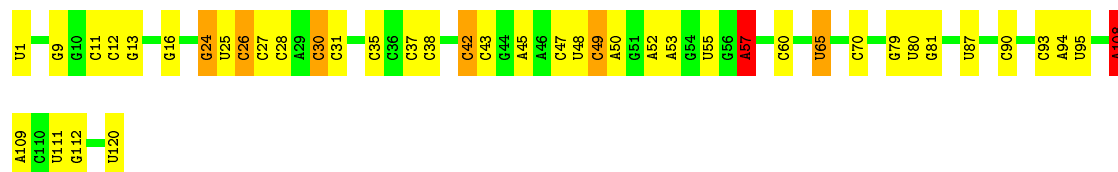


| | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2663 | G2567 | A2478 | G2375 | A2173 | C2104 | C1905 | A1668 | A1569 | A1469 | G1250 | A1142 |
| U2684 | U2568 | U2479 | A2378 | C2174 | U2105 | G1906 | A1669 | A1570 | A1470 | C1251 | A1143 |
| G2689 | A2572 | C2480 | G2378 | C2175 | U2106 | G1907 | A1670 | A1571 | A1353 | G1252 | |
| U2690 | G2573 | G2481 | G2383 | A2176 | G2107 | A1913 | G1673 | A1572 | G1475 | A1254 | G1149 |
| C2691 | G2574 | C2482 | U2384 | C2177 | A2108 | G1914 | G1674 | A1359 | A1476 | C1255 | C1150 |
| | G2575 | G2483 | C2385 | C2178 | U2109 | G1915 | C1675 | A1359 | A1477 | G1256 | A1151 |
| U2698 | G2576 | G2484 | U2390 | C2179 | G2110 | A1916 | | A1365 | G1478 | C1257 | C1152 |
| C2699 | | G2485 | U2391 | U2180 | U2111 | | U1680 | | G1482 | U1258 | C1153 |
| A2700 | U2579 | G2488 | U2393 | U2181 | G2112 | C1924 | U1681 | A1378 | A1485 | G1259 | G1154 |
| U2701 | U2580 | C2394 | A2183 | U2182 | U2113 | A1927 | U1682 | A1379 | A1486 | A1260 | A1155 |
| G2702 | G2581 | U2184 | U2185 | A2186 | A2114 | G1928 | G1687 | G1380 | U1487 | C1261 | |
| | G2582 | G2186 | U2187 | U2187 | A2115 | G1929 | | | | | |
| U2707 | U2583 | U2402 | U2403 | U2188 | A2116 | G1930 | | | | | |
| | U2584 | U2404 | A2405 | U2189 | G2117 | | | | | | |
| C2710 | U2585 | A2406 | A2407 | G2120 | A2118 | | | | | | |
| | | A2407 | | G2121 | A2119 | | | | | | |
| G2714 | C2591 | U2500 | U2408 | G2122 | A2120 | C1934 | | | | | |
| C2715 | G2592 | G2502 | U2409 | G2123 | G2125 | G1935 | | | | | |
| G2716 | | A2503 | A2411 | G2127 | A2126 | A1936 | | | | | |
| G2717 | G2595 | U2504 | | U2128 | G2128 | A1937 | | | | | |
| G2718 | A2598 | G2505 | C2416 | C2129 | U2130 | U1938 | | | | | |
| G2719 | G2599 | U2506 | | U2131 | U2131 | G1811 | | | | | |
| U2720 | A2600 | | U2419 | U2132 | C2044 | U1940 | | | | | |
| | C2601 | C2512 | | G2133 | C2045 | C1942 | | | | | |
| A2726 | A2602 | A2513 | C2427 | A2134 | G2046 | U1943 | | | | | |
| G2733 | U2603 | G2514 | G2428 | A2135 | C2047 | | | | | | |
| G2734 | U2604 | G2515 | G2429 | A2136 | U2048 | U1955 | | | | | |
| | U2605 | A2516 | A2430 | G2136 | A2051 | U1956 | | | | | |
| U2739 | C2606 | U2517 | A2434 | G2140 | A2052 | C1957 | | | | | |
| | | U2519 | A2435 | G2141 | | G1958 | | | | | |
| U2742 | U2609 | G2520 | A2436 | A2142 | C2055 | G1959 | | | | | |
| U2743 | C2610 | U2521 | | C2143 | G2056 | A1960 | | | | | |
| U2744 | U2613 | U2522 | | G2144 | G2057 | C1961 | | | | | |
| U2745 | U2614 | | U2441 | C2145 | A2058 | U1963 | | | | | |
| U2746 | U2615 | G2525 | C2442 | C2146 | A2059 | G1964 | | | | | |
| | U2617 | | G2443 | A2147 | A2060 | | | | | | |
| C2752 | C2616 | U2529 | G2444 | | | | | | | | |
| U2755 | U2617 | A2530 | G2445 | C2150 | A2062 | C1967 | | | | | |
| A2757 | C2626 | U2531 | G2446 | U2151 | C2065 | U1971 | | | | | |
| | | G2532 | G2447 | G2152 | C2066 | G1972 | | | | | |
| U2759 | U2629 | A2542 | A2448 | G2156 | | | | | | | |
| | G2630 | | G2455 | G2157 | G2069 | U1976 | | | | | |
| | | U2547 | C2456 | A2158 | A2070 | | | | | | |
| A2764 | C2636 | A2548 | U2457 | G2159 | A2071 | U1982 | | | | | |
| A2765 | U2637 | G2549 | | C2160 | | | | | | | |
| U2766 | G2638 | G2550 | C2462 | C2161 | U1990 | C1990 | | | | | |
| | A2639 | | | G2162 | U1991 | G1992 | | | | | |
| C2773 | | U2554 | C2466 | A2163 | G1993 | U1993 | | | | | |
| | | U2555 | | C2164 | A1985 | | | | | | |
| A2778 | C2645 | C2556 | A2469 | U2165 | U1986 | C1995 | | | | | |
| | U2647 | G2557 | G2470 | U2166 | C1996 | C1996 | | | | | |
| G2782 | G2648 | C2558 | | U2167 | G2087 | U1997 | | | | | |
| | C2649 | | U2473 | G2168 | A2088 | A1998 | | | | | |
| C2788 | | U2562 | U2474 | A2169 | G2100 | | | | | | |
| | U2656 | A2565 | C2475 | A2170 | | G2002 | | | | | |
| G2791 | A2657 | A2566 | U2477 | A2171 | C2103 | U2007 | | | | | |
| A2792 | | | | U2172 | | | | | | | |



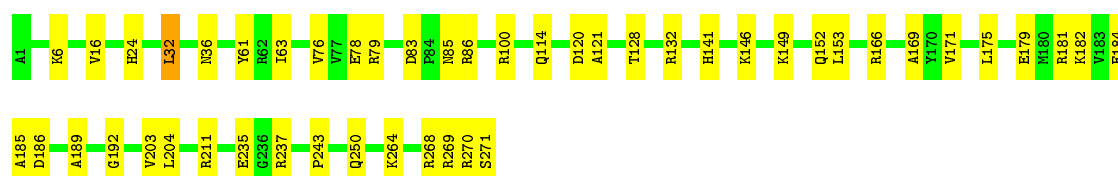
• Molecule 27: 5S ribosomal RNA

Chain B: 64% 29% 5% .



• Molecule 28: 50S ribosomal protein L2

Chain C: 82% 17%



• Molecule 29: 50S ribosomal protein L3

Chain D: 78% 22%



• Molecule 30: 50S ribosomal protein L4

Chain E: 87% 13%



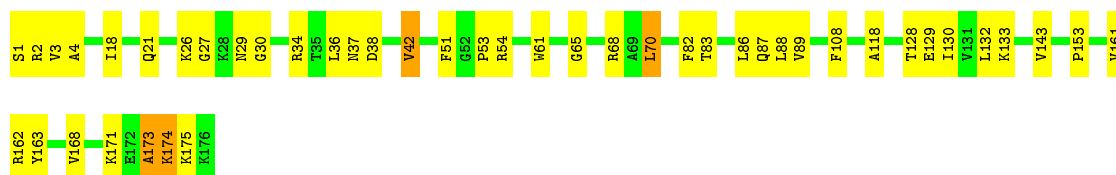
• Molecule 31: 50S ribosomal protein L5

Chain F: 81% 18%



• Molecule 32: 50S ribosomal protein L6

Chain G: 74% 23%



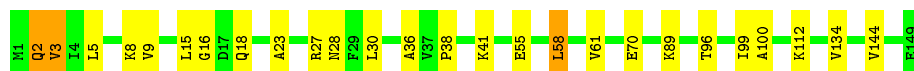
- Molecule 33: 50S ribosomal protein L11

Chain I: 78% 21% ..



- Molecule 34: 50S ribosomal protein L9

Chain H: 83% 15% .



- Molecule 35: 50S ribosomal protein L13

Chain J: 82% 17% .



- Molecule 36: 50S ribosomal protein L14

Chain K: 78% 21% .



- Molecule 37: 50S ribosomal protein L15

Chain L: 78% 22% .



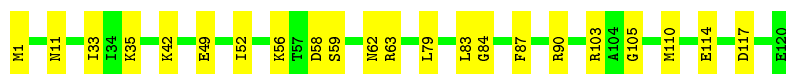
- Molecule 38: 50S ribosomal protein L16

Chain M: 81% 18% .



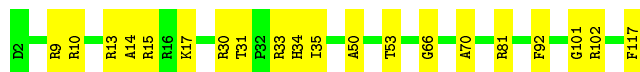
- Molecule 39: 50S ribosomal protein L17

Chain N: 82% 18%



- Molecule 40: 50S ribosomal protein L18

Chain O: 83% 17%



- Molecule 41: 50S ribosomal protein L19

Chain P: 81% 19%



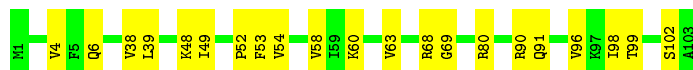
- Molecule 42: 50S ribosomal protein L20

Chain Q: 85% 15%



- Molecule 43: 50S ribosomal protein L21

Chain R: 80% 20%



- Molecule 44: 50S ribosomal protein L22

Chain S: 87% 11%



- Molecule 45: 50S ribosomal protein L23

Chain T: 75% 24%

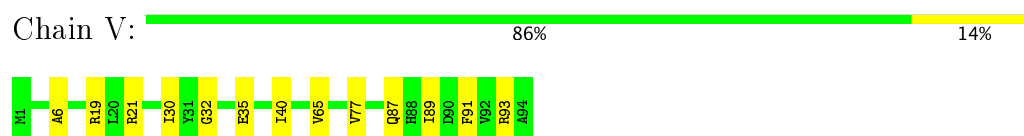


- Molecule 46: 50S ribosomal protein L24

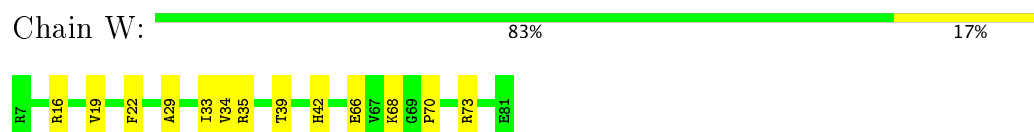
Chain U: 67% 31%



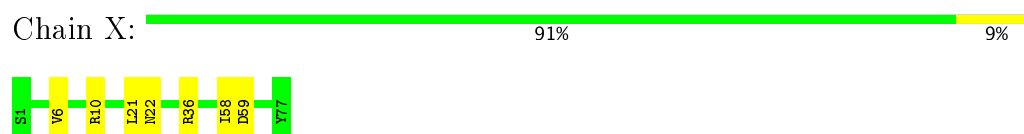
- Molecule 47: 50S ribosomal protein L25



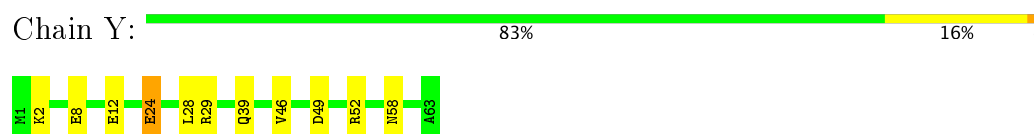
- Molecule 48: 50S ribosomal protein L27



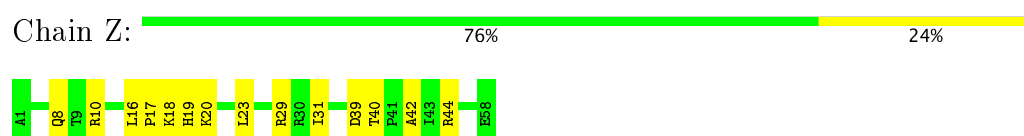
- Molecule 49: 50S ribosomal protein L28



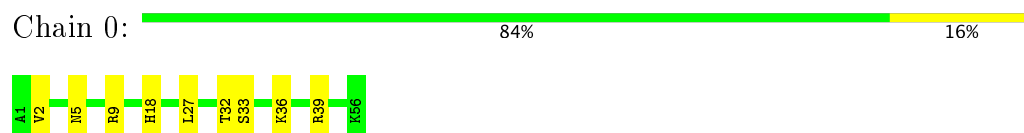
- Molecule 50: 50S ribosomal protein L29



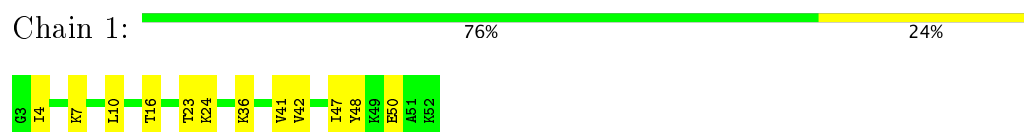
- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



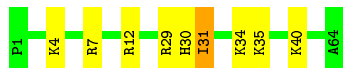
- Molecule 54: 50S ribosomal protein L34





- Molecule 55: 50S ribosomal protein L35

Chain 3: 86% 13% .



- Molecule 56: 50S ribosomal protein L36

Chain 4: 82% 16% .



- Molecule 57: 50S ribosomal protein L31

Chain 6: 73% 21% 6%



- Molecule 58: CCA 3' end of E-site tRNA^{Sec} (low occupancy)

Chain w: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

| Property | Value | Source |
|--------------------------------------|--|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 8002 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 30 | Depositor |
| Minimum defocus (nm) | 700 | Depositor |
| Maximum defocus (nm) | 2600 | Depositor |
| Magnification | 59000 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 0.58 | 3/36701 (0.0%) | 1.30 | 392/57246 (0.7%) |
| 10 | j | 0.44 | 0/797 | 0.87 | 1/1077 (0.1%) |
| 11 | k | 0.48 | 0/886 | 0.87 | 3/1195 (0.3%) |
| 12 | l | 0.43 | 0/969 | 0.79 | 1/1300 (0.1%) |
| 13 | m | 0.42 | 0/893 | 0.90 | 1/1193 (0.1%) |
| 14 | n | 0.45 | 0/806 | 0.82 | 1/1074 (0.1%) |
| 15 | o | 0.42 | 0/722 | 0.81 | 3/964 (0.3%) |
| 16 | p | 0.55 | 0/659 | 0.78 | 0/884 |
| 17 | q | 0.45 | 0/658 | 0.88 | 0/881 |
| 18 | r | 0.36 | 0/512 | 0.67 | 0/689 |
| 19 | s | 0.37 | 0/653 | 0.73 | 2/877 (0.2%) |
| 2 | b | 0.45 | 0/1736 | 0.85 | 4/2338 (0.2%) |
| 20 | t | 0.43 | 0/671 | 0.77 | 0/888 |
| 21 | u | 0.43 | 0/501 | 0.85 | 1/668 (0.1%) |
| 22 | v | 0.62 | 2/1745 (0.1%) | 1.33 | 25/2716 (0.9%) |
| 23 | x | 0.88 | 1/1145 (0.1%) | 1.84 | 45/1781 (2.5%) |
| 24 | y | 0.89 | 2/2168 (0.1%) | 1.92 | 110/3375 (3.3%) |
| 25 | z | 0.47 | 0/4963 | 0.89 | 12/6727 (0.2%) |
| 26 | A | 0.57 | 13/69240 (0.0%) | 1.24 | 539/108014 (0.5%) |
| 27 | B | 0.58 | 1/2873 (0.0%) | 1.24 | 27/4478 (0.6%) |
| 28 | C | 0.42 | 0/2122 | 0.77 | 1/2852 (0.0%) |
| 29 | D | 0.45 | 0/1586 | 0.75 | 0/2134 |
| 3 | c | 0.41 | 0/1652 | 0.76 | 3/2225 (0.1%) |
| 30 | E | 0.43 | 0/1571 | 0.75 | 2/2113 (0.1%) |
| 31 | F | 0.52 | 1/1435 (0.1%) | 0.90 | 4/1926 (0.2%) |
| 32 | G | 0.47 | 0/1343 | 0.82 | 3/1816 (0.2%) |
| 33 | I | 0.49 | 0/1046 | 0.97 | 5/1410 (0.4%) |
| 34 | H | 0.40 | 0/1122 | 0.74 | 1/1515 (0.1%) |
| 35 | J | 0.42 | 0/1152 | 0.70 | 2/1551 (0.1%) |
| 36 | K | 0.47 | 0/948 | 0.75 | 0/1268 |
| 37 | L | 0.42 | 0/1054 | 0.75 | 0/1403 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 38 | M | 0.43 | 0/1093 | 0.74 | 1/1460 (0.1%) |
| 39 | N | 0.43 | 0/974 | 0.68 | 0/1301 |
| 4 | d | 0.49 | 0/1665 | 0.93 | 3/2227 (0.1%) |
| 40 | O | 0.43 | 0/902 | 0.72 | 0/1209 |
| 41 | P | 0.43 | 0/929 | 0.72 | 1/1242 (0.1%) |
| 42 | Q | 0.41 | 0/960 | 0.58 | 1/1278 (0.1%) |
| 43 | R | 0.42 | 0/829 | 0.79 | 0/1107 |
| 44 | S | 0.39 | 0/864 | 0.80 | 2/1156 (0.2%) |
| 45 | T | 0.44 | 0/745 | 0.77 | 0/994 |
| 46 | U | 0.43 | 0/788 | 0.91 | 1/1051 (0.1%) |
| 47 | V | 0.47 | 0/766 | 0.72 | 0/1025 |
| 48 | W | 0.39 | 0/582 | 0.69 | 0/769 |
| 49 | X | 0.35 | 0/635 | 0.70 | 1/848 (0.1%) |
| 5 | e | 0.45 | 0/1170 | 0.88 | 0/1573 |
| 50 | Y | 0.48 | 0/510 | 0.92 | 2/677 (0.3%) |
| 51 | Z | 0.40 | 0/453 | 0.72 | 1/605 (0.2%) |
| 52 | 0 | 0.44 | 0/450 | 0.80 | 0/599 |
| 53 | 1 | 0.36 | 0/417 | 0.77 | 0/554 |
| 54 | 2 | 0.40 | 0/380 | 0.69 | 0/498 |
| 55 | 3 | 0.40 | 0/513 | 0.63 | 0/676 |
| 56 | 4 | 0.48 | 0/303 | 0.80 | 1/397 (0.3%) |
| 57 | 6 | 0.46 | 0/532 | 1.01 | 5/709 (0.7%) |
| 58 | w | 0.32 | 0/68 | 0.98 | 0/103 |
| 6 | f | 0.51 | 0/836 | 0.85 | 1/1128 (0.1%) |
| 7 | g | 0.46 | 0/1196 | 0.81 | 2/1602 (0.1%) |
| 8 | h | 0.43 | 0/989 | 0.78 | 1/1326 (0.1%) |
| 9 | i | 0.47 | 0/1034 | 0.84 | 0/1375 |
| All | All | 0.55 | 23/164912 (0.0%) | 1.17 | 1211/246067 (0.5%) |

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 |
|-----|-------|---------------------|---------------------|
| 1 | a | 2 | 0 |
| 10 | j | 0 | 2 |
| 11 | k | 0 | 1 |
| 12 | l | 0 | 2 |
| 13 | m | 0 | 2 |
| 15 | o | 0 | 1 |
| 18 | r | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | b | 0 | 2 |
| 25 | z | 0 | 3 |
| 26 | A | 2 | 0 |
| 28 | C | 0 | 1 |
| 33 | I | 0 | 2 |
| 34 | H | 0 | 3 |
| 36 | K | 0 | 1 |
| 38 | M | 0 | 1 |
| 44 | S | 0 | 1 |
| 46 | U | 0 | 2 |
| 5 | e | 0 | 1 |
| 55 | 3 | 0 | 1 |
| All | All | 4 | 28 |

All (23) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 24 | y | 1 | G | OP3-P | -10.71 | 1.48 | 1.61 |
| 22 | v | 1 | C | OP3-P | -10.67 | 1.48 | 1.61 |
| 23 | x | 87 | A | OP3-P | -10.65 | 1.48 | 1.61 |
| 1 | a | 2 | A | OP3-P | -10.60 | 1.48 | 1.61 |
| 27 | B | 1 | U | OP3-P | -10.57 | 1.48 | 1.61 |
| 26 | A | 1 | G | OP3-P | -10.57 | 1.48 | 1.61 |
| 26 | A | 2169 | A | C8-N7 | -9.34 | 1.25 | 1.31 |
| 26 | A | 571 | U | C4-O4 | 8.22 | 1.30 | 1.23 |
| 1 | a | 723 | U | C4-O4 | -6.98 | 1.18 | 1.23 |
| 26 | A | 2059 | A | N9-C4 | -6.42 | 1.34 | 1.37 |
| 26 | A | 1171 | G | C6-N1 | 6.16 | 1.43 | 1.39 |
| 26 | A | 2167 | U | N1-C2 | -6.15 | 1.33 | 1.38 |
| 26 | A | 1085 | A | N7-C5 | -6.04 | 1.35 | 1.39 |
| 31 | F | 11 | VAL | CB-CG1 | -5.89 | 1.40 | 1.52 |
| 26 | A | 2169 | A | N7-C5 | -5.56 | 1.35 | 1.39 |
| 26 | A | 1313 | U | N1-C2 | 5.49 | 1.43 | 1.38 |
| 24 | y | 61 | C | C5-C6 | -5.45 | 1.29 | 1.34 |
| 26 | A | 574 | A | N9-C4 | -5.16 | 1.34 | 1.37 |
| 26 | A | 1178 | C | N3-C4 | -5.09 | 1.30 | 1.33 |
| 26 | A | 101 | A | N9-C4 | -5.08 | 1.34 | 1.37 |
| 22 | v | 57 | A | N7-C5 | -5.07 | 1.36 | 1.39 |
| 26 | A | 278 | A | N9-C4 | 5.03 | 1.40 | 1.37 |
| 1 | a | 80 | A | N9-C4 | -5.00 | 1.34 | 1.37 |

All (1211) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|--------|-------------|----------|
| 1 | a | 452 | A | O5'-P-OP1 | -19.89 | 86.83 | 110.70 |
| 1 | a | 450 | G | O5'-P-OP1 | 16.99 | 131.09 | 110.70 |
| 26 | A | 1026 | G | O5'-P-OP1 | -15.92 | 91.37 | 105.70 |
| 26 | A | 2169 | A | C5-N7-C8 | 15.84 | 111.82 | 103.90 |
| 26 | A | 1178 | C | N1-C2-O2 | 15.82 | 128.39 | 118.90 |
| 26 | A | 1178 | C | N3-C2-O2 | -15.14 | 111.30 | 121.90 |
| 26 | A | 120 | U | C5-C4-O4 | -14.70 | 117.08 | 125.90 |
| 26 | A | 2059 | A | N1-C2-N3 | -14.28 | 122.16 | 129.30 |
| 26 | A | 890 | C | N1-C2-O2 | 14.17 | 127.40 | 118.90 |
| 1 | a | 1158 | C | N1-C2-O2 | 13.98 | 127.29 | 118.90 |
| 26 | A | 1171 | G | N3-C2-N2 | -13.97 | 110.12 | 119.90 |
| 26 | A | 120 | U | N3-C4-O4 | 13.94 | 129.16 | 119.40 |
| 26 | A | 1313 | U | N1-C2-O2 | 13.34 | 132.14 | 122.80 |
| 26 | A | 1071 | G | C5-C6-O6 | -13.14 | 120.72 | 128.60 |
| 1 | a | 1158 | C | N3-C2-O2 | -12.84 | 112.92 | 121.90 |
| 1 | a | 1304 | G | O5'-P-OP2 | -12.64 | 94.32 | 105.70 |
| 26 | A | 1313 | U | N3-C2-O2 | -12.56 | 113.41 | 122.20 |
| 24 | y | 47(I) | G | O5'-P-OP2 | -12.20 | 94.72 | 105.70 |
| 26 | A | 2146 | C | O5'-P-OP1 | 12.19 | 125.33 | 110.70 |
| 26 | A | 1186 | G | O5'-P-OP2 | 12.09 | 125.20 | 110.70 |
| 1 | a | 1198 | G | O5'-P-OP2 | -11.90 | 94.99 | 105.70 |
| 24 | y | 61 | C | C6-N1-C2 | -11.44 | 115.72 | 120.30 |
| 26 | A | 1313 | U | C2-N1-C1' | 11.27 | 131.22 | 117.70 |
| 1 | a | 1197 | A | O5'-P-OP1 | -11.26 | 95.57 | 105.70 |
| 26 | A | 2109 | U | C5-C6-N1 | 11.05 | 128.23 | 122.70 |
| 46 | U | 51 | LEU | CA-CB-CG | 10.88 | 140.32 | 115.30 |
| 23 | x | 117 | C | N1-C2-O2 | 10.85 | 125.41 | 118.90 |
| 26 | A | 1093 | G | C5-C6-O6 | -10.75 | 122.15 | 128.60 |
| 26 | A | 2169 | A | C4-C5-N7 | -10.70 | 105.35 | 110.70 |
| 22 | v | 51 | C | C6-N1-C2 | -10.52 | 116.09 | 120.30 |
| 24 | y | 61 | C | C4-C5-C6 | 10.45 | 122.62 | 117.40 |
| 24 | y | 61 | C | N3-C4-C5 | -10.39 | 117.74 | 121.90 |
| 24 | y | 41 | C | C5-C6-N1 | 10.34 | 126.17 | 121.00 |
| 26 | A | 2305 | U | C5-C4-O4 | -10.29 | 119.72 | 125.90 |
| 24 | y | 47(D) | C | C6-N1-C2 | -10.19 | 116.22 | 120.30 |
| 24 | y | 47(D) | C | C5-C6-N1 | 10.13 | 126.06 | 121.00 |
| 26 | A | 1071 | G | N1-C6-O6 | 10.10 | 125.96 | 119.90 |
| 1 | a | 1054 | C | O5'-P-OP2 | -10.06 | 96.65 | 105.70 |
| 23 | x | 117 | C | N3-C2-O2 | -10.02 | 114.89 | 121.90 |
| 1 | a | 968 | A | N1-C6-N6 | -9.97 | 112.61 | 118.60 |
| 26 | A | 647 | G | O5'-P-OP1 | -9.92 | 96.77 | 105.70 |
| 1 | a | 1296 | C | C6-N1-C2 | -9.89 | 116.34 | 120.30 |
| 26 | A | 436 | C | O5'-P-OP2 | -9.84 | 96.84 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 22 | v | 51 | C | C5-C6-N1 | 9.80 | 125.90 | 121.00 |
| 26 | A | 1993 | U | N3-C2-O2 | -9.78 | 115.35 | 122.20 |
| 26 | A | 2059 | A | C6-N1-C2 | 9.73 | 124.44 | 118.60 |
| 26 | A | 1186 | G | O5'-P-OP1 | -9.71 | 96.96 | 105.70 |
| 26 | A | 887 | U | N3-C2-O2 | -9.71 | 115.41 | 122.20 |
| 26 | A | 2637 | U | C5-C6-N1 | 9.70 | 127.55 | 122.70 |
| 26 | A | 2583 | G | O5'-P-OP2 | -9.70 | 96.97 | 105.70 |
| 24 | y | 48 | G | N1-C6-O6 | 9.62 | 125.67 | 119.90 |
| 33 | I | 32 | VAL | CG1-CB-CG2 | -9.59 | 95.56 | 110.90 |
| 1 | a | 656 | G | N3-C2-N2 | -9.58 | 113.19 | 119.90 |
| 24 | y | 48 | G | C5-C6-O6 | -9.58 | 122.85 | 128.60 |
| 24 | y | 43 | G | O4'-C1'-N9 | 9.54 | 115.83 | 108.20 |
| 26 | A | 67 | U | C5-C4-O4 | -9.48 | 120.21 | 125.90 |
| 26 | A | 1539 | U | C5-C6-N1 | 9.46 | 127.43 | 122.70 |
| 26 | A | 1093 | G | N9-C4-C5 | -9.42 | 101.63 | 105.40 |
| 26 | A | 1079 | C | N1-C2-O2 | 9.38 | 124.53 | 118.90 |
| 1 | a | 414 | A | N1-C6-N6 | -9.35 | 112.99 | 118.60 |
| 26 | A | 2147 | A | C8-N9-C4 | -9.34 | 102.06 | 105.80 |
| 1 | a | 597 | G | O5'-P-OP2 | -9.30 | 97.33 | 105.70 |
| 1 | a | 214 | C | C5-C6-N1 | 9.29 | 125.65 | 121.00 |
| 1 | a | 1158 | C | C6-N1-C2 | -9.27 | 116.59 | 120.30 |
| 24 | y | 41 | C | C6-N1-C2 | -9.22 | 116.61 | 120.30 |
| 57 | 6 | 18 | CYS | CA-CB-SG | -9.22 | 97.40 | 114.00 |
| 26 | A | 890 | C | C2-N3-C4 | 9.16 | 124.48 | 119.90 |
| 26 | A | 2302 | U | N3-C2-O2 | -9.16 | 115.79 | 122.20 |
| 26 | A | 281 | C | C5-C6-N1 | 9.15 | 125.58 | 121.00 |
| 1 | a | 214 | C | C6-N1-C2 | -9.14 | 116.64 | 120.30 |
| 24 | y | 47(N) | C | C6-N1-C2 | -9.14 | 116.64 | 120.30 |
| 23 | x | 117 | C | C6-N1-C2 | -9.10 | 116.66 | 120.30 |
| 26 | A | 1783 | A | O5'-P-OP2 | -9.09 | 97.52 | 105.70 |
| 1 | a | 72 | A | O5'-P-OP2 | -9.08 | 97.53 | 105.70 |
| 1 | a | 1158 | C | C2-N1-C1' | 9.05 | 128.75 | 118.80 |
| 26 | A | 67 | U | N3-C4-O4 | 9.03 | 125.72 | 119.40 |
| 26 | A | 545 | U | C6-N1-C2 | -9.03 | 115.58 | 121.00 |
| 23 | x | 125 | G | N9-C1'-C2' | -9.02 | 102.07 | 112.00 |
| 26 | A | 2150 | C | C6-N1-C2 | -8.94 | 116.72 | 120.30 |
| 24 | y | 61 | C | N1-C2-O2 | 8.94 | 124.27 | 118.90 |
| 26 | A | 2428 | G | O5'-P-OP1 | 8.94 | 121.43 | 110.70 |
| 26 | A | 1171 | G | N9-C4-C5 | 8.92 | 108.97 | 105.40 |
| 24 | y | 47(C) | C | C6-N1-C2 | -8.87 | 116.75 | 120.30 |
| 26 | A | 2359 | C | C6-N1-C2 | -8.84 | 116.76 | 120.30 |
| 26 | A | 2617 | U | N3-C2-O2 | -8.79 | 116.04 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24 | y | 62 | C | N3-C2-O2 | -8.79 | 115.75 | 121.90 |
| 26 | A | 2325 | G | O5'-P-OP1 | 8.68 | 121.11 | 110.70 |
| 1 | a | 1241 | G | C2-N3-C4 | 8.66 | 116.23 | 111.90 |
| 26 | A | 281 | C | C6-N1-C2 | -8.65 | 116.84 | 120.30 |
| 26 | A | 647 | G | O5'-P-OP2 | 8.63 | 121.06 | 110.70 |
| 24 | y | 61 | C | N3-C2-O2 | -8.63 | 115.86 | 121.90 |
| 1 | a | 528 | C | N1-C2-O2 | 8.60 | 124.06 | 118.90 |
| 26 | A | 887 | U | N1-C2-O2 | 8.60 | 128.82 | 122.80 |
| 1 | a | 563 | A | N9-C4-C5 | -8.54 | 102.38 | 105.80 |
| 24 | y | 48 | G | O4'-C1'-N9 | -8.54 | 101.36 | 108.20 |
| 3 | c | 33 | ASP | CB-CG-OD1 | 8.52 | 125.97 | 118.30 |
| 26 | A | 545 | U | C5-C6-N1 | 8.49 | 126.95 | 122.70 |
| 24 | y | 73 | G | C4-C5-N7 | 8.42 | 114.17 | 110.80 |
| 26 | A | 1042 | G | P-O3'-C3' | 8.40 | 129.78 | 119.70 |
| 1 | a | 1412 | C | C6-N1-C2 | -8.37 | 116.95 | 120.30 |
| 26 | A | 1104 | C | C6-N1-C2 | -8.35 | 116.96 | 120.30 |
| 26 | A | 546 | U | C5-C6-N1 | 8.35 | 126.87 | 122.70 |
| 24 | y | 60 | U | N1-C2-O2 | -8.32 | 116.98 | 122.80 |
| 26 | A | 610 | C | C6-N1-C2 | -8.32 | 116.97 | 120.30 |
| 1 | a | 392 | C | C6-N1-C2 | -8.32 | 116.97 | 120.30 |
| 23 | x | 127 | U | P-O3'-C3' | 8.31 | 129.67 | 119.70 |
| 26 | A | 571 | U | N3-C4-C5 | -8.31 | 109.61 | 114.60 |
| 24 | y | 57 | G | O5'-P-OP2 | 8.24 | 120.59 | 110.70 |
| 26 | A | 1093 | G | C4-C5-N7 | 8.24 | 114.10 | 110.80 |
| 21 | u | 15 | LEU | CA-CB-CG | 8.23 | 134.23 | 115.30 |
| 1 | a | 1296 | C | N1-C2-O2 | 8.22 | 123.83 | 118.90 |
| 1 | a | 972 | C | C6-N1-C2 | -8.22 | 117.01 | 120.30 |
| 24 | y | 30 | G | N9-C4-C5 | -8.21 | 102.12 | 105.40 |
| 27 | B | 24 | G | C5-C6-O6 | -8.19 | 123.69 | 128.60 |
| 26 | A | 2150 | C | C5-C6-N1 | 8.18 | 125.09 | 121.00 |
| 25 | z | 328 | ALA | N-CA-C | -8.18 | 88.92 | 111.00 |
| 26 | A | 1080 | A | C8-N9-C4 | -8.18 | 102.53 | 105.80 |
| 26 | A | 1076 | C | C6-N1-C2 | -8.14 | 117.05 | 120.30 |
| 26 | A | 2714 | G | O5'-P-OP2 | 8.13 | 120.46 | 110.70 |
| 1 | a | 1296 | C | C5-C6-N1 | 8.12 | 125.06 | 121.00 |
| 1 | a | 723 | U | N3-C4-C5 | 8.12 | 119.47 | 114.60 |
| 26 | A | 2109 | U | C6-N1-C2 | -8.11 | 116.13 | 121.00 |
| 26 | A | 2502 | G | O5'-P-OP2 | 8.11 | 120.43 | 110.70 |
| 26 | A | 1076 | C | C5-C6-N1 | 8.07 | 125.04 | 121.00 |
| 15 | o | 30 | LEU | CB-CG-CD2 | -8.06 | 97.30 | 111.00 |
| 1 | a | 1397 | C | C6-N1-C2 | 8.05 | 123.52 | 120.30 |
| 24 | y | 61 | C | C2-N1-C1' | 8.05 | 127.66 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | A | 2267 | A | C2-N3-C4 | 8.05 | 114.63 | 110.60 |
| 26 | A | 2169 | A | N7-C8-N9 | -8.05 | 109.78 | 113.80 |
| 26 | A | 2147 | A | N7-C8-N9 | 8.02 | 117.81 | 113.80 |
| 26 | A | 2109 | U | C2-N3-C4 | 7.99 | 131.79 | 127.00 |
| 1 | a | 477 | C | C6-N1-C2 | -7.97 | 117.11 | 120.30 |
| 1 | a | 419 | C | C6-N1-C2 | -7.96 | 117.12 | 120.30 |
| 26 | A | 84 | A | C8-N9-C4 | 7.96 | 108.98 | 105.80 |
| 26 | A | 2269 | G | O5'-P-OP1 | -7.93 | 98.56 | 105.70 |
| 1 | a | 799 | G | N1-C6-O6 | -7.92 | 115.15 | 119.90 |
| 24 | y | 61 | C | N3-C4-N4 | 7.90 | 123.53 | 118.00 |
| 1 | a | 34 | C | C6-N1-C2 | -7.89 | 117.14 | 120.30 |
| 27 | B | 24 | G | N1-C6-O6 | 7.89 | 124.63 | 119.90 |
| 1 | a | 1395 | C | N1-C2-O2 | 7.88 | 123.63 | 118.90 |
| 26 | A | 2637 | U | C6-N1-C2 | -7.88 | 116.28 | 121.00 |
| 26 | A | 891 | G | C5-C6-O6 | -7.87 | 123.88 | 128.60 |
| 26 | A | 890 | C | C4-C5-C6 | -7.85 | 113.47 | 117.40 |
| 26 | A | 1047 | G | O4'-C1'-N9 | 7.85 | 114.48 | 108.20 |
| 23 | x | 117 | C | C2-N1-C1' | 7.84 | 127.43 | 118.80 |
| 26 | A | 2466 | C | O5'-P-OP1 | -7.84 | 98.65 | 105.70 |
| 1 | a | 750 | C | C6-N1-C2 | -7.83 | 117.17 | 120.30 |
| 1 | a | 392 | C | N1-C2-O2 | 7.82 | 123.59 | 118.90 |
| 26 | A | 1386 | C | C5-C6-N1 | 7.79 | 124.90 | 121.00 |
| 26 | A | 962 | G | O5'-P-OP1 | -7.78 | 98.70 | 105.70 |
| 1 | a | 513 | C | C6-N1-C2 | -7.76 | 117.19 | 120.30 |
| 6 | f | 72 | ASP | CB-CG-OD1 | 7.76 | 125.28 | 118.30 |
| 26 | A | 2758 | A | N1-C6-N6 | -7.75 | 113.95 | 118.60 |
| 26 | A | 669 | G | N3-C4-C5 | -7.74 | 124.73 | 128.60 |
| 26 | A | 885 | C | C6-N1-C2 | -7.73 | 117.21 | 120.30 |
| 26 | A | 1270 | C | C5-C6-N1 | 7.73 | 124.86 | 121.00 |
| 26 | A | 883 | G | C6-C5-N7 | -7.72 | 125.77 | 130.40 |
| 26 | A | 1564 | C | C5-C6-N1 | 7.72 | 124.86 | 121.00 |
| 26 | A | 2359 | C | C5-C6-N1 | 7.72 | 124.86 | 121.00 |
| 26 | A | 1656 | C | C5-C6-N1 | 7.71 | 124.86 | 121.00 |
| 26 | A | 2474 | U | N3-C2-O2 | -7.71 | 116.80 | 122.20 |
| 33 | I | 64 | ARG | CA-CB-CG | 7.71 | 130.35 | 113.40 |
| 26 | A | 546 | U | C6-N1-C2 | -7.70 | 116.38 | 121.00 |
| 13 | m | 57 | ASP | CB-CG-OD1 | 7.68 | 125.21 | 118.30 |
| 1 | a | 1397 | C | N3-C4-N4 | -7.65 | 112.65 | 118.00 |
| 26 | A | 2166 | U | C6-N1-C2 | -7.64 | 116.42 | 121.00 |
| 1 | a | 924 | C | C6-N1-C2 | -7.64 | 117.25 | 120.30 |
| 26 | A | 2416 | C | C5-C6-N1 | 7.64 | 124.82 | 121.00 |
| 26 | A | 571 | U | C5-C4-O4 | 7.63 | 130.48 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | A | 1074 | G | N3-C2-N2 | -7.62 | 114.56 | 119.90 |
| 26 | A | 1656 | C | C6-N1-C2 | -7.62 | 117.25 | 120.30 |
| 1 | a | 754 | C | C2-N1-C1' | 7.61 | 127.17 | 118.80 |
| 7 | g | 139 | ASP | CB-CG-OD1 | 7.61 | 125.14 | 118.30 |
| 1 | a | 492 | C | C5-C6-N1 | 7.60 | 124.80 | 121.00 |
| 1 | a | 993 | G | N9-C4-C5 | -7.59 | 102.36 | 105.40 |
| 4 | d | 190 | LEU | CB-CG-CD1 | 7.59 | 123.90 | 111.00 |
| 27 | B | 11 | C | C6-N1-C2 | -7.59 | 117.27 | 120.30 |
| 1 | a | 430 | A | O5'-P-OP1 | -7.58 | 98.88 | 105.70 |
| 1 | a | 993 | G | N3-C4-N9 | 7.56 | 130.54 | 126.00 |
| 1 | a | 34 | C | C5-C6-N1 | 7.56 | 124.78 | 121.00 |
| 26 | A | 1271 | G | O4'-C1'-N9 | 7.55 | 114.24 | 108.20 |
| 26 | A | 2143 | C | C6-N1-C2 | -7.53 | 117.29 | 120.30 |
| 26 | A | 2896 | C | C5-C6-N1 | 7.53 | 124.76 | 121.00 |
| 1 | a | 1034 | G | C4-C5-N7 | 7.51 | 113.81 | 110.80 |
| 24 | y | 27 | C | C6-N1-C2 | -7.49 | 117.30 | 120.30 |
| 26 | A | 1171 | G | N1-C2-N2 | 7.49 | 122.94 | 116.20 |
| 1 | a | 476 | U | C5-C6-N1 | 7.47 | 126.44 | 122.70 |
| 24 | y | 30 | G | N3-C4-N9 | 7.46 | 130.48 | 126.00 |
| 1 | a | 737 | C | C6-N1-C2 | -7.42 | 117.33 | 120.30 |
| 1 | a | 1102 | A | N9-C4-C5 | -7.42 | 102.83 | 105.80 |
| 26 | A | 231 | A | N9-C4-C5 | -7.42 | 102.83 | 105.80 |
| 26 | A | 53 | A | C5-C6-N6 | -7.41 | 117.77 | 123.70 |
| 26 | A | 647 | G | OP1-P-OP2 | -7.41 | 108.49 | 119.60 |
| 1 | a | 968 | A | O5'-P-OP2 | -7.41 | 99.03 | 105.70 |
| 26 | A | 890 | C | N3-C4-N4 | -7.40 | 112.82 | 118.00 |
| 26 | A | 1171 | G | C6-N1-C2 | -7.40 | 120.66 | 125.10 |
| 26 | A | 2165 | C | O5'-P-OP2 | -7.38 | 99.06 | 105.70 |
| 1 | a | 563 | A | N1-C2-N3 | -7.38 | 125.61 | 129.30 |
| 24 | y | 47 | G | C8-N9-C4 | -7.38 | 103.45 | 106.40 |
| 1 | a | 490 | C | C6-N1-C2 | -7.38 | 117.35 | 120.30 |
| 1 | a | 878 | A | N9-C4-C5 | -7.38 | 102.85 | 105.80 |
| 1 | a | 1034 | G | N9-C4-C5 | -7.38 | 102.45 | 105.40 |
| 26 | A | 2562 | U | N3-C2-O2 | -7.37 | 117.04 | 122.20 |
| 1 | a | 180 | U | C5-C6-N1 | 7.36 | 126.38 | 122.70 |
| 26 | A | 1665 | A | O5'-P-OP2 | -7.35 | 99.09 | 105.70 |
| 26 | A | 669 | G | N3-C4-N9 | 7.34 | 130.40 | 126.00 |
| 26 | A | 1982 | U | O5'-P-OP2 | -7.34 | 99.09 | 105.70 |
| 1 | a | 1263 | C | C5-C6-N1 | 7.33 | 124.67 | 121.00 |
| 1 | a | 1397 | C | N3-C4-C5 | 7.33 | 124.83 | 121.90 |
| 14 | n | 32 | ASP | CB-CG-OD1 | 7.33 | 124.90 | 118.30 |
| 26 | A | 1079 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1 | a | 575 | G | N3-C2-N2 | -7.32 | 114.77 | 119.90 |
| 1 | a | 1027 | C | N1-C2-O2 | 7.30 | 123.28 | 118.90 |
| 1 | a | 1262 | C | N1-C2-O2 | 7.29 | 123.28 | 118.90 |
| 26 | A | 813 | U | N3-C2-O2 | -7.29 | 117.10 | 122.20 |
| 26 | A | 2473 | U | N3-C2-O2 | -7.28 | 117.10 | 122.20 |
| 24 | y | 59 | C | C5-C6-N1 | 7.27 | 124.64 | 121.00 |
| 25 | z | 398 | LEU | CA-CB-CG | 7.26 | 132.01 | 115.30 |
| 26 | A | 2746 | U | C5-C6-N1 | 7.26 | 126.33 | 122.70 |
| 27 | B | 60 | C | C6-N1-C2 | -7.26 | 117.40 | 120.30 |
| 26 | A | 1171 | G | N3-C4-N9 | -7.26 | 121.65 | 126.00 |
| 26 | A | 2582 | G | OP2-P-O3' | 7.25 | 121.16 | 105.20 |
| 1 | a | 1071 | C | C6-N1-C2 | -7.25 | 117.40 | 120.30 |
| 2 | b | 81 | ASP | CB-CG-OD1 | 7.24 | 124.82 | 118.30 |
| 26 | A | 1386 | C | C6-N1-C2 | -7.24 | 117.41 | 120.30 |
| 1 | a | 1148 | U | N3-C2-O2 | -7.24 | 117.14 | 122.20 |
| 24 | y | 59 | C | C6-N1-C2 | -7.22 | 117.41 | 120.30 |
| 24 | y | 47(B) | G | N7-C8-N9 | 7.21 | 116.71 | 113.10 |
| 26 | A | 1060 | U | O5'-P-OP1 | -7.20 | 99.22 | 105.70 |
| 1 | a | 1493 | A | N1-C2-N3 | -7.20 | 125.70 | 129.30 |
| 1 | a | 620 | C | N1-C2-O2 | 7.19 | 123.21 | 118.90 |
| 1 | a | 472 | U | C5-C6-N1 | 7.16 | 126.28 | 122.70 |
| 26 | A | 2161 | C | N1-C2-O2 | -7.15 | 114.61 | 118.90 |
| 26 | A | 1476 | U | N3-C2-O2 | -7.13 | 117.20 | 122.20 |
| 1 | a | 217 | C | C5-C6-N1 | 7.13 | 124.57 | 121.00 |
| 1 | a | 414 | A | C2-N3-C4 | 7.12 | 114.16 | 110.60 |
| 26 | A | 2110 | G | N3-C4-N9 | -7.12 | 121.73 | 126.00 |
| 1 | a | 419 | C | N3-C2-O2 | -7.11 | 116.92 | 121.90 |
| 26 | A | 1080 | A | N7-C8-N9 | 7.11 | 117.36 | 113.80 |
| 24 | y | 47(P) | C | C6-N1-C2 | -7.11 | 117.46 | 120.30 |
| 31 | F | 88 | VAL | CG1-CB-CG2 | -7.11 | 99.52 | 110.90 |
| 1 | a | 80 | A | C6-N1-C2 | 7.11 | 122.86 | 118.60 |
| 1 | a | 477 | C | C5-C6-N1 | 7.10 | 124.55 | 121.00 |
| 24 | y | 47(N) | C | C5-C6-N1 | 7.10 | 124.55 | 121.00 |
| 27 | B | 60 | C | C5-C6-N1 | 7.10 | 124.55 | 121.00 |
| 50 | Y | 49 | ASP | CB-CG-OD1 | 7.08 | 124.67 | 118.30 |
| 24 | y | 55 | PSU | P-O3'-C3' | 7.07 | 128.19 | 119.70 |
| 1 | a | 163 | C | C6-N1-C2 | -7.07 | 117.47 | 120.30 |
| 1 | a | 392 | C | C5-C6-N1 | 7.07 | 124.53 | 121.00 |
| 26 | A | 183 | C | N1-C2-O2 | 7.07 | 123.14 | 118.90 |
| 30 | E | 82 | GLY | N-CA-C | 7.07 | 130.76 | 113.10 |
| 1 | a | 397 | A | C2-N3-C4 | 7.06 | 114.13 | 110.60 |
| 22 | v | 39 | C | C5-C6-N1 | 7.05 | 124.53 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1 | a | 1202 | U | N3-C2-O2 | -7.05 | 117.27 | 122.20 |
| 1 | a | 397 | A | N3-C4-N9 | 7.04 | 133.03 | 127.40 |
| 1 | a | 409 | U | C5-C6-N1 | 7.04 | 126.22 | 122.70 |
| 26 | A | 1074 | G | N1-C2-N2 | 7.03 | 122.53 | 116.20 |
| 1 | a | 512 | U | C5-C6-N1 | 7.03 | 126.21 | 122.70 |
| 24 | y | 30 | G | C6-C5-N7 | -7.01 | 126.19 | 130.40 |
| 1 | a | 492 | C | C6-N1-C2 | -7.00 | 117.50 | 120.30 |
| 24 | y | 47(C) | C | C5-C6-N1 | 6.97 | 124.49 | 121.00 |
| 23 | x | 126 | G | P-O3'-C3' | 6.97 | 128.06 | 119.70 |
| 26 | A | 114 | U | N1-C2-O2 | 6.97 | 127.68 | 122.80 |
| 26 | A | 79 | C | C6-N1-C2 | -6.96 | 117.52 | 120.30 |
| 25 | z | 328 | ALA | N-CA-CB | 6.94 | 119.82 | 110.10 |
| 1 | a | 392 | C | C2-N1-C1' | 6.93 | 126.43 | 118.80 |
| 24 | y | 73 | G | N9-C4-C5 | -6.93 | 102.63 | 105.40 |
| 26 | A | 1936 | A | N1-C6-N6 | -6.92 | 114.45 | 118.60 |
| 26 | A | 1313 | U | C6-N1-C1' | -6.91 | 111.52 | 121.20 |
| 26 | A | 2442 | C | N1-C2-O2 | 6.91 | 123.05 | 118.90 |
| 26 | A | 1071 | G | N9-C4-C5 | -6.91 | 102.64 | 105.40 |
| 31 | F | 11 | VAL | CG1-CB-CG2 | -6.90 | 99.86 | 110.90 |
| 26 | A | 2474 | U | N1-C2-O2 | 6.89 | 127.62 | 122.80 |
| 25 | z | 445 | LEU | CB-CG-CD2 | -6.88 | 99.30 | 111.00 |
| 26 | A | 1104 | C | C5-C6-N1 | 6.87 | 124.43 | 121.00 |
| 26 | A | 2195 | U | N3-C2-O2 | -6.87 | 117.39 | 122.20 |
| 26 | A | 53 | A | N1-C6-N6 | 6.86 | 122.71 | 118.60 |
| 1 | a | 1448 | C | N1-C2-O2 | 6.85 | 123.01 | 118.90 |
| 26 | A | 2636 | C | N1-C2-O2 | 6.85 | 123.01 | 118.90 |
| 26 | A | 445 | C | N3-C2-O2 | -6.85 | 117.11 | 121.90 |
| 26 | A | 2755 | C | N1-C2-O2 | 6.85 | 123.01 | 118.90 |
| 26 | A | 1294 | U | N3-C2-O2 | -6.83 | 117.42 | 122.20 |
| 26 | A | 883 | G | N7-C8-N9 | 6.83 | 116.52 | 113.10 |
| 24 | y | 48 | G | C4-C5-N7 | 6.83 | 113.53 | 110.80 |
| 1 | a | 1296 | C | N3-C2-O2 | -6.82 | 117.12 | 121.90 |
| 26 | A | 884 | U | N1-C2-N3 | 6.82 | 118.99 | 114.90 |
| 22 | v | 32 | C | N1-C2-O2 | 6.82 | 122.99 | 118.90 |
| 33 | I | 79 | LEU | CB-CG-CD2 | -6.82 | 99.41 | 111.00 |
| 1 | a | 868 | C | C6-N1-C2 | -6.82 | 117.57 | 120.30 |
| 22 | v | 50 | U | C5-C6-N1 | 6.82 | 126.11 | 122.70 |
| 26 | A | 2167 | U | N1-C2-O2 | -6.82 | 118.03 | 122.80 |
| 1 | a | 1034 | G | N1-C6-O6 | 6.81 | 123.99 | 119.90 |
| 24 | y | 40 | C | C5-C6-N1 | 6.81 | 124.41 | 121.00 |
| 24 | y | 47(G) | C | N1-C2-O2 | -6.81 | 114.81 | 118.90 |
| 1 | a | 88 | U | C6-N1-C2 | -6.81 | 116.92 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | x | 118 | G | N7-C8-N9 | 6.81 | 116.50 | 113.10 |
| 44 | S | 64 | ALA | N-CA-CB | 6.80 | 119.62 | 110.10 |
| 1 | a | 1263 | C | C6-N1-C2 | -6.80 | 117.58 | 120.30 |
| 26 | A | 2326 | C | C6-N1-C2 | -6.79 | 117.58 | 120.30 |
| 26 | A | 2512 | C | C6-N1-C2 | -6.79 | 117.58 | 120.30 |
| 27 | B | 120 | U | N3-C2-O2 | -6.79 | 117.45 | 122.20 |
| 1 | a | 407 | U | O5'-P-OP2 | 6.78 | 118.84 | 110.70 |
| 26 | A | 2069 | G7M | P-O3'-C3' | 6.77 | 127.82 | 119.70 |
| 26 | A | 84 | A | N7-C8-N9 | -6.75 | 110.42 | 113.80 |
| 26 | A | 140 | C | C6-N1-C2 | -6.75 | 117.60 | 120.30 |
| 1 | a | 428 | G | N3-C4-N9 | -6.72 | 121.97 | 126.00 |
| 26 | A | 1071 | G | C4-C5-N7 | 6.72 | 113.49 | 110.80 |
| 1 | a | 429 | U | OP1-P-O3' | 6.71 | 119.97 | 105.20 |
| 26 | A | 546 | U | N3-C2-O2 | -6.71 | 117.50 | 122.20 |
| 27 | B | 55 | U | N3-C2-O2 | -6.71 | 117.51 | 122.20 |
| 1 | a | 923 | A | N7-C8-N9 | 6.71 | 117.15 | 113.80 |
| 26 | A | 283 | G | N3-C2-N2 | -6.69 | 115.22 | 119.90 |
| 24 | y | 20 | G | C2-N3-C4 | -6.69 | 108.56 | 111.90 |
| 1 | a | 526 | C | C6-N1-C2 | -6.68 | 117.63 | 120.30 |
| 26 | A | 2080 | A | N9-C4-C5 | -6.68 | 103.13 | 105.80 |
| 1 | a | 407 | U | C6-N1-C2 | -6.67 | 117.00 | 121.00 |
| 23 | x | 133 | C | C6-N1-C2 | -6.67 | 117.63 | 120.30 |
| 24 | y | 48 | G | N9-C4-C5 | -6.67 | 102.73 | 105.40 |
| 26 | A | 2574 | G | O5'-P-OP1 | 6.67 | 118.71 | 110.70 |
| 26 | A | 2163 | A | O5'-P-OP1 | 6.66 | 118.70 | 110.70 |
| 27 | B | 57 | A | N7-C8-N9 | 6.66 | 117.13 | 113.80 |
| 26 | A | 8 | C | C5-C6-N1 | 6.66 | 124.33 | 121.00 |
| 26 | A | 2267 | A | N1-C6-N6 | -6.66 | 114.60 | 118.60 |
| 1 | a | 1344 | C | C6-N1-C2 | -6.64 | 117.64 | 120.30 |
| 1 | a | 1466 | C | N3-C2-O2 | -6.63 | 117.25 | 121.90 |
| 26 | A | 1178 | C | C6-N1-C2 | -6.63 | 117.65 | 120.30 |
| 22 | v | 19 | G | O4'-C1'-N9 | -6.62 | 102.90 | 108.20 |
| 26 | A | 890 | C | N3-C2-O2 | -6.62 | 117.27 | 121.90 |
| 1 | a | 397 | A | N9-C4-C5 | -6.62 | 103.15 | 105.80 |
| 1 | a | 1105 | A | N9-C4-C5 | -6.62 | 103.15 | 105.80 |
| 22 | v | 32 | C | N3-C2-O2 | -6.62 | 117.27 | 121.90 |
| 26 | A | 208 | C | C5-C6-N1 | 6.62 | 124.31 | 121.00 |
| 1 | a | 88 | U | C5-C6-N1 | 6.61 | 126.01 | 122.70 |
| 26 | A | 528 | A | N7-C8-N9 | 6.61 | 117.11 | 113.80 |
| 26 | A | 1664 | A | O5'-P-OP1 | 6.61 | 118.63 | 110.70 |
| 26 | A | 1083 | U | N1-C2-O2 | -6.60 | 118.18 | 122.80 |
| 1 | a | 1037 | C | C6-N1-C2 | -6.60 | 117.66 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 27 | B | 42 | C | N1-C2-O2 | 6.60 | 122.86 | 118.90 |
| 26 | A | 528 | A | C8-N9-C4 | -6.60 | 103.16 | 105.80 |
| 1 | a | 1393 | U | N3-C2-O2 | -6.60 | 117.58 | 122.20 |
| 26 | A | 642 | U | C6-N1-C2 | -6.60 | 117.04 | 121.00 |
| 26 | A | 399 | U | N3-C2-O2 | -6.60 | 117.58 | 122.20 |
| 1 | a | 443 | C | C5-C6-N1 | 6.59 | 124.30 | 121.00 |
| 1 | a | 1109 | C | N1-C2-O2 | 6.59 | 122.85 | 118.90 |
| 1 | a | 993 | G | C6-C5-N7 | -6.59 | 126.45 | 130.40 |
| 26 | A | 889 | C | N1-C2-O2 | 6.59 | 122.85 | 118.90 |
| 23 | x | 109 | C | C6-N1-C2 | -6.58 | 117.67 | 120.30 |
| 26 | A | 1313 | U | C5-C6-N1 | 6.58 | 125.99 | 122.70 |
| 1 | a | 1497 | G | N3-C4-N9 | 6.58 | 129.95 | 126.00 |
| 24 | y | 72 | C | C2-N1-C1' | 6.58 | 126.03 | 118.80 |
| 1 | a | 136 | C | C2-N1-C1' | 6.57 | 126.02 | 118.80 |
| 1 | a | 527 | G7M | P-O3'-C3' | 6.57 | 127.58 | 119.70 |
| 1 | a | 611 | C | N1-C2-O2 | 6.57 | 122.84 | 118.90 |
| 26 | A | 2626 | C | C5-C6-N1 | 6.56 | 124.28 | 121.00 |
| 1 | a | 592 | G | C8-N9-C4 | -6.56 | 103.78 | 106.40 |
| 26 | A | 534 | U | C5-C6-N1 | 6.56 | 125.98 | 122.70 |
| 1 | a | 536 | C | C6-N1-C2 | -6.56 | 117.68 | 120.30 |
| 26 | A | 1093 | G | C8-N9-C4 | 6.55 | 109.02 | 106.40 |
| 1 | a | 1109 | C | C6-N1-C2 | -6.55 | 117.68 | 120.30 |
| 26 | A | 837 | C | N3-C2-O2 | -6.55 | 117.31 | 121.90 |
| 1 | a | 1195 | C | C6-N1-C2 | -6.55 | 117.68 | 120.30 |
| 26 | A | 231 | A | C8-N9-C4 | 6.55 | 108.42 | 105.80 |
| 26 | A | 806 | C | C6-N1-C2 | -6.54 | 117.69 | 120.30 |
| 26 | A | 1072 | C | O5'-P-OP2 | -6.54 | 99.81 | 105.70 |
| 1 | a | 620 | C | N3-C2-O2 | -6.53 | 117.33 | 121.90 |
| 26 | A | 1075 | C | N1-C2-O2 | 6.53 | 122.82 | 118.90 |
| 26 | A | 1093 | G | N1-C6-O6 | 6.53 | 123.82 | 119.90 |
| 26 | A | 1669 | A | N3-C4-N9 | 6.51 | 132.61 | 127.40 |
| 1 | a | 563 | A | C4-C5-N7 | 6.51 | 113.95 | 110.70 |
| 26 | A | 2502 | G | O5'-P-OP1 | -6.50 | 99.85 | 105.70 |
| 26 | A | 1064 | C | N1-C2-O2 | -6.50 | 115.00 | 118.90 |
| 1 | a | 136 | C | N1-C2-O2 | 6.50 | 122.80 | 118.90 |
| 1 | a | 418 | C | C6-N1-C2 | -6.49 | 117.70 | 120.30 |
| 1 | a | 1427 | C | C6-N1-C2 | -6.49 | 117.70 | 120.30 |
| 26 | A | 2162 | G | N1-C6-O6 | -6.49 | 116.01 | 119.90 |
| 1 | a | 513 | C | C5-C6-N1 | 6.49 | 124.24 | 121.00 |
| 1 | a | 1517 | G | N3-C2-N2 | -6.47 | 115.37 | 119.90 |
| 26 | A | 1075 | C | C2-N1-C1' | 6.47 | 125.92 | 118.80 |
| 27 | B | 37 | C | N1-C2-O2 | 6.47 | 122.78 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | a | 90 | C | C6-N1-C2 | -6.47 | 117.71 | 120.30 |
| 26 | A | 445 | C | N1-C2-O2 | 6.47 | 122.78 | 118.90 |
| 26 | A | 571 | U | C4-C5-C6 | 6.47 | 123.58 | 119.70 |
| 1 | a | 661 | G | N9-C4-C5 | -6.46 | 102.81 | 105.40 |
| 26 | A | 2060 | A | OP2-P-O3' | 6.45 | 119.39 | 105.20 |
| 1 | a | 1469 | C | N1-C2-O2 | 6.45 | 122.77 | 118.90 |
| 56 | 4 | 14 | CYS | CA-CB-SG | 6.45 | 125.60 | 114.00 |
| 26 | A | 1956 | U | N3-C2-O2 | -6.44 | 117.69 | 122.20 |
| 23 | x | 109 | C | C5-C6-N1 | 6.44 | 124.22 | 121.00 |
| 1 | a | 475 | C | C6-N1-C2 | -6.43 | 117.73 | 120.30 |
| 26 | A | 1056 | G | N1-C6-O6 | 6.43 | 123.76 | 119.90 |
| 26 | A | 2702 | G | N1-C6-O6 | -6.43 | 116.05 | 119.90 |
| 1 | a | 656 | G | C6-N1-C2 | -6.42 | 121.25 | 125.10 |
| 26 | A | 183 | C | N3-C2-O2 | -6.42 | 117.40 | 121.90 |
| 24 | y | 30 | G | C8-N9-C1' | -6.42 | 118.65 | 127.00 |
| 26 | A | 2188 | U | C5-C6-N1 | 6.42 | 125.91 | 122.70 |
| 1 | a | 493 | A | C8-N9-C4 | -6.42 | 103.23 | 105.80 |
| 1 | a | 449 | G | C4-C5-N7 | 6.41 | 113.37 | 110.80 |
| 1 | a | 744 | C | C5-C6-N1 | 6.41 | 124.21 | 121.00 |
| 26 | A | 669 | G | C2-N3-C4 | 6.41 | 115.11 | 111.90 |
| 26 | A | 1294 | U | N1-C2-O2 | 6.41 | 127.29 | 122.80 |
| 1 | a | 217 | C | C6-N1-C2 | -6.41 | 117.74 | 120.30 |
| 1 | a | 1027 | C | C5-C6-N1 | 6.41 | 124.20 | 121.00 |
| 26 | A | 560 | C | C5-C6-N1 | 6.41 | 124.20 | 121.00 |
| 26 | A | 891 | G | C6-C5-N7 | -6.41 | 126.56 | 130.40 |
| 1 | a | 963 | G | N3-C2-N2 | -6.40 | 115.42 | 119.90 |
| 26 | A | 1064 | C | C6-N1-C2 | -6.40 | 117.74 | 120.30 |
| 33 | I | 64 | ARG | N-CA-CB | -6.39 | 99.10 | 110.60 |
| 26 | A | 646 | U | OP2-P-O3' | 6.39 | 119.25 | 105.20 |
| 26 | A | 615 | U | C5-C4-O4 | -6.39 | 122.07 | 125.90 |
| 23 | x | 124 | A | N9-C4-C5 | -6.38 | 103.25 | 105.80 |
| 1 | a | 110 | C | N1-C2-O2 | 6.38 | 122.73 | 118.90 |
| 1 | a | 723 | U | N1-C2-O2 | 6.38 | 127.27 | 122.80 |
| 23 | x | 104 | U | N3-C2-O2 | -6.38 | 117.74 | 122.20 |
| 26 | A | 399 | U | N1-C2-O2 | 6.37 | 127.26 | 122.80 |
| 26 | A | 783 | A | C2-N3-C4 | 6.37 | 113.79 | 110.60 |
| 26 | A | 1059 | G | C5-C6-O6 | -6.37 | 124.78 | 128.60 |
| 26 | A | 891 | G | N3-C4-N9 | 6.37 | 129.82 | 126.00 |
| 1 | a | 896 | C | C5-C6-N1 | 6.37 | 124.18 | 121.00 |
| 24 | y | 56 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 26 | A | 1075 | C | N3-C2-O2 | -6.36 | 117.45 | 121.90 |
| 26 | A | 1348 | C | N1-C2-O2 | 6.36 | 122.72 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 24 | y | 20 | G | N1-C2-N3 | 6.36 | 127.72 | 123.90 |
| 26 | A | 114 | U | N3-C2-O2 | -6.36 | 117.75 | 122.20 |
| 1 | a | 419 | C | C6-N1-C1' | 6.36 | 128.43 | 120.80 |
| 26 | A | 2110 | G | C5-C6-O6 | 6.36 | 132.41 | 128.60 |
| 24 | y | 47(K) | G | N3-C4-C5 | 6.36 | 131.78 | 128.60 |
| 1 | a | 307 | C | N1-C2-O2 | 6.35 | 122.71 | 118.90 |
| 1 | a | 1326 | U | N3-C2-O2 | -6.35 | 117.76 | 122.20 |
| 24 | y | 65 | U | O5'-P-OP1 | -6.34 | 99.99 | 105.70 |
| 26 | A | 2011 | U | N3-C2-O2 | -6.34 | 117.76 | 122.20 |
| 1 | a | 1202 | U | N1-C2-O2 | 6.34 | 127.24 | 122.80 |
| 26 | A | 2305 | U | C6-N1-C2 | 6.34 | 124.80 | 121.00 |
| 26 | A | 1025 | G | OP1-P-O3' | 6.33 | 119.13 | 105.20 |
| 1 | a | 754 | C | C6-N1-C1' | -6.33 | 113.20 | 120.80 |
| 1 | a | 868 | C | C5-C6-N1 | 6.33 | 124.17 | 121.00 |
| 1 | a | 1404 | C | N1-C2-O2 | 6.33 | 122.69 | 118.90 |
| 1 | a | 968 | A | C5-C6-N6 | 6.32 | 128.75 | 123.70 |
| 26 | A | 2840 | C | C5-C6-N1 | 6.32 | 124.16 | 121.00 |
| 27 | B | 26 | C | N3-C2-O2 | -6.32 | 117.48 | 121.90 |
| 26 | A | 2160 | C | C6-N1-C2 | -6.31 | 117.78 | 120.30 |
| 1 | a | 177 | G | N3-C4-C5 | -6.31 | 125.45 | 128.60 |
| 26 | A | 2267 | A | N1-C2-N3 | -6.30 | 126.15 | 129.30 |
| 26 | A | 1669 | A | N9-C4-C5 | -6.30 | 103.28 | 105.80 |
| 24 | y | 48 | G | C6-C5-N7 | -6.29 | 126.62 | 130.40 |
| 8 | h | 95 | MET | CA-CB-CG | 6.29 | 124.00 | 113.30 |
| 26 | A | 1539 | U | C5-C4-O4 | -6.29 | 122.12 | 125.90 |
| 1 | a | 177 | G | C2-N3-C4 | 6.29 | 115.05 | 111.90 |
| 26 | A | 1101 | U | N3-C2-O2 | -6.29 | 117.80 | 122.20 |
| 1 | a | 1066 | C | N3-C2-O2 | -6.29 | 117.50 | 121.90 |
| 2 | b | 134 | LEU | CA-CB-CG | 6.29 | 129.76 | 115.30 |
| 26 | A | 1200 | C | C6-N1-C2 | -6.29 | 117.79 | 120.30 |
| 26 | A | 1178 | C | C5-C4-N4 | 6.28 | 124.60 | 120.20 |
| 26 | A | 2691 | C | C5-C6-N1 | 6.28 | 124.14 | 121.00 |
| 27 | B | 49 | C | C6-N1-C2 | -6.28 | 117.79 | 120.30 |
| 26 | A | 2394 | C | C6-N1-C2 | -6.28 | 117.79 | 120.30 |
| 25 | z | 559 | ASP | CB-CG-OD1 | 6.28 | 123.95 | 118.30 |
| 1 | a | 1412 | C | C5-C6-N1 | 6.27 | 124.14 | 121.00 |
| 26 | A | 1096 | A | C8-N9-C4 | -6.27 | 103.29 | 105.80 |
| 26 | A | 2442 | C | N3-C2-O2 | -6.27 | 117.51 | 121.90 |
| 1 | a | 1302 | C | C6-N1-C2 | 6.26 | 122.80 | 120.30 |
| 1 | a | 979 | C | N1-C2-O2 | 6.26 | 122.65 | 118.90 |
| 26 | A | 898 | C | C6-N1-C2 | -6.25 | 117.80 | 120.30 |
| 1 | a | 1302 | C | OP1-P-O3' | -6.25 | 91.45 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 27 | B | 26 | C | N1-C2-O2 | 6.25 | 122.65 | 118.90 |
| 26 | A | 357 | C | C6-N1-C2 | -6.25 | 117.80 | 120.30 |
| 26 | A | 1313 | U | C6-N1-C2 | -6.24 | 117.26 | 121.00 |
| 11 | k | 96 | ILE | CG1-CB-CG2 | -6.24 | 97.68 | 111.40 |
| 27 | B | 26 | C | C6-N1-C2 | -6.24 | 117.81 | 120.30 |
| 26 | A | 1787 | A | N9-C4-C5 | -6.24 | 103.31 | 105.80 |
| 26 | A | 140 | C | C5-C6-N1 | 6.23 | 124.11 | 121.00 |
| 26 | A | 2572 | A | O5'-P-OP1 | -6.22 | 100.10 | 105.70 |
| 26 | A | 234 | U | N3-C2-O2 | -6.22 | 117.85 | 122.20 |
| 26 | A | 1101 | U | N1-C2-O2 | 6.21 | 127.15 | 122.80 |
| 26 | A | 1012 | U | N1-C2-O2 | -6.20 | 118.46 | 122.80 |
| 1 | a | 977 | A | C2-N3-C4 | 6.20 | 113.70 | 110.60 |
| 26 | A | 2394 | C | N1-C2-O2 | 6.20 | 122.62 | 118.90 |
| 23 | x | 129 | U | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 26 | A | 1096 | A | N7-C8-N9 | 6.18 | 116.89 | 113.80 |
| 26 | A | 2044 | C | C6-N1-C2 | -6.18 | 117.83 | 120.30 |
| 1 | a | 516 | PSU | O3'-P-O5' | -6.17 | 92.28 | 104.00 |
| 1 | a | 795 | C | C6-N1-C2 | -6.17 | 117.83 | 120.30 |
| 4 | d | 189 | ASP | CB-CG-OD1 | 6.16 | 123.84 | 118.30 |
| 1 | a | 989 | U | N3-C2-O2 | -6.16 | 117.89 | 122.20 |
| 1 | a | 1296 | C | C2-N1-C1' | 6.15 | 125.57 | 118.80 |
| 1 | a | 660 | C | C5-C6-N1 | 6.14 | 124.07 | 121.00 |
| 1 | a | 180 | U | C6-N1-C2 | -6.14 | 117.32 | 121.00 |
| 26 | A | 231 | A | C5-C6-N6 | -6.14 | 118.79 | 123.70 |
| 26 | A | 444 | C | C6-N1-C2 | -6.14 | 117.84 | 120.30 |
| 26 | A | 1611 | C | C6-N1-C2 | -6.14 | 117.85 | 120.30 |
| 23 | x | 121 | U | N3-C2-O2 | -6.13 | 117.91 | 122.20 |
| 26 | A | 1075 | C | C6-N1-C2 | -6.13 | 117.85 | 120.30 |
| 24 | y | 30 | G | N1-C6-O6 | 6.12 | 123.58 | 119.90 |
| 26 | A | 2617 | U | N1-C2-O2 | 6.12 | 127.09 | 122.80 |
| 1 | a | 1497 | G | N3-C4-C5 | -6.12 | 125.54 | 128.60 |
| 26 | A | 2043 | C | C2-N1-C1' | 6.12 | 125.53 | 118.80 |
| 1 | a | 397 | A | N1-C2-N3 | -6.12 | 126.24 | 129.30 |
| 26 | A | 891 | G | N1-C6-O6 | 6.11 | 123.57 | 119.90 |
| 23 | x | 118 | G | C6-C5-N7 | -6.11 | 126.73 | 130.40 |
| 26 | A | 1021 | A | C2-N3-C4 | 6.11 | 113.66 | 110.60 |
| 1 | a | 1493 | A | C6-N1-C2 | 6.10 | 122.26 | 118.60 |
| 24 | y | 47(D) | C | C2-N3-C4 | 6.10 | 122.95 | 119.90 |
| 23 | x | 104 | U | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 26 | A | 1171 | G | C4-C5-N7 | -6.09 | 108.36 | 110.80 |
| 1 | a | 1284 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 24 | y | 45 | U | P-O3'-C3' | 6.08 | 127.00 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | A | 2103 | C | N3-C2-O2 | -6.08 | 117.64 | 121.90 |
| 26 | A | 2766 | A | N9-C4-C5 | -6.08 | 103.37 | 105.80 |
| 24 | y | 50 | C | C5-C6-N1 | 6.08 | 124.04 | 121.00 |
| 1 | a | 1109 | C | N3-C2-O2 | -6.08 | 117.65 | 121.90 |
| 24 | y | 40 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 1 | a | 679 | C | C6-N1-C2 | -6.07 | 117.87 | 120.30 |
| 24 | y | 56 | C | C5-C6-N1 | 6.07 | 124.03 | 121.00 |
| 1 | a | 993 | G | C4-C5-N7 | 6.06 | 113.23 | 110.80 |
| 26 | A | 2755 | C | N3-C2-O2 | -6.06 | 117.66 | 121.90 |
| 26 | A | 889 | C | N3-C2-O2 | -6.06 | 117.66 | 121.90 |
| 3 | c | 117 | ASP | CB-CG-OD1 | 6.05 | 123.75 | 118.30 |
| 1 | a | 1466 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 23 | x | 129 | U | N3-C2-O2 | -6.05 | 117.97 | 122.20 |
| 26 | A | 283 | G | C6-C5-N7 | 6.05 | 134.03 | 130.40 |
| 1 | a | 1195 | C | C5-C6-N1 | 6.04 | 124.02 | 121.00 |
| 1 | a | 536 | C | C5-C6-N1 | 6.03 | 124.02 | 121.00 |
| 23 | x | 108 | A | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 26 | A | 1181 | U | N3-C2-O2 | -6.03 | 117.98 | 122.20 |
| 24 | y | 16 | C | C6-N1-C1' | 6.02 | 128.03 | 120.80 |
| 22 | v | 36 | U | N3-C2-O2 | -6.02 | 117.99 | 122.20 |
| 26 | A | 1056 | G | C5-C6-O6 | -6.01 | 124.99 | 128.60 |
| 22 | v | 51 | C | C2-N1-C1' | 6.01 | 125.41 | 118.80 |
| 26 | A | 198 | C | C5-C6-N1 | 6.00 | 124.00 | 121.00 |
| 24 | y | 30 | G | C4-C5-N7 | 6.00 | 113.20 | 110.80 |
| 1 | a | 207 | C | C6-N1-C2 | -6.00 | 117.90 | 120.30 |
| 26 | A | 1723 | G | N1-C6-O6 | -5.99 | 116.31 | 119.90 |
| 1 | a | 438 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 1 | a | 968 | A | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 26 | A | 1279 | G | C4-C5-N7 | 5.99 | 113.19 | 110.80 |
| 23 | x | 131 | C | O4'-C1'-N1 | 5.98 | 112.99 | 108.20 |
| 1 | a | 799 | G | C2-N3-C4 | 5.98 | 114.89 | 111.90 |
| 1 | a | 1393 | U | N1-C2-O2 | 5.98 | 126.98 | 122.80 |
| 26 | A | 435 | C | OP1-P-OP2 | -5.98 | 110.63 | 119.60 |
| 1 | a | 464 | U | C5-C6-N1 | 5.97 | 125.69 | 122.70 |
| 24 | y | 46 | G | N3-C2-N2 | -5.97 | 115.72 | 119.90 |
| 26 | A | 2837 | A | O5'-P-OP2 | -5.97 | 100.33 | 105.70 |
| 1 | a | 1326 | U | N1-C2-O2 | 5.97 | 126.98 | 122.80 |
| 1 | a | 52 | C | C6-N1-C2 | -5.96 | 117.91 | 120.30 |
| 1 | a | 1262 | C | N3-C2-O2 | -5.96 | 117.73 | 121.90 |
| 1 | a | 968 | A | N9-C4-C5 | 5.96 | 108.19 | 105.80 |
| 1 | a | 612 | C | N1-C2-O2 | 5.96 | 122.47 | 118.90 |
| 26 | A | 1348 | C | C6-N1-C2 | -5.96 | 117.92 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | a | 980 | C | C6-N1-C2 | -5.95 | 117.92 | 120.30 |
| 12 | l | 80 | LEU | CA-CB-CG | 5.95 | 128.99 | 115.30 |
| 24 | y | 56 | C | OP2-P-O3' | -5.95 | 92.11 | 105.20 |
| 26 | A | 1092 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 1 | a | 354 | G | N9-C4-C5 | -5.95 | 103.02 | 105.40 |
| 26 | A | 2160 | C | N3-C2-O2 | -5.95 | 117.74 | 121.90 |
| 49 | X | 21 | LEU | CA-CB-CG | 5.94 | 128.97 | 115.30 |
| 26 | A | 2394 | C | N3-C2-O2 | -5.94 | 117.74 | 121.90 |
| 26 | A | 1585 | C | N1-C2-O2 | 5.93 | 122.46 | 118.90 |
| 26 | A | 2162 | G | C5-C6-O6 | 5.93 | 132.16 | 128.60 |
| 26 | A | 2473 | U | N1-C2-O2 | 5.93 | 126.95 | 122.80 |
| 23 | x | 128 | C | C3'-C2'-C1' | 5.92 | 106.24 | 101.50 |
| 27 | B | 120 | U | N1-C2-O2 | 5.92 | 126.95 | 122.80 |
| 23 | x | 101 | A | N1-C2-N3 | -5.92 | 126.34 | 129.30 |
| 26 | A | 2179 | C | C6-N1-C2 | -5.92 | 117.93 | 120.30 |
| 26 | A | 1775 | U | N3-C2-O2 | -5.92 | 118.06 | 122.20 |
| 1 | a | 578 | C | C6-N1-C2 | -5.91 | 117.93 | 120.30 |
| 22 | v | 34 | C | N1-C2-O2 | 5.91 | 122.45 | 118.90 |
| 1 | a | 423 | G | C5-C6-O6 | -5.91 | 125.05 | 128.60 |
| 1 | a | 16 | A | C6-N1-C2 | 5.91 | 122.14 | 118.60 |
| 24 | y | 43 | G | C4-N9-C1' | -5.90 | 118.83 | 126.50 |
| 1 | a | 1027 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 1 | a | 1448 | C | C2-N1-C1' | 5.90 | 125.29 | 118.80 |
| 26 | A | 231 | A | C4-C5-N7 | 5.90 | 113.65 | 110.70 |
| 1 | a | 528 | C | C2-N1-C1' | 5.90 | 125.28 | 118.80 |
| 26 | A | 130 | C | C6-N1-C2 | -5.89 | 117.94 | 120.30 |
| 26 | A | 687 | C | N1-C2-O2 | 5.89 | 122.44 | 118.90 |
| 1 | a | 494 | G | C5-C6-O6 | -5.89 | 125.06 | 128.60 |
| 1 | a | 483 | C | C6-N1-C2 | -5.89 | 117.94 | 120.30 |
| 26 | A | 890 | C | C5-C4-N4 | 5.88 | 124.32 | 120.20 |
| 26 | A | 2550 | G | O5'-P-OP1 | -5.88 | 100.40 | 105.70 |
| 26 | A | 885 | C | C5-C6-N1 | 5.88 | 123.94 | 121.00 |
| 1 | a | 368 | U | N3-C2-O2 | -5.88 | 118.09 | 122.20 |
| 1 | a | 346 | G | C2-N3-C4 | 5.87 | 114.84 | 111.90 |
| 11 | k | 112 | VAL | CA-CB-CG1 | 5.87 | 119.71 | 110.90 |
| 27 | B | 49 | C | C5-C6-N1 | 5.87 | 123.94 | 121.00 |
| 26 | A | 560 | C | C6-N1-C2 | -5.86 | 117.96 | 120.30 |
| 1 | a | 166 | U | N3-C2-O2 | -5.86 | 118.10 | 122.20 |
| 26 | A | 1093 | G | N3-C4-N9 | 5.85 | 129.51 | 126.00 |
| 27 | B | 37 | C | N3-C2-O2 | -5.85 | 117.80 | 121.90 |
| 1 | a | 1162 | C | C6-N1-C2 | -5.85 | 117.96 | 120.30 |
| 24 | y | 48 | G | C8-N9-C1' | -5.85 | 119.40 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|----------|-------|-------------|----------|
| 26 | A | 234 | U | N1-C2-O2 | 5.85 | 126.89 | 122.80 |
| 26 | A | 257 | C | C6-N1-C2 | -5.85 | 117.96 | 120.30 |
| 1 | a | 188 | C | C6-N1-C2 | -5.85 | 117.96 | 120.30 |
| 1 | a | 400 | C | C5-C6-N1 | 5.85 | 123.92 | 121.00 |
| 26 | A | 1171 | G | C8-N9-C4 | -5.85 | 104.06 | 106.40 |
| 1 | a | 923 | A | C6-C5-N7 | -5.84 | 128.21 | 132.30 |
| 25 | z | 257 | LEU | CA-CB-CG | 5.84 | 128.74 | 115.30 |
| 1 | a | 808 | C | C6-N1-C2 | -5.84 | 117.96 | 120.30 |
| 26 | A | 302 | C | C6-N1-C2 | -5.84 | 117.96 | 120.30 |
| 26 | A | 397 | U | C5-C6-N1 | 5.84 | 125.62 | 122.70 |
| 26 | A | 2254 | C | N1-C2-O2 | 5.84 | 122.40 | 118.90 |
| 1 | a | 346 | G | N3-C4-N9 | 5.84 | 129.50 | 126.00 |
| 26 | A | 1063 | G | N3-C4-C5 | -5.84 | 125.68 | 128.60 |
| 1 | a | 1455 | G | N3-C4-N9 | 5.83 | 129.50 | 126.00 |
| 26 | A | 1494 | A | N7-C8-N9 | 5.83 | 116.72 | 113.80 |
| 44 | S | 64 | ALA | N-CA-C | -5.83 | 95.25 | 111.00 |
| 24 | y | 47(G) | C | C6-N1-C2 | -5.83 | 117.97 | 120.30 |
| 24 | y | 47(B) | G | C8-N9-C4 | -5.83 | 104.07 | 106.40 |
| 26 | A | 2649 | C | C5-C6-N1 | 5.82 | 123.91 | 121.00 |
| 1 | a | 82 | G | N3-C4-N9 | 5.82 | 129.49 | 126.00 |
| 1 | a | 879 | C | N1-C2-O2 | 5.82 | 122.39 | 118.90 |
| 26 | A | 2606 | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |
| 24 | y | 27 | C | C5-C6-N1 | 5.82 | 123.91 | 121.00 |
| 26 | A | 1049 | C | N3-C4-N4 | -5.81 | 113.93 | 118.00 |
| 23 | x | 130 | G | N7-C8-N9 | 5.81 | 116.01 | 113.10 |
| 1 | a | 497 | G | N3-C2-N2 | -5.81 | 115.83 | 119.90 |
| 1 | a | 582 | C | C6-N1-C2 | -5.81 | 117.98 | 120.30 |
| 1 | a | 658 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 1 | a | 1382 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 26 | A | 2292 | U | C5-C6-N1 | 5.81 | 125.60 | 122.70 |
| 1 | a | 735 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 22 | v | 57 | A | C5-N7-C8 | 5.80 | 106.80 | 103.90 |
| 26 | A | 1993 | U | N1-C2-O2 | 5.80 | 126.86 | 122.80 |
| 26 | A | 2896 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 1 | a | 679 | C | C5-C6-N1 | 5.80 | 123.90 | 121.00 |
| 26 | A | 383 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 26 | A | 1081 | U | C6-N1-C2 | -5.80 | 117.52 | 121.00 |
| 1 | a | 980 | C | N3-C2-O2 | -5.80 | 117.84 | 121.90 |
| 1 | a | 684 | U | N3-C2-O2 | -5.79 | 118.14 | 122.20 |
| 26 | A | 229 | C | C6-N1-C2 | -5.79 | 117.98 | 120.30 |
| 26 | A | 1113 | U | N3-C2-O2 | -5.79 | 118.14 | 122.20 |
| 26 | A | 1113 | U | N1-C2-O2 | 5.79 | 126.85 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 26 | A | 876 | C | C6-N1-C2 | -5.79 | 117.98 | 120.30 |
| 26 | A | 889 | C | C6-N1-C2 | -5.79 | 117.98 | 120.30 |
| 26 | A | 668 | A | N9-C4-C5 | -5.79 | 103.48 | 105.80 |
| 26 | A | 1314 | C | C6-N1-C2 | -5.79 | 117.98 | 120.30 |
| 23 | x | 118 | G | N3-C4-N9 | 5.79 | 129.47 | 126.00 |
| 1 | a | 556 | C | C5-C6-N1 | 5.78 | 123.89 | 121.00 |
| 24 | y | 57 | G | N1-C2-N2 | 5.78 | 121.41 | 116.20 |
| 26 | A | 1103 | A | C2-N3-C4 | 5.78 | 113.49 | 110.60 |
| 26 | A | 2120 | G | O5'-P-OP1 | -5.78 | 100.49 | 105.70 |
| 1 | a | 1494 | G | O5'-P-OP1 | -5.78 | 100.50 | 105.70 |
| 24 | y | 15 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 1 | a | 90 | C | C5-C6-N1 | 5.78 | 123.89 | 121.00 |
| 25 | z | 26 | ASP | CB-CG-OD1 | 5.77 | 123.50 | 118.30 |
| 26 | A | 1539 | U | N3-C4-O4 | 5.77 | 123.44 | 119.40 |
| 26 | A | 2310 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 24 | y | 73 | G | N1-C6-O6 | 5.77 | 123.36 | 119.90 |
| 26 | A | 2147 | A | O5'-P-OP1 | -5.77 | 100.51 | 105.70 |
| 32 | G | 70 | LEU | CA-CB-CG | 5.77 | 128.57 | 115.30 |
| 24 | y | 56 | C | C2-N1-C1' | 5.76 | 125.14 | 118.80 |
| 26 | A | 2305 | U | N3-C4-C5 | 5.76 | 118.06 | 114.60 |
| 26 | A | 2146 | C | OP1-P-O3' | -5.76 | 92.52 | 105.20 |
| 26 | A | 2215 | C | C6-N1-C2 | -5.76 | 118.00 | 120.30 |
| 23 | x | 115 | A | O4'-C1'-N9 | -5.76 | 103.59 | 108.20 |
| 24 | y | 31 | A | OP2-P-O3' | 5.76 | 117.87 | 105.20 |
| 1 | a | 1034 | G | C5-C6-O6 | -5.76 | 125.15 | 128.60 |
| 24 | y | 47(D) | C | N1-C2-O2 | 5.75 | 122.35 | 118.90 |
| 26 | A | 1905 | C | N1-C2-O2 | 5.75 | 122.35 | 118.90 |
| 26 | A | 1494 | A | C8-N9-C4 | -5.75 | 103.50 | 105.80 |
| 26 | A | 1760 | C | N1-C2-O2 | 5.75 | 122.35 | 118.90 |
| 23 | x | 126 | G | N1-C2-N2 | -5.74 | 111.03 | 116.20 |
| 1 | a | 1226 | C | N3-C2-O2 | -5.74 | 117.88 | 121.90 |
| 24 | y | 30 | G | C5-C6-O6 | -5.74 | 125.16 | 128.60 |
| 26 | A | 1267 | U | N3-C2-O2 | -5.74 | 118.18 | 122.20 |
| 26 | A | 1380 | G | N3-C4-N9 | 5.74 | 129.44 | 126.00 |
| 27 | B | 30 | C | C6-N1-C2 | -5.74 | 118.00 | 120.30 |
| 26 | A | 1054 | A | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 1 | a | 656 | G | N9-C4-C5 | 5.74 | 107.69 | 105.40 |
| 1 | a | 1378 | C | N1-C2-O2 | 5.74 | 122.34 | 118.90 |
| 57 | 6 | 40 | CYS | N-CA-CB | 5.74 | 120.92 | 110.60 |
| 22 | v | 32 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 26 | A | 1279 | G | N9-C4-C5 | -5.73 | 103.11 | 105.40 |
| 1 | a | 491 | G | C8-N9-C1' | -5.73 | 119.55 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | a | 689 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 26 | A | 1270 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 1 | a | 866 | C | C5-C6-N1 | 5.72 | 123.86 | 121.00 |
| 1 | a | 575 | G | N9-C4-C5 | 5.72 | 107.69 | 105.40 |
| 24 | y | 1 | G | N9-C4-C5 | -5.71 | 103.11 | 105.40 |
| 26 | A | 2804 | U | N3-C2-O2 | -5.71 | 118.20 | 122.20 |
| 1 | a | 330 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 1 | a | 1197 | A | N9-C4-C5 | -5.71 | 103.52 | 105.80 |
| 26 | A | 1565 | C | C6-N1-C2 | -5.71 | 118.02 | 120.30 |
| 26 | A | 2043 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 1 | a | 1536 | C | C6-N1-C2 | -5.71 | 118.02 | 120.30 |
| 26 | A | 1582 | C | C6-N1-C2 | -5.71 | 118.02 | 120.30 |
| 26 | A | 2103 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 24 | y | 43 | G | C8-N9-C1' | 5.71 | 134.42 | 127.00 |
| 24 | y | 65 | U | OP2-P-O3' | 5.71 | 117.75 | 105.20 |
| 26 | A | 1083 | U | C2-N1-C1' | -5.71 | 110.85 | 117.70 |
| 28 | C | 32 | LEU | CA-CB-CG | 5.71 | 128.43 | 115.30 |
| 1 | a | 392 | C | N3-C2-O2 | -5.70 | 117.91 | 121.90 |
| 1 | a | 723 | U | N3-C4-O4 | -5.70 | 115.41 | 119.40 |
| 23 | x | 104 | U | OP2-P-O3' | 5.70 | 117.74 | 105.20 |
| 1 | a | 993 | G | C8-N9-C1' | -5.70 | 119.59 | 127.00 |
| 1 | a | 1028 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 24 | y | 10 | C | C6-N1-C2 | -5.70 | 118.02 | 120.30 |
| 1 | a | 14 | U | C6-N1-C2 | -5.69 | 117.58 | 121.00 |
| 26 | A | 2512 | C | C5-C6-N1 | 5.68 | 123.84 | 121.00 |
| 1 | a | 87 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 26 | A | 729 | G | C4-N9-C1' | 5.68 | 133.88 | 126.50 |
| 26 | A | 1257 | C | C5-C6-N1 | 5.68 | 123.84 | 121.00 |
| 1 | a | 968 | A | N9-C1'-C2' | -5.68 | 105.75 | 112.00 |
| 35 | J | 81 | ILE | CG1-CB-CG2 | -5.68 | 98.91 | 111.40 |
| 23 | x | 118 | G | C4-C5-N7 | 5.67 | 113.07 | 110.80 |
| 26 | A | 680 | C | C5-C6-N1 | 5.67 | 123.84 | 121.00 |
| 26 | A | 1760 | C | C5-C6-N1 | 5.67 | 123.84 | 121.00 |
| 1 | a | 426 | U | N3-C2-O2 | -5.67 | 118.23 | 122.20 |
| 26 | A | 2080 | A | N1-C2-N3 | -5.67 | 126.46 | 129.30 |
| 1 | a | 923 | A | C5-N7-C8 | -5.67 | 101.07 | 103.90 |
| 1 | a | 1149 | C | C6-N1-C2 | -5.66 | 118.03 | 120.30 |
| 26 | A | 1380 | G | C6-C5-N7 | -5.66 | 127.00 | 130.40 |
| 26 | A | 2065 | C | C6-N1-C2 | -5.66 | 118.04 | 120.30 |
| 26 | A | 1053 | C | C6-N1-C2 | -5.65 | 118.04 | 120.30 |
| 26 | A | 2558 | C | C5-C6-N1 | 5.65 | 123.83 | 121.00 |
| 26 | A | 2765 | A | C2-N3-C4 | 5.65 | 113.42 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-------------|-------|-------------|----------|
| 24 | y | 60 | U | N3-C2-O2 | 5.65 | 126.15 | 122.20 |
| 25 | z | 461 | LEU | CB-CG-CD1 | -5.65 | 101.40 | 111.00 |
| 26 | A | 883 | G | C4-C5-N7 | 5.65 | 113.06 | 110.80 |
| 26 | A | 2720 | U | N3-C2-O2 | -5.65 | 118.25 | 122.20 |
| 1 | a | 514 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 1 | a | 1317 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 26 | A | 209 | C | C5-C6-N1 | 5.64 | 123.82 | 121.00 |
| 1 | a | 449 | G | C5-C6-O6 | -5.64 | 125.21 | 128.60 |
| 1 | a | 799 | G | N3-C2-N2 | -5.64 | 115.95 | 119.90 |
| 26 | A | 503 | A | C8-N9-C4 | 5.64 | 108.06 | 105.80 |
| 26 | A | 1267 | U | N1-C2-O2 | 5.64 | 126.75 | 122.80 |
| 24 | y | 15 | C | C2-N1-C1' | 5.64 | 125.00 | 118.80 |
| 26 | A | 558 | U | O5'-P-OP1 | -5.64 | 100.63 | 105.70 |
| 1 | a | 513 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 23 | x | 125 | G | C3'-C2'-C1' | 5.63 | 106.00 | 101.50 |
| 1 | a | 407 | U | C5-C6-N1 | 5.62 | 125.51 | 122.70 |
| 26 | A | 243 | U | N1-C2-O2 | 5.62 | 126.73 | 122.80 |
| 26 | A | 729 | G | O4'-C1'-N9 | 5.62 | 112.69 | 108.20 |
| 24 | y | 17 | G | N3-C4-N9 | -5.61 | 122.63 | 126.00 |
| 26 | A | 2180 | U | C2-N3-C4 | 5.61 | 130.37 | 127.00 |
| 1 | a | 322 | C | C6-N1-C2 | -5.61 | 118.06 | 120.30 |
| 1 | a | 611 | C | N3-C2-O2 | -5.61 | 117.97 | 121.90 |
| 26 | A | 243 | U | N3-C2-O2 | -5.61 | 118.28 | 122.20 |
| 26 | A | 2710 | C | C6-N1-C2 | -5.61 | 118.06 | 120.30 |
| 26 | A | 2637 | U | N3-C2-O2 | -5.60 | 118.28 | 122.20 |
| 1 | a | 54 | C | N1-C2-O2 | 5.60 | 122.26 | 118.90 |
| 1 | a | 1303 | C | OP2-P-O3' | 5.60 | 117.53 | 105.20 |
| 24 | y | 5 | G | N3-C2-N2 | -5.60 | 115.98 | 119.90 |
| 27 | B | 70 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 1 | a | 920 | U | N3-C2-O2 | -5.60 | 118.28 | 122.20 |
| 26 | A | 2416 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 32 | G | 42 | VAL | CG1-CB-CG2 | -5.60 | 101.94 | 110.90 |
| 1 | a | 1469 | C | N3-C2-O2 | -5.59 | 117.98 | 121.90 |
| 26 | A | 2066 | C | C6-N1-C2 | -5.59 | 118.06 | 120.30 |
| 26 | A | 806 | C | C5-C6-N1 | 5.58 | 123.79 | 121.00 |
| 1 | a | 1009 | U | N3-C4-O4 | -5.58 | 115.50 | 119.40 |
| 26 | A | 837 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 32 | G | 173 | ALA | C-N-CA | 5.58 | 135.65 | 121.70 |
| 24 | y | 47(G) | C | C6-N1-C1' | 5.58 | 127.49 | 120.80 |
| 1 | a | 1133 | G | N3-C2-N2 | -5.58 | 116.00 | 119.90 |
| 26 | A | 279 | A | C5-C6-N6 | -5.58 | 119.24 | 123.70 |
| 26 | A | 1180 | U | C2-N1-C1' | 5.57 | 124.39 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 1 | a | 354 | G | N3-C4-N9 | 5.57 | 129.34 | 126.00 |
| 1 | a | 723 | U | C4-C5-C6 | -5.57 | 116.36 | 119.70 |
| 1 | a | 799 | G | N9-C4-C5 | 5.57 | 107.63 | 105.40 |
| 26 | A | 2626 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 1 | a | 502 | A | N9-C4-C5 | -5.57 | 103.57 | 105.80 |
| 24 | y | 16 | C | C2-N1-C1' | -5.57 | 112.68 | 118.80 |
| 1 | a | 110 | C | N3-C2-O2 | -5.56 | 118.00 | 121.90 |
| 26 | A | 2044 | C | C5-C6-N1 | 5.56 | 123.78 | 121.00 |
| 26 | A | 198 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |
| 26 | A | 2214 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 24 | y | 47(H) | A | O5'-P-OP2 | -5.55 | 100.71 | 105.70 |
| 26 | A | 1594 | U | C5-C6-N1 | 5.55 | 125.47 | 122.70 |
| 1 | a | 647 | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 26 | A | 1103 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 26 | A | 84 | A | C5-N7-C8 | 5.54 | 106.67 | 103.90 |
| 26 | A | 1076 | C | C2-N3-C4 | 5.54 | 122.67 | 119.90 |
| 26 | A | 2179 | C | N3-C2-O2 | -5.54 | 118.02 | 121.90 |
| 1 | a | 443 | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 1 | a | 956 | U | N3-C2-O2 | -5.54 | 118.32 | 122.20 |
| 22 | v | 1 | C | C2-N3-C4 | 5.54 | 122.67 | 119.90 |
| 26 | A | 2276 | G | N3-C2-N2 | -5.54 | 116.02 | 119.90 |
| 1 | a | 312 | C | C2-N1-C1' | 5.53 | 124.89 | 118.80 |
| 1 | a | 1161 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 26 | A | 610 | C | C5-C6-N1 | 5.53 | 123.77 | 121.00 |
| 1 | a | 737 | C | C5-C6-N1 | 5.53 | 123.77 | 121.00 |
| 1 | a | 1460 | C | C5-C6-N1 | 5.53 | 123.77 | 121.00 |
| 26 | A | 2562 | U | N1-C2-O2 | 5.53 | 126.67 | 122.80 |
| 51 | Z | 23 | LEU | CB-CG-CD1 | -5.53 | 101.60 | 111.00 |
| 1 | a | 536 | C | C2-N1-C1' | 5.53 | 124.88 | 118.80 |
| 26 | A | 890 | C | N1-C2-N3 | -5.53 | 115.33 | 119.20 |
| 26 | A | 1971 | U | N1-C2-O2 | -5.53 | 118.93 | 122.80 |
| 1 | a | 90 | C | N3-C2-O2 | -5.53 | 118.03 | 121.90 |
| 1 | a | 960 | U | N1-C2-O2 | 5.53 | 126.67 | 122.80 |
| 23 | x | 101 | A | N9-C4-C5 | -5.52 | 103.59 | 105.80 |
| 26 | A | 948 | C | C5-C6-N1 | 5.52 | 123.76 | 121.00 |
| 26 | A | 1071 | G | OP1-P-O3' | 5.52 | 117.35 | 105.20 |
| 26 | A | 1564 | C | C6-N1-C2 | -5.52 | 118.09 | 120.30 |
| 26 | A | 1775 | U | N1-C2-O2 | 5.52 | 126.67 | 122.80 |
| 1 | a | 307 | C | C6-N1-C2 | -5.52 | 118.09 | 120.30 |
| 23 | x | 125 | G | C8-N9-C4 | -5.52 | 104.19 | 106.40 |
| 26 | A | 2075 | U | N3-C4-O4 | 5.52 | 123.26 | 119.40 |
| 26 | A | 2573 | C | O5'-P-OP1 | 5.51 | 117.32 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-------------|-------|-------------|----------|
| 26 | A | 2707 | U | N1-C2-O2 | 5.51 | 126.66 | 122.80 |
| 26 | A | 231 | A | N1-C6-N6 | 5.51 | 121.91 | 118.60 |
| 26 | A | 642 | U | N3-C2-O2 | -5.51 | 118.34 | 122.20 |
| 1 | a | 1395 | C | N3-C2-O2 | -5.51 | 118.04 | 121.90 |
| 26 | A | 393 | C | C6-N1-C2 | -5.51 | 118.10 | 120.30 |
| 1 | a | 662 | U | C5-C4-O4 | -5.50 | 122.60 | 125.90 |
| 24 | y | 47(K) | G | N3-C4-N9 | -5.50 | 122.70 | 126.00 |
| 26 | A | 559 | G | N7-C8-N9 | 5.50 | 115.85 | 113.10 |
| 26 | A | 2462 | C | C5-C6-N1 | 5.50 | 123.75 | 121.00 |
| 24 | y | 47(B) | G | C4-N9-C1' | 5.49 | 133.64 | 126.50 |
| 26 | A | 901 | C | N1-C2-O2 | 5.49 | 122.20 | 118.90 |
| 1 | a | 491 | G | C4-N9-C1' | 5.49 | 133.64 | 126.50 |
| 1 | a | 868 | C | C2-N1-C1' | 5.49 | 124.84 | 118.80 |
| 1 | a | 514 | C | C5-C6-N1 | 5.49 | 123.74 | 121.00 |
| 1 | a | 1071 | C | C2-N1-C1' | 5.49 | 124.84 | 118.80 |
| 26 | A | 852 | U | C5-C4-O4 | -5.49 | 122.61 | 125.90 |
| 1 | a | 896 | C | C6-N1-C2 | -5.49 | 118.11 | 120.30 |
| 23 | x | 126 | G | C2'-C3'-O3' | -5.48 | 97.44 | 109.50 |
| 26 | A | 1158 | C | O5'-P-OP2 | -5.48 | 100.76 | 105.70 |
| 1 | a | 513 | C | C2-N1-C1' | 5.48 | 124.83 | 118.80 |
| 26 | A | 2805 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 1 | a | 598 | U | N3-C2-O2 | -5.48 | 118.36 | 122.20 |
| 26 | A | 125 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 26 | A | 1244 | A | N9-C4-C5 | -5.48 | 103.61 | 105.80 |
| 26 | A | 822 | G | N7-C8-N9 | 5.48 | 115.84 | 113.10 |
| 26 | A | 2134 | A | N1-C6-N6 | -5.47 | 115.32 | 118.60 |
| 1 | a | 334 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 26 | A | 415 | A | N9-C4-C5 | -5.47 | 103.61 | 105.80 |
| 26 | A | 717 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 1 | a | 418 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 24 | y | 47(O) | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 26 | A | 1314 | C | C5-C6-N1 | 5.47 | 123.73 | 121.00 |
| 41 | P | 113 | LEU | CA-CB-CG | 5.46 | 127.87 | 115.30 |
| 1 | a | 90 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 26 | A | 1548 | A | N9-C4-C5 | -5.46 | 103.61 | 105.80 |
| 1 | a | 1521 | C | C5-C6-N1 | 5.46 | 123.73 | 121.00 |
| 22 | v | 67 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 26 | A | 1061 | U | OP2-P-O3' | 5.46 | 117.21 | 105.20 |
| 1 | a | 103 | U | N3-C2-O2 | -5.45 | 118.38 | 122.20 |
| 24 | y | 48 | G | C5-N7-C8 | -5.45 | 101.57 | 104.30 |
| 1 | a | 984 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 26 | A | 1578 | U | N3-C2-O2 | -5.45 | 118.38 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-------------|-------|-------------|----------|
| 57 | 6 | 32 | LEU | CB-CG-CD1 | 5.45 | 120.26 | 111.00 |
| 1 | a | 211 | G | N3-C4-C5 | -5.44 | 125.88 | 128.60 |
| 1 | a | 34 | C | C2-N1-C1' | 5.44 | 124.78 | 118.80 |
| 1 | a | 1066 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 24 | y | 57 | G | N9-C4-C5 | 5.43 | 107.57 | 105.40 |
| 26 | A | 1340 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 26 | A | 2766 | A | C5-C6-N6 | -5.43 | 119.35 | 123.70 |
| 1 | a | 610 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 2 | b | 56 | LEU | CA-CB-CG | 5.43 | 127.78 | 115.30 |
| 26 | A | 1624 | U | N3-C2-O2 | -5.42 | 118.40 | 122.20 |
| 1 | a | 16 | A | N1-C2-N3 | -5.42 | 126.59 | 129.30 |
| 1 | a | 322 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 22 | v | 68 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 26 | A | 120 | U | C4-C5-C6 | 5.42 | 122.95 | 119.70 |
| 26 | A | 669 | G | C4-N9-C1' | 5.42 | 133.55 | 126.50 |
| 1 | a | 1487 | G | N3-C2-N2 | -5.42 | 116.11 | 119.90 |
| 1 | a | 1131 | G | C4-C5-N7 | 5.42 | 112.97 | 110.80 |
| 24 | y | 45 | U | C6-N1-C2 | -5.42 | 117.75 | 121.00 |
| 24 | y | 48 | G | C4-N9-C1' | 5.42 | 133.54 | 126.50 |
| 1 | a | 723 | U | N3-C2-O2 | -5.41 | 118.41 | 122.20 |
| 24 | y | 47(E) | G | N1-C6-O6 | -5.41 | 116.65 | 119.90 |
| 57 | 6 | 4 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 26 | A | 1348 | C | N3-C2-O2 | -5.41 | 118.11 | 121.90 |
| 26 | A | 2118 | U | C5-C4-O4 | -5.41 | 122.66 | 125.90 |
| 26 | A | 1070 | A | O5'-P-OP2 | 5.40 | 117.19 | 110.70 |
| 1 | a | 87 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 23 | x | 124 | A | N3-C4-N9 | 5.40 | 131.72 | 127.40 |
| 26 | A | 2254 | C | N3-C2-O2 | -5.40 | 118.12 | 121.90 |
| 26 | A | 2305 | U | C6-N1-C1' | -5.40 | 113.64 | 121.20 |
| 26 | A | 278 | A | C2-N3-C4 | 5.39 | 113.30 | 110.60 |
| 26 | A | 1708 | C | C5-C6-N1 | 5.39 | 123.70 | 121.00 |
| 1 | a | 307 | C | N3-C2-O2 | -5.39 | 118.13 | 121.90 |
| 26 | A | 2902 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 23 | x | 129 | U | C5'-C4'-C3' | 5.39 | 124.62 | 116.00 |
| 27 | B | 108 | A | N1-C6-N6 | 5.38 | 121.83 | 118.60 |
| 26 | A | 2699 | C | C5-C6-N1 | 5.38 | 123.69 | 121.00 |
| 1 | a | 680 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 26 | A | 1914 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 26 | A | 867 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 24 | y | 47(G) | C | N1-C2-N3 | 5.38 | 122.97 | 119.20 |
| 26 | A | 141 | G | N3-C4-N9 | 5.38 | 129.23 | 126.00 |
| 1 | a | 71 | A | OP2-P-O3' | 5.38 | 117.03 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27 | B | 65 | U | N3-C2-O2 | -5.38 | 118.44 | 122.20 |
| 23 | x | 126 | G | N3-C2-N2 | 5.38 | 123.66 | 119.90 |
| 22 | v | 62 | C | C5-C6-N1 | 5.37 | 123.69 | 121.00 |
| 26 | A | 827 | U | O5'-P-OP1 | -5.37 | 100.86 | 105.70 |
| 26 | A | 365 | U | C5-C4-O4 | -5.37 | 122.68 | 125.90 |
| 27 | B | 25 | U | N3-C2-O2 | -5.37 | 118.44 | 122.20 |
| 26 | A | 1476 | U | C2-N1-C1' | 5.37 | 124.14 | 117.70 |
| 1 | a | 661 | G | C4-C5-N7 | 5.37 | 112.95 | 110.80 |
| 19 | s | 15 | LEU | CA-CB-CG | 5.37 | 127.64 | 115.30 |
| 26 | A | 1723 | G | C5-C6-N1 | 5.37 | 114.18 | 111.50 |
| 1 | a | 582 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 26 | A | 1670 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 26 | A | 658 | U | C5-C6-N1 | 5.36 | 125.38 | 122.70 |
| 26 | A | 1927 | A | OP2-P-O3' | 5.36 | 116.99 | 105.20 |
| 1 | a | 923 | A | C4-C5-N7 | 5.36 | 113.38 | 110.70 |
| 23 | x | 110 | G | P-O3'-C3' | -5.36 | 113.27 | 119.70 |
| 1 | a | 470 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 1 | a | 1158 | C | C6-N1-C1' | -5.36 | 114.37 | 120.80 |
| 1 | a | 979 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 26 | A | 1585 | C | N3-C2-O2 | -5.35 | 118.15 | 121.90 |
| 1 | a | 1302 | C | N3-C4-C5 | 5.35 | 124.04 | 121.90 |
| 26 | A | 230 | G | N9-C4-C5 | -5.35 | 103.26 | 105.40 |
| 26 | A | 2165 | C | N1-C2-O2 | 5.35 | 122.11 | 118.90 |
| 22 | v | 40 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 1 | a | 967 | 5MC | OP2-P-O3' | 5.35 | 116.96 | 105.20 |
| 1 | a | 1389 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 26 | A | 717 | C | C5-C6-N1 | 5.35 | 123.67 | 121.00 |
| 24 | y | 41 | C | C2-N1-C1' | 5.35 | 124.68 | 118.80 |
| 26 | A | 1886 | U | N3-C2-O2 | -5.35 | 118.46 | 122.20 |
| 1 | a | 413 | G | N3-C4-C5 | 5.34 | 131.27 | 128.60 |
| 26 | A | 1043 | C | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 1 | a | 420 | U | C2-N1-C1' | 5.34 | 124.11 | 117.70 |
| 26 | A | 444 | C | C5-C6-N1 | 5.33 | 123.67 | 121.00 |
| 1 | a | 1102 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 1 | a | 1241 | G | C8-N9-C4 | -5.33 | 104.27 | 106.40 |
| 26 | A | 2428 | G | OP1-P-OP2 | -5.33 | 111.60 | 119.60 |
| 1 | a | 440 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 26 | A | 2180 | U | C5-C6-N1 | 5.33 | 125.36 | 122.70 |
| 1 | a | 178 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 1 | a | 225 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 1 | a | 431 | A | N1-C6-N6 | -5.33 | 115.40 | 118.60 |
| 1 | a | 1460 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26 | A | 148 | U | C5-C4-O4 | -5.33 | 122.70 | 125.90 |
| 24 | y | 62 | C | N3-C4-N4 | -5.33 | 114.27 | 118.00 |
| 25 | z | 338 | VAL | CG1-CB-CG2 | -5.33 | 102.38 | 110.90 |
| 1 | a | 751 | U | N3-C2-O2 | -5.33 | 118.47 | 122.20 |
| 26 | A | 947 | A | N9-C4-C5 | -5.32 | 103.67 | 105.80 |
| 23 | x | 131 | C | C3'-C2'-C1' | 5.32 | 105.76 | 101.50 |
| 26 | A | 2302 | U | N1-C2-O2 | 5.32 | 126.53 | 122.80 |
| 26 | A | 1498 | C | C5-C6-N1 | 5.32 | 123.66 | 121.00 |
| 1 | a | 610 | U | N1-C2-O2 | 5.32 | 126.52 | 122.80 |
| 1 | a | 1382 | C | N3-C2-O2 | -5.32 | 118.18 | 121.90 |
| 24 | y | 53 | G | C2-N3-C4 | -5.31 | 109.24 | 111.90 |
| 26 | A | 1990 | C | C6-N1-C2 | -5.31 | 118.17 | 120.30 |
| 33 | I | 10 | LEU | CA-CB-CG | 5.31 | 127.52 | 115.30 |
| 1 | a | 80 | A | C5-C6-N1 | -5.31 | 115.05 | 117.70 |
| 1 | a | 1138 | G | C2-N3-C4 | 5.31 | 114.55 | 111.90 |
| 22 | v | 40 | C | N1-C2-O2 | 5.31 | 122.08 | 118.90 |
| 26 | A | 2081 | U | C5-C6-N1 | 5.31 | 125.35 | 122.70 |
| 1 | a | 323 | U | C5-C4-O4 | -5.30 | 122.72 | 125.90 |
| 1 | a | 764 | C | C5-C6-N1 | 5.30 | 123.65 | 121.00 |
| 1 | a | 878 | A | C4-C5-N7 | 5.30 | 113.35 | 110.70 |
| 1 | a | 879 | C | C5-C6-N1 | 5.30 | 123.65 | 121.00 |
| 1 | a | 1504 | G | N3-C4-N9 | -5.30 | 122.82 | 126.00 |
| 24 | y | 57 | G | N3-C4-N9 | -5.30 | 122.82 | 126.00 |
| 26 | A | 1629 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 26 | A | 2007 | U | C5-C6-N1 | 5.30 | 125.35 | 122.70 |
| 1 | a | 924 | C | C5-C6-N1 | 5.29 | 123.65 | 121.00 |
| 42 | Q | 108 | LEU | CA-CB-CG | 5.29 | 127.47 | 115.30 |
| 24 | y | 72 | C | C6-N1-C2 | -5.29 | 118.19 | 120.30 |
| 26 | A | 2080 | A | N1-C6-N6 | 5.29 | 121.77 | 118.60 |
| 26 | A | 1548 | A | N1-C2-N3 | -5.29 | 126.66 | 129.30 |
| 1 | a | 528 | C | C5-C6-N1 | 5.28 | 123.64 | 121.00 |
| 26 | A | 1229 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 24 | y | 58 | A | O5'-P-OP2 | -5.28 | 100.95 | 105.70 |
| 31 | F | 162 | ASP | CB-CG-OD1 | 5.28 | 123.05 | 118.30 |
| 1 | a | 439 | U | N3-C2-O2 | -5.27 | 118.51 | 122.20 |
| 26 | A | 2231 | U | C5-C6-N1 | 5.27 | 125.33 | 122.70 |
| 24 | y | 40 | C | C2-N1-C1' | 5.27 | 124.60 | 118.80 |
| 27 | B | 47 | C | C6-N1-C2 | -5.27 | 118.19 | 120.30 |
| 23 | x | 117 | C | C5-C6-N1 | 5.27 | 123.63 | 121.00 |
| 26 | A | 233 | A | N9-C4-C5 | -5.27 | 103.69 | 105.80 |
| 1 | a | 620 | C | C6-N1-C2 | -5.26 | 118.19 | 120.30 |
| 26 | A | 283 | G | N3-C4-N9 | -5.26 | 122.84 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 22 | v | 67 | C | C5-C6-N1 | 5.26 | 123.63 | 121.00 |
| 26 | A | 302 | C | C5-C6-N1 | 5.26 | 123.63 | 121.00 |
| 24 | y | 30 | G | C4-N9-C1' | 5.25 | 133.33 | 126.50 |
| 26 | A | 1512 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 1 | a | 968 | A | C6-C5-N7 | 5.25 | 135.97 | 132.30 |
| 1 | a | 169 | C | N3-C2-O2 | -5.25 | 118.23 | 121.90 |
| 26 | A | 1399 | C | C5-C6-N1 | 5.25 | 123.62 | 121.00 |
| 1 | a | 528 | C | N3-C2-O2 | -5.24 | 118.23 | 121.90 |
| 1 | a | 1263 | C | N1-C2-O2 | 5.24 | 122.05 | 118.90 |
| 1 | a | 1410 | A | N9-C4-C5 | -5.24 | 103.70 | 105.80 |
| 26 | A | 2259 | U | N3-C2-O2 | -5.24 | 118.53 | 122.20 |
| 1 | a | 1086 | U | C5-C6-N1 | 5.24 | 125.32 | 122.70 |
| 26 | A | 2254 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 26 | A | 1059 | G | OP1-P-O3' | 5.24 | 116.73 | 105.20 |
| 1 | a | 552 | U | C5-C6-N1 | 5.24 | 125.32 | 122.70 |
| 26 | A | 283 | G | N1-C6-O6 | -5.24 | 116.76 | 119.90 |
| 26 | A | 1644 | C | N1-C2-O2 | 5.24 | 122.04 | 118.90 |
| 26 | A | 1118 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 26 | A | 209 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 26 | A | 1257 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 25 | z | 610 | LEU | CA-CB-CG | 5.23 | 127.33 | 115.30 |
| 1 | a | 449 | G | N9-C4-C5 | -5.23 | 103.31 | 105.40 |
| 1 | a | 1317 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 1 | a | 956 | U | N1-C2-O2 | 5.23 | 126.46 | 122.80 |
| 26 | A | 101 | A | C2-N3-C4 | -5.23 | 107.99 | 110.60 |
| 10 | j | 75 | ASP | CB-CG-OD1 | 5.23 | 123.00 | 118.30 |
| 26 | A | 2565 | A | C8-N9-C4 | -5.23 | 103.71 | 105.80 |
| 26 | A | 143 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 1 | a | 1412 | C | C2-N1-C1' | 5.22 | 124.54 | 118.80 |
| 27 | B | 42 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 1 | a | 1464 | U | N3-C2-O2 | -5.22 | 118.55 | 122.20 |
| 26 | A | 1958 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 1 | a | 580 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 1 | a | 582 | C | C5-C6-N1 | 5.22 | 123.61 | 121.00 |
| 26 | A | 56 | A | N9-C4-C5 | -5.22 | 103.71 | 105.80 |
| 26 | A | 898 | C | C5-C6-N1 | 5.21 | 123.61 | 121.00 |
| 1 | a | 493 | A | N7-C8-N9 | 5.21 | 116.41 | 113.80 |
| 26 | A | 813 | U | N1-C2-O2 | 5.21 | 126.45 | 122.80 |
| 1 | a | 920 | U | N1-C2-O2 | 5.21 | 126.44 | 122.80 |
| 26 | A | 890 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 26 | A | 2086 | U | N3-C2-O2 | -5.21 | 118.56 | 122.20 |
| 24 | y | 73 | G | C5-C6-O6 | -5.20 | 125.48 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 22 | v | 39 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 26 | A | 2028 | U | C5-C6-N1 | 5.20 | 125.30 | 122.70 |
| 57 | 6 | 40 | CYS | CB-CA-C | -5.20 | 100.00 | 110.40 |
| 1 | a | 397 | A | C4-C5-N7 | 5.20 | 113.30 | 110.70 |
| 25 | z | 457 | LEU | CA-CB-CG | 5.20 | 127.26 | 115.30 |
| 26 | A | 2556 | C | N3-C2-O2 | -5.20 | 118.26 | 121.90 |
| 1 | a | 866 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 24 | y | 40 | C | O5'-P-OP2 | -5.20 | 101.02 | 105.70 |
| 1 | a | 274 | A | N1-C2-N3 | -5.19 | 126.70 | 129.30 |
| 1 | a | 127 | G | N9-C4-C5 | -5.19 | 103.32 | 105.40 |
| 24 | y | 1 | G | C4-C5-N7 | 5.19 | 112.88 | 110.80 |
| 26 | A | 435 | C | OP2-P-O3' | 5.19 | 116.62 | 105.20 |
| 26 | A | 891 | G | N3-C4-C5 | -5.19 | 126.00 | 128.60 |
| 26 | A | 933 | A | N3-C4-N9 | 5.19 | 131.55 | 127.40 |
| 26 | A | 346 | A | OP2-P-O3' | 5.19 | 116.62 | 105.20 |
| 26 | A | 314 | C | C5-C6-N1 | 5.19 | 123.59 | 121.00 |
| 26 | A | 1077 | A | C5-C6-N1 | 5.19 | 120.29 | 117.70 |
| 26 | A | 2226 | C | N1-C2-O2 | 5.19 | 122.01 | 118.90 |
| 50 | Y | 28 | LEU | CA-CB-CG | 5.18 | 127.22 | 115.30 |
| 26 | A | 1093 | G | C6-C5-N7 | -5.18 | 127.29 | 130.40 |
| 26 | A | 119 | A | C4-C5-C6 | -5.18 | 114.41 | 117.00 |
| 26 | A | 883 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 23 | x | 119 | G | N9-C4-C5 | 5.18 | 107.47 | 105.40 |
| 30 | E | 82 | GLY | CA-C-O | -5.18 | 111.28 | 120.60 |
| 22 | v | 50 | U | C6-N1-C2 | -5.18 | 117.89 | 121.00 |
| 24 | y | 32 | C | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 26 | A | 2136 | G | C5-C6-O6 | -5.17 | 125.50 | 128.60 |
| 26 | A | 2766 | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 1 | a | 219 | U | C5-C6-N1 | 5.17 | 125.29 | 122.70 |
| 24 | y | 47(P) | C | N3-C2-O2 | -5.17 | 118.28 | 121.90 |
| 15 | o | 55 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 26 | A | 2310 | C | N3-C2-O2 | -5.17 | 118.28 | 121.90 |
| 1 | a | 431 | A | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 26 | A | 1243 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 23 | x | 110 | G | C4-N9-C1' | 5.16 | 133.21 | 126.50 |
| 31 | F | 50 | ASP | CB-CG-OD1 | 5.16 | 122.95 | 118.30 |
| 1 | a | 1148 | U | C6-N1-C2 | -5.16 | 117.90 | 121.00 |
| 1 | a | 1109 | C | C5-C6-N1 | 5.16 | 123.58 | 121.00 |
| 24 | y | 47(F) | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 26 | A | 2430 | A | C2-N3-C4 | 5.16 | 113.18 | 110.60 |
| 1 | a | 1003 | G | C8-N9-C4 | -5.16 | 104.34 | 106.40 |
| 15 | o | 86 | LEU | CA-CB-CG | 5.16 | 127.16 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | a | 413 | G | O4'-C1'-N9 | -5.15 | 104.08 | 108.20 |
| 26 | A | 888 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 1 | a | 1034 | G | C6-C5-N7 | -5.15 | 127.31 | 130.40 |
| 26 | A | 687 | C | N3-C2-O2 | -5.15 | 118.29 | 121.90 |
| 26 | A | 1075 | C | C6-N1-C1' | -5.15 | 114.62 | 120.80 |
| 1 | a | 634 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 26 | A | 946 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 26 | A | 1771 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 1 | a | 199 | A | N9-C4-C5 | -5.14 | 103.74 | 105.80 |
| 1 | a | 1241 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 26 | A | 314 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 26 | A | 1043 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 26 | A | 1081 | U | C5-C6-N1 | 5.14 | 125.27 | 122.70 |
| 26 | A | 2469 | A | C5-C6-N6 | -5.14 | 119.59 | 123.70 |
| 1 | a | 340 | U | N3-C2-O2 | -5.14 | 118.60 | 122.20 |
| 1 | a | 1411 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 26 | A | 897 | C | N3-C2-O2 | -5.14 | 118.30 | 121.90 |
| 26 | A | 2065 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 1 | a | 414 | A | C5-C6-N1 | 5.14 | 120.27 | 117.70 |
| 1 | a | 1237 | C | C5-C6-N1 | 5.13 | 123.57 | 121.00 |
| 1 | a | 1263 | C | C2-N1-C1' | 5.13 | 124.45 | 118.80 |
| 11 | k | 84 | MET | CA-CB-CG | 5.13 | 122.03 | 113.30 |
| 1 | a | 1032 | G | N3-C4-N9 | 5.13 | 129.08 | 126.00 |
| 1 | a | 418 | C | C5-C6-N1 | 5.13 | 123.57 | 121.00 |
| 1 | a | 923 | A | N9-C4-C5 | -5.13 | 103.75 | 105.80 |
| 23 | x | 119 | G | N3-C2-N2 | -5.13 | 116.31 | 119.90 |
| 26 | A | 2146 | C | OP1-P-OP2 | -5.13 | 111.90 | 119.60 |
| 27 | B | 28 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 23 | x | 118 | G | C5-N7-C8 | -5.13 | 101.73 | 104.30 |
| 1 | a | 697 | U | N3-C2-O2 | -5.13 | 118.61 | 122.20 |
| 26 | A | 1181 | U | C6-N1-C2 | -5.13 | 117.92 | 121.00 |
| 26 | A | 283 | G | N9-C4-C5 | 5.13 | 107.45 | 105.40 |
| 26 | A | 889 | C | C2-N1-C1' | 5.13 | 124.44 | 118.80 |
| 25 | z | 177 | LEU | CB-CG-CD2 | -5.12 | 102.29 | 111.00 |
| 4 | d | 4 | LEU | CB-CG-CD2 | -5.12 | 102.29 | 111.00 |
| 1 | a | 207 | C | N3-C2-O2 | -5.12 | 118.32 | 121.90 |
| 1 | a | 428 | G | N3-C4-C5 | 5.12 | 131.16 | 128.60 |
| 7 | g | 39 | GLU | CA-CB-CG | 5.12 | 124.66 | 113.40 |
| 26 | A | 1350 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 26 | A | 1499 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 26 | A | 1990 | C | C5-C6-N1 | 5.12 | 123.56 | 121.00 |
| 27 | B | 120 | U | C2-N1-C1' | 5.12 | 123.84 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | a | 1524 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 26 | A | 851 | C | C5-C6-N1 | 5.11 | 123.56 | 121.00 |
| 24 | y | 16 | C | N3-C4-N4 | -5.11 | 114.42 | 118.00 |
| 1 | a | 55 | A | C2-N3-C4 | 5.11 | 113.16 | 110.60 |
| 1 | a | 1342 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 26 | A | 2548 | U | C5-C6-N1 | 5.11 | 125.26 | 122.70 |
| 34 | H | 58 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 26 | A | 278 | A | N3-C4-C5 | -5.11 | 123.22 | 126.80 |
| 26 | A | 668 | A | N1-C2-N3 | -5.11 | 126.75 | 129.30 |
| 3 | c | 30 | ASP | CB-CG-OD1 | 5.11 | 122.89 | 118.30 |
| 26 | A | 283 | G | N1-C2-N2 | 5.11 | 120.79 | 116.20 |
| 1 | a | 409 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 26 | A | 665 | U | C5-C6-N1 | 5.10 | 125.25 | 122.70 |
| 26 | A | 807 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 26 | A | 2656 | U | N1-C2-O2 | 5.10 | 126.37 | 122.80 |
| 26 | A | 867 | C | N3-C2-O2 | -5.10 | 118.33 | 121.90 |
| 26 | A | 1680 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 1 | a | 1500 | A | C6-N1-C2 | 5.10 | 121.66 | 118.60 |
| 2 | b | 17 | HIS | N-CA-C | 5.10 | 124.77 | 111.00 |
| 22 | v | 28 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 1 | a | 419 | C | N1-C2-N3 | 5.09 | 122.76 | 119.20 |
| 26 | A | 1476 | U | C6-N1-C2 | -5.09 | 117.94 | 121.00 |
| 26 | A | 53 | A | C4-C5-N7 | 5.09 | 113.25 | 110.70 |
| 26 | A | 392 | U | N3-C2-O2 | -5.09 | 118.64 | 122.20 |
| 26 | A | 1158 | C | C5-C6-N1 | 5.09 | 123.55 | 121.00 |
| 1 | a | 54 | C | N3-C2-O2 | -5.09 | 118.34 | 121.90 |
| 26 | A | 208 | C | C6-N1-C2 | -5.09 | 118.27 | 120.30 |
| 26 | A | 373 | U | C6-N1-C2 | -5.09 | 117.95 | 121.00 |
| 26 | A | 610 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 26 | A | 2558 | C | C6-N1-C2 | -5.09 | 118.27 | 120.30 |
| 26 | A | 2756 | U | OP1-P-O3' | 5.09 | 116.39 | 105.20 |
| 1 | a | 294 | U | C5-C6-N1 | 5.08 | 125.24 | 122.70 |
| 1 | a | 1489 | G | N3-C2-N2 | -5.08 | 116.34 | 119.90 |
| 26 | A | 1578 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 38 | M | 65 | ILE | CG1-CB-CG2 | -5.08 | 100.21 | 111.40 |
| 26 | A | 2716 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 26 | A | 1812 | U | N3-C2-O2 | -5.08 | 118.64 | 122.20 |
| 26 | A | 2086 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 26 | A | 1830 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 27 | B | 57 | A | C8-N9-C4 | -5.08 | 103.77 | 105.80 |
| 26 | A | 2234 | G | N7-C8-N9 | 5.07 | 115.64 | 113.10 |
| 24 | y | 35 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1 | a | 750 | C | N1-C2-N3 | 5.07 | 122.75 | 119.20 |
| 26 | A | 1113 | U | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |
| 1 | a | 489 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 1 | a | 879 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 26 | A | 1093 | G | C5-C6-N1 | 5.07 | 114.03 | 111.50 |
| 26 | A | 2103 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 1 | a | 418 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 23 | x | 118 | G | C4-N9-C1' | 5.07 | 133.09 | 126.50 |
| 24 | y | 32 | C | C6-N1-C1' | 5.07 | 126.88 | 120.80 |
| 26 | A | 2480 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 1 | a | 392 | C | N3-C4-N4 | 5.06 | 121.54 | 118.00 |
| 22 | v | 57 | A | N7-C8-N9 | -5.06 | 111.27 | 113.80 |
| 24 | y | 47(J) | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 1 | a | 796 | C | C6-N1-C2 | -5.06 | 118.28 | 120.30 |
| 26 | A | 1052 | C | C5-C6-N1 | 5.06 | 123.53 | 121.00 |
| 26 | A | 2739 | U | N3-C2-O2 | -5.06 | 118.66 | 122.20 |
| 35 | J | 17 | VAL | CG1-CB-CG2 | -5.06 | 102.81 | 110.90 |
| 26 | A | 883 | G | C5-N7-C8 | -5.05 | 101.77 | 104.30 |
| 26 | A | 2119 | A | C5-C6-N6 | -5.05 | 119.66 | 123.70 |
| 1 | a | 1455 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 26 | A | 1437 | C | C5-C6-N1 | 5.05 | 123.53 | 121.00 |
| 26 | A | 1646 | C | OP1-P-O3' | 5.05 | 116.31 | 105.20 |
| 1 | a | 1226 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 26 | A | 358 | U | N3-C2-O2 | -5.05 | 118.67 | 122.20 |
| 1 | a | 1448 | C | C5-C6-N1 | 5.05 | 123.52 | 121.00 |
| 26 | A | 2636 | C | N3-C2-O2 | -5.05 | 118.37 | 121.90 |
| 23 | x | 101 | A | C6-N1-C2 | 5.04 | 121.63 | 118.60 |
| 1 | a | 80 | A | N3-C4-C5 | 5.04 | 130.33 | 126.80 |
| 1 | a | 623 | C | C6-N1-C2 | -5.04 | 118.28 | 120.30 |
| 1 | a | 979 | C | N3-C2-O2 | -5.04 | 118.37 | 121.90 |
| 23 | x | 114 | C | O5'-P-OP2 | -5.04 | 101.16 | 105.70 |
| 26 | A | 2895 | G | N9-C4-C5 | -5.04 | 103.38 | 105.40 |
| 1 | a | 1379 | G | N3-C2-N2 | -5.04 | 116.37 | 119.90 |
| 22 | v | 25 | C | C6-N1-C2 | -5.04 | 118.28 | 120.30 |
| 26 | A | 2405 | G | OP2-P-O3' | 5.04 | 116.29 | 105.20 |
| 26 | A | 832 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 26 | A | 1716 | U | C6-N1-C2 | -5.04 | 117.98 | 121.00 |
| 26 | A | 2782 | G | N3-C4-N9 | 5.04 | 129.02 | 126.00 |
| 26 | A | 2880 | C | C6-N1-C2 | -5.04 | 118.28 | 120.30 |
| 1 | a | 550 | G | N3-C4-C5 | -5.03 | 126.08 | 128.60 |
| 26 | A | 852 | U | C5-C6-N1 | 5.03 | 125.22 | 122.70 |
| 26 | A | 1956 | U | N1-C2-O2 | 5.03 | 126.32 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1 | a | 88 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 1 | a | 817 | C | C2-N1-C1' | 5.03 | 124.33 | 118.80 |
| 26 | A | 141 | G | N3-C4-C5 | -5.03 | 126.09 | 128.60 |
| 26 | A | 1539 | U | C2-N1-C1' | 5.03 | 123.73 | 117.70 |
| 26 | A | 2065 | C | N3-C2-O2 | -5.03 | 118.38 | 121.90 |
| 19 | s | 4 | LEU | CA-CB-CG | 5.02 | 126.86 | 115.30 |
| 26 | A | 193 | U | N3-C2-O2 | -5.02 | 118.68 | 122.20 |
| 26 | A | 915 | C | C2-N1-C1' | 5.02 | 124.33 | 118.80 |
| 1 | a | 71 | A | OP1-P-OP2 | -5.02 | 112.07 | 119.60 |
| 26 | A | 1774 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 26 | A | 1279 | G | N1-C6-O6 | 5.02 | 122.91 | 119.90 |
| 26 | A | 595 | C | C5-C6-N1 | 5.02 | 123.51 | 121.00 |
| 24 | y | 72 | C | C5-C6-N1 | 5.02 | 123.51 | 121.00 |
| 1 | a | 218 | U | C5-C6-N1 | 5.02 | 125.21 | 122.70 |
| 26 | A | 49 | A | O4'-C1'-N9 | -5.02 | 104.19 | 108.20 |
| 26 | A | 2752 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 1 | a | 905 | U | C6-N1-C2 | -5.01 | 117.99 | 121.00 |
| 26 | A | 2305 | U | C2-N3-C4 | -5.01 | 123.99 | 127.00 |
| 26 | A | 2656 | U | N3-C2-O2 | -5.01 | 118.69 | 122.20 |
| 1 | a | 674 | G | N7-C8-N9 | 5.01 | 115.61 | 113.10 |
| 1 | a | 346 | G | C5-C6-N1 | 5.01 | 114.00 | 111.50 |
| 24 | y | 47(B) | G | C6-C5-N7 | -5.01 | 127.39 | 130.40 |
| 26 | A | 2238 | G | N3-C4-N9 | 5.01 | 129.00 | 126.00 |
| 1 | a | 1348 | U | N1-C2-O2 | 5.01 | 126.31 | 122.80 |
| 1 | a | 94 | G | C5-C6-O6 | -5.01 | 125.60 | 128.60 |
| 22 | v | 17 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 26 | A | 2556 | C | N1-C2-O2 | 5.01 | 121.90 | 118.90 |
| 24 | y | 67(A) | U | C5-C6-N1 | 5.00 | 125.20 | 122.70 |
| 1 | a | 689 | C | C2-N1-C1' | 5.00 | 124.30 | 118.80 |
| 26 | A | 2110 | G | N3-C4-C5 | 5.00 | 131.10 | 128.60 |
| 26 | A | 2279 | G | N9-C4-C5 | -5.00 | 103.40 | 105.40 |
| 1 | a | 136 | C | C5-C6-N1 | 5.00 | 123.50 | 121.00 |
| 1 | a | 656 | G | N1-C2-N3 | 5.00 | 126.90 | 123.90 |
| 26 | A | 919 | U | N1-C2-O2 | 5.00 | 126.30 | 122.80 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|---------|
| 1 | a | 527 | G7M | C4',C3' |
| 26 | A | 2069 | G7M | C4',C3' |

All (28) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 55 | 3 | 30 | HIS | Peptide |
| 28 | C | 120 | ASP | Peptide |
| 34 | H | 2 | GLN | Peptide |
| 34 | H | 8 | LYS | Mainchain,Peptide |
| 33 | I | 23 | VAL | Peptide |
| 33 | I | 63 | ASP | Peptide |
| 36 | K | 34 | GLY | Peptide |
| 38 | M | 57 | VAL | Mainchain |
| 44 | S | 63 | GLY | Peptide |
| 46 | U | 5 | ARG | Peptide |
| 46 | U | 50 | ALA | Peptide |
| 2 | b | 16 | GLY | Peptide |
| 2 | b | 17 | HIS | Mainchain |
| 5 | e | 92 | ARG | Peptide |
| 10 | j | 33 | GLY | Peptide |
| 10 | j | 56 | HIS | Peptide |
| 11 | k | 91 | GLY | Peptide |
| 12 | l | 100 | ALA | Peptide |
| 12 | l | 74 | GLN | Peptide |
| 13 | m | 3 | ILE | Peptide |
| 13 | m | 4 | ALA | Mainchain |
| 15 | o | 87 | ARG | Mainchain |
| 18 | r | 10 | CYS | Peptide |
| 18 | r | 16 | GLY | Peptide |
| 25 | z | 190 | LEU | Peptide |
| 25 | z | 300 | LEU | Peptide |
| 25 | z | 327 | SER | Mainchain |

5.2 Too-close contacts ⓘ

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 | 33029 | 0 | 16643 | 0 | 0 |
| 2 | b | 1705 | 0 | 1732 | 0 | 0 |
| 3 | c | 1625 | 0 | 1699 | 0 | 0 |
| 4 | d | 1643 | 0 | 1710 | 0 | 0 |
| 5 | e | 1157 | 0 | 1199 | 0 | 0 |
| 6 | f | 818 | 0 | 808 | 0 | 0 |
| 7 | g | 1182 | 0 | 1240 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8 | h | 979 | 0 | 1034 | 0 | 0 |
| 9 | i | 1022 | 0 | 1070 | 0 | 0 |
| 10 | j | 787 | 0 | 828 | 0 | 0 |
| 11 | k | 870 | 0 | 878 | 0 | 0 |
| 12 | l | 955 | 0 | 1019 | 0 | 0 |
| 13 | m | 884 | 0 | 944 | 0 | 0 |
| 14 | n | 794 | 0 | 836 | 0 | 0 |
| 15 | o | 714 | 0 | 737 | 0 | 0 |
| 16 | p | 649 | 0 | 666 | 0 | 0 |
| 17 | q | 649 | 0 | 691 | 0 | 0 |
| 18 | r | 505 | 0 | 502 | 0 | 0 |
| 19 | s | 638 | 0 | 665 | 0 | 0 |
| 20 | t | 665 | 0 | 714 | 0 | 0 |
| 21 | u | 496 | 0 | 486 | 0 | 0 |
| 22 | v | 1642 | 0 | 839 | 0 | 0 |
| 23 | x | 1025 | 0 | 518 | 0 | 0 |
| 24 | y | 2031 | 0 | 1039 | 0 | 0 |
| 25 | z | 4863 | 0 | 4837 | 0 | 0 |
| 26 | A | 62335 | 0 | 31375 | 421 | 0 |
| 27 | B | 2570 | 0 | 1301 | 20 | 0 |
| 28 | C | 2083 | 0 | 2157 | 30 | 0 |
| 29 | D | 1565 | 0 | 1616 | 32 | 0 |
| 30 | E | 1552 | 0 | 1619 | 16 | 0 |
| 31 | F | 1411 | 0 | 1447 | 20 | 0 |
| 32 | G | 1323 | 0 | 1374 | 29 | 0 |
| 33 | I | 1032 | 0 | 1088 | 15 | 0 |
| 34 | H | 1111 | 0 | 1148 | 13 | 0 |
| 35 | J | 1129 | 0 | 1162 | 14 | 0 |
| 36 | K | 939 | 0 | 1012 | 16 | 0 |
| 37 | L | 1045 | 0 | 1117 | 21 | 0 |
| 38 | M | 1074 | 0 | 1157 | 17 | 0 |
| 39 | N | 961 | 0 | 1000 | 14 | 0 |
| 40 | O | 892 | 0 | 923 | 14 | 0 |
| 41 | P | 917 | 0 | 965 | 13 | 0 |
| 42 | Q | 947 | 0 | 1022 | 14 | 0 |
| 43 | R | 816 | 0 | 839 | 12 | 0 |
| 44 | S | 857 | 0 | 922 | 9 | 0 |
| 45 | T | 739 | 0 | 807 | 16 | 0 |
| 46 | U | 780 | 0 | 834 | 16 | 0 |
| 47 | V | 753 | 0 | 780 | 10 | 0 |
| 48 | W | 575 | 0 | 592 | 9 | 0 |
| 49 | X | 625 | 0 | 655 | 6 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 50 | Y | 509 | 0 | 543 | 8 | 0 |
| 51 | Z | 449 | 0 | 491 | 10 | 0 |
| 52 | 0 | 444 | 0 | 461 | 6 | 0 |
| 53 | 1 | 410 | 0 | 440 | 7 | 0 |
| 54 | 2 | 377 | 0 | 418 | 4 | 0 |
| 55 | 3 | 504 | 0 | 574 | 7 | 0 |
| 56 | 4 | 302 | 0 | 340 | 6 | 0 |
| 57 | 6 | 523 | 0 | 521 | 10 | 0 |
| 58 | w | 62 | 0 | 34 | 0 | 0 |
| 59 | v | 10 | 0 | 10 | 0 | 0 |
| 60 | y | 6 | 0 | 3 | 0 | 0 |
| 61 | z | 32 | 0 | 13 | 0 | 0 |
| 62 | z | 1 | 0 | 0 | 0 | 0 |
| 63 | 4 | 1 | 0 | 0 | 0 | 0 |
| 63 | 6 | 1 | 0 | 0 | 0 | 0 |
| 64 | z | 2 | 0 | 0 | 0 | 0 |
| All | All | 152991 | 0 | 104094 | 728 | 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 6.

All (728) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 26:A:279:A:N6 | 26:A:361:G:N3 | 2.04 | 1.05 |
| 26:A:2166:U:O2 | 26:A:2170:A:N6 | 2.08 | 0.85 |
| 36:K:35:VAL:HG21 | 36:K:69:VAL:HG12 | 1.69 | 0.74 |
| 26:A:1072:C:OP1 | 26:A:1077:A:N6 | 2.23 | 0.72 |
| 26:A:410:G:N3 | 26:A:432:A:N6 | 41.67 | 0.72 |
| 47:V:32:GLY:O | 47:V:93:ARG:NH2 | 2.24 | 0.70 |
| 39:N:35:LYS:NZ | 39:N:110:MET:SD | 2.64 | 0.70 |
| 32:G:88:LEU:HG | 32:G:161:VAL:HG22 | 1.74 | 0.68 |
| 26:A:1250:G:N7 | 37:L:18:ARG:NH2 | 2.40 | 0.68 |
| 26:A:585:G:N7 | 42:Q:5:ARG:NH1 | 2.43 | 0.66 |
| 26:A:2296:U:OP2 | 40:O:9:ARG:NH2 | 2.28 | 0.66 |
| 26:A:956:G:N7 | 38:M:14:LYS:NZ | 2.43 | 0.65 |
| 26:A:1311:G:H21 | 26:A:1603:A:H62 | 1.43 | 0.65 |
| 57:6:28:VAL:HG11 | 57:6:32:LEU:HD23 | 1.79 | 0.64 |
| 43:R:48:LYS:NZ | 43:R:49:ILE:O | 2.30 | 0.64 |
| 26:A:1060:U:O2' | 35:J:58:ASN:ND2 | 81.07 | 0.64 |
| 29:D:128:ARG:NH1 | 29:D:129:THR:O | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:I:32:VAL:HG23 | 33:I:60:VAL:HG13 | 1.79 | 0.64 |
| 28:C:181:ARG:NH1 | 28:C:182:LYS:O | 2.31 | 0.64 |
| 26:A:994:C:OP1 | 42:Q:52:ARG:NH2 | 2.31 | 0.64 |
| 26:A:2848:G:O2' | 26:A:2867:G:N2 | 2.31 | 0.64 |
| 26:A:850:U:OP1 | 51:Z:18:LYS:NZ | 2.31 | 0.63 |
| 26:A:1454:C:OP1 | 39:N:63:ARG:NH2 | 2.31 | 0.63 |
| 26:A:910:A:N3 | 26:A:2264:C:O2' | 2.29 | 0.63 |
| 26:A:2743:U:OP2 | 26:A:2755:C:N4 | 2.32 | 0.63 |
| 26:A:2250:G:O2' | 26:A:2496:C:OP1 | 2.16 | 0.63 |
| 26:A:475:C:O2 | 26:A:479:A:N6 | 2.31 | 0.63 |
| 27:B:30:C:H1' | 27:B:57:A:H61 | 1.64 | 0.63 |
| 40:O:50:ALA:O | 40:O:81:ARG:NH2 | 2.32 | 0.63 |
| 26:A:764:A:N3 | 28:C:211:ARG:NH1 | 2.47 | 0.62 |
| 27:B:48:U:OP1 | 40:O:30:ARG:NH2 | 2.31 | 0.62 |
| 31:F:31:GLU:OE2 | 31:F:158:THR:OG1 | 2.18 | 0.62 |
| 31:F:101:ARG:NH1 | 57:6:9:TYR:OH | 2.33 | 0.62 |
| 26:A:516:C:OP1 | 52:0:9:ARG:NH1 | 2.33 | 0.61 |
| 29:D:37:VAL:HA | 29:D:48:ILE:HG22 | 1.83 | 0.61 |
| 26:A:24:G:N2 | 44:S:78:GLU:OE2 | 2.34 | 0.61 |
| 26:A:961:C:OP1 | 26:A:2456:C:O2' | 2.19 | 0.61 |
| 29:D:97:SER:OG | 29:D:99:GLU:OE1 | 2.18 | 0.61 |
| 26:A:2830:C:OP2 | 29:D:59:ARG:NH2 | 2.34 | 0.61 |
| 26:A:545:U:O2 | 26:A:548:G:O6 | 2.19 | 0.61 |
| 33:I:17:ALA:HB1 | 33:I:38:CYS:HA | 1.81 | 0.61 |
| 26:A:200:U:O2 | 26:A:386:G:N2 | 2.32 | 0.61 |
| 26:A:245:G:N7 | 55:3:7:ARG:NH2 | 2.48 | 0.61 |
| 35:J:105:VAL:HG12 | 35:J:109:LEU:HD23 | 1.83 | 0.61 |
| 31:F:177:ARG:O | 57:6:47:LYS:NZ | 2.33 | 0.61 |
| 43:R:69:GLY:O | 43:R:90:ARG:NE | 2.29 | 0.61 |
| 26:A:1056:G:O2' | 26:A:1103:A:N6 | 2.34 | 0.60 |
| 26:A:2334:U:O2' | 40:O:13:ARG:NH2 | 2.34 | 0.60 |
| 26:A:453:A:N3 | 26:A:457:A:O2' | 2.34 | 0.60 |
| 26:A:908:C:OP2 | 38:M:22:GLN:NE2 | 2.34 | 0.60 |
| 26:A:1737:G:N2 | 26:A:1737:G:OP2 | 2.34 | 0.60 |
| 41:P:8:GLU:HG2 | 41:P:54:LEU:HD23 | 1.84 | 0.60 |
| 26:A:750:A:OP1 | 26:A:1615:C:N4 | 2.35 | 0.60 |
| 32:G:21:GLN:NE2 | 32:G:37:ASN:O | 2.35 | 0.60 |
| 28:C:182:LYS:NZ | 28:C:264:LYS:O | 2.34 | 0.60 |
| 26:A:491:G:O6 | 44:S:49:LYS:NZ | 2.34 | 0.60 |
| 26:A:877:A:O2' | 26:A:900:A:N6 | 2.31 | 0.60 |
| 26:A:1753:G:N2 | 26:A:1756:G:OP2 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:A:1000:A:OP2 | 26:A:1154:G:N1 | 2.32 | 0.59 |
| 26:A:771:G:OP2 | 54:2:11:LYS:NZ | 2.35 | 0.59 |
| 26:A:2746:U:N3 | 26:A:2756:U:O4 | 2.34 | 0.59 |
| 26:A:959:A:N3 | 26:A:2457:PSU:O2' | 2.32 | 0.59 |
| 26:A:1528:A:OP2 | 26:A:1543:G:N2 | 2.34 | 0.59 |
| 26:A:837:C:N3 | 26:A:941:A:N6 | 2.50 | 0.59 |
| 32:G:53:PRO:HG3 | 32:G:61:TRP:CE2 | 2.37 | 0.59 |
| 57:6:14:ALA:HB3 | 57:6:22:MET:HB2 | 1.84 | 0.59 |
| 53:1:16:THR:HG21 | 53:1:41:VAL:HG11 | 1.83 | 0.59 |
| 26:A:2344:U:OP1 | 53:1:36:LYS:NZ | 2.35 | 0.59 |
| 26:A:2576:G:O2' | 26:A:2579:C:OP2 | 2.21 | 0.59 |
| 26:A:1997:C:OP2 | 29:D:128:ARG:NH1 | 2.35 | 0.59 |
| 36:K:69:VAL:O | 36:K:76:VAL:HA | 2.03 | 0.59 |
| 26:A:1084:A:H2' | 26:A:1085:A:C8 | 2.37 | 0.58 |
| 26:A:1392:A:N6 | 45:T:18:GLU:OE1 | 2.35 | 0.58 |
| 26:A:297:G:N2 | 26:A:300:A:OP2 | 12.69 | 0.58 |
| 26:A:612:G:OP2 | 26:A:614:A:N6 | 2.36 | 0.58 |
| 26:A:2394:C:OP1 | 55:3:29:ARG:NH1 | 2.36 | 0.58 |
| 35:J:118:MET:HA | 35:J:121:LYS:HZ3 | 1.67 | 0.58 |
| 26:A:807:U:O2' | 26:A:2060:A:N1 | 2.37 | 0.58 |
| 43:R:63:VAL:HG12 | 43:R:96:VAL:HG12 | 1.85 | 0.58 |
| 27:B:57:A:N3 | 31:F:26:GLN:NE2 | 2.52 | 0.58 |
| 32:G:4:ALA:HA | 32:G:68:ARG:HE | 1.67 | 0.58 |
| 26:A:1666:G:HO2' | 36:K:6:THR:HG1 | 1.52 | 0.58 |
| 26:A:684:G:O2' | 26:A:788:A:N7 | 2.35 | 0.58 |
| 28:C:83:ASP:OD2 | 28:C:86:ARG:NH1 | 2.36 | 0.58 |
| 28:C:61:TYR:HA | 28:C:85:ASN:HD21 | 1.67 | 0.58 |
| 26:A:2742:G:OP1 | 56:4:36:ARG:NH1 | 2.37 | 0.57 |
| 26:A:1127:A:N7 | 26:A:2488:G:O2' | 2.35 | 0.57 |
| 26:A:2520:C:O2' | 26:A:2565:A:O2' | 2.21 | 0.57 |
| 26:A:956:G:N2 | 26:A:960:A:OP2 | 2.35 | 0.57 |
| 26:A:1288:G:OP2 | 26:A:1288:G:N2 | 2.32 | 0.57 |
| 51:Z:8:GLN:NE2 | 51:Z:10:ARG:O | 2.36 | 0.57 |
| 26:A:63:A:O2' | 45:T:77:ARG:NE | 2.36 | 0.57 |
| 40:O:14:ALA:HA | 40:O:17:LYS:HE3 | 1.87 | 0.57 |
| 26:A:1992:G:O2' | 26:A:1997:C:N4 | 2.37 | 0.57 |
| 28:C:78:GLU:OE2 | 28:C:100:ARG:NH1 | 2.38 | 0.57 |
| 43:R:58:VAL:H | 43:R:102:SER:HB2 | 1.70 | 0.57 |
| 26:A:1068:G:N3 | 26:A:1095:A:O2' | 2.37 | 0.57 |
| 26:A:660:C:O2' | 37:L:13:LYS:NZ | 2.38 | 0.57 |
| 26:A:2406:A:OP2 | 26:A:2411:A:N6 | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 32:G:38:ASP:O | 32:G:54:ARG:NH1 | 2.36 | 0.57 |
| 35:J:49:ASP:OD1 | 35:J:121:LYS:NZ | 2.38 | 0.57 |
| 26:A:1365:A:O2' | 49:X:10:ARG:NH2 | 2.37 | 0.57 |
| 26:A:2051:A:N6 | 26:A:2614:A:O2' | 2.38 | 0.57 |
| 26:A:1156:A:OP1 | 42:Q:54:ARG:NH1 | 2.38 | 0.56 |
| 26:A:2835:A:N6 | 26:A:2879:A:O4' | 2.38 | 0.56 |
| 26:A:563:A:N6 | 26:A:884:U:O2 | 105.61 | 0.56 |
| 28:C:243:PRO:O | 28:C:250:GLN:NE2 | 2.38 | 0.56 |
| 34:H:2:GLN:NE2 | 34:H:18:GLN:OE1 | 2.38 | 0.56 |
| 26:A:2788:C:O2' | 26:A:2809:A:N3 | 2.32 | 0.56 |
| 41:P:47:ILE:HA | 41:P:96:LEU:HD12 | 1.87 | 0.56 |
| 26:A:536:G:H4' | 42:Q:56:PHE:HZ | 1.70 | 0.56 |
| 26:A:279:A:H61 | 26:A:361:G:H1' | 1.69 | 0.56 |
| 45:T:80:TRP:HZ3 | 45:T:82:LYS:HB3 | 1.70 | 0.56 |
| 26:A:545:U:O2 | 26:A:548:G:C6 | 2.59 | 0.56 |
| 26:A:301:G:OP2 | 46:U:81:ARG:NH1 | 2.38 | 0.56 |
| 26:A:196:A:OP2 | 37:L:47:ARG:NH1 | 2.39 | 0.56 |
| 46:U:49:PRO:O | 46:U:53:GLN:NE2 | 2.38 | 0.56 |
| 26:A:2320:U:O2' | 26:A:2333:A:N6 | 2.39 | 0.56 |
| 36:K:76:VAL:H | 41:P:72:VAL:HG22 | 1.70 | 0.56 |
| 26:A:1315:C:O2' | 26:A:1392:A:N3 | 2.36 | 0.56 |
| 26:A:2522:U:O2' | 26:A:2647:U:OP1 | 2.23 | 0.56 |
| 53:1:36:LYS:HB3 | 53:1:47:ILE:HD13 | 1.88 | 0.56 |
| 26:A:859:G:OP2 | 26:A:869:G:N1 | 23.51 | 0.56 |
| 29:D:8:LYS:NZ | 29:D:195:GLY:O | 2.35 | 0.56 |
| 29:D:32:ASN:OD1 | 29:D:52:THR:OG1 | 2.21 | 0.56 |
| 38:M:17:ASN:O | 38:M:38:ARG:NH1 | 2.38 | 0.56 |
| 26:A:221:A:N1 | 26:A:265:A:O2' | 2.35 | 0.56 |
| 35:J:73:VAL:HG12 | 35:J:88:THR:HG22 | 1.88 | 0.56 |
| 36:K:21:CYS:HA | 36:K:41:ILE:HG22 | 1.88 | 0.56 |
| 26:A:1088:A:N6 | 33:I:134:SER:OG | 2.39 | 0.55 |
| 26:A:1378:A:O2' | 26:A:1380:G:OP2 | 2.23 | 0.55 |
| 43:R:6:GLN:HE22 | 43:R:39:LEU:HD11 | 1.70 | 0.55 |
| 26:A:1807:G:N2 | 26:A:1810:A:OP2 | 2.38 | 0.55 |
| 51:Z:40:THR:HG22 | 51:Z:42:ALA:H | 1.71 | 0.55 |
| 28:C:132:ARG:NH1 | 28:C:186:ASP:OD1 | 2.35 | 0.55 |
| 32:G:88:LEU:N | 32:G:128:THR:O | 2.33 | 0.55 |
| 40:O:53:THR:HG21 | 40:O:70:ALA:HB1 | 1.87 | 0.55 |
| 26:A:1071:G:H1' | 26:A:1089:A:H2' | 1.88 | 0.55 |
| 31:F:56:LEU:HD22 | 31:F:64:PRO:HG3 | 1.88 | 0.55 |
| 26:A:1437:C:HO2' | 26:A:1516:G:HO2' | 1.54 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:A:2419:U:OP1 | 55:3:40:LYS:NZ | 2.40 | 0.55 |
| 28:C:32:LEU:HD13 | 28:C:63:ILE:HB | 1.89 | 0.55 |
| 39:N:58:ASP:OD1 | 39:N:63:ARG:NE | 2.38 | 0.55 |
| 49:X:6:VAL:HG21 | 49:X:58:ILE:HD11 | 1.89 | 0.55 |
| 26:A:298:G:N1 | 26:A:339:U:OP2 | 2.39 | 0.55 |
| 36:K:25:LEU:O | 36:K:30:ARG:NH1 | 2.39 | 0.55 |
| 26:A:1153:C:OP1 | 42:Q:91:ARG:NH2 | 2.39 | 0.55 |
| 30:E:117:ARG:NH2 | 30:E:183:PHE:O | 2.40 | 0.54 |
| 32:G:1:SER:OG | 32:G:2:ARG:N | 2.40 | 0.54 |
| 26:A:1869:G:N2 | 26:A:1872:A:OP2 | 2.40 | 0.54 |
| 26:A:1889:A:N3 | 26:A:2086:U:O2' | 2.37 | 0.54 |
| 26:A:743:A:O2' | 26:A:1659:G:OP1 | 2.24 | 0.54 |
| 26:A:2172:U:OP1 | 26:A:2174:C:N4 | 2.39 | 0.54 |
| 32:G:26:LYS:NZ | 32:G:27:GLY:O | 2.38 | 0.54 |
| 33:I:64:ARG:NH1 | 33:I:65:SER:OG | 2.40 | 0.54 |
| 45:T:40:LYS:HA | 45:T:43:ILE:HG12 | 1.88 | 0.54 |
| 26:A:197:A:N6 | 26:A:2430:A:O2' | 2.41 | 0.54 |
| 26:A:2469:A:O4' | 38:M:55:ARG:NH1 | 2.40 | 0.54 |
| 28:C:16:VAL:HG12 | 28:C:203:VAL:HG22 | 1.90 | 0.54 |
| 26:A:270:A:N1 | 26:A:369:U:O2' | 2.40 | 0.54 |
| 26:A:635:C:O2' | 26:A:639:U:OP1 | 2.26 | 0.54 |
| 26:A:1798:U:OP2 | 28:C:270:ARG:NH2 | 2.41 | 0.54 |
| 26:A:27:G:O2' | 26:A:512:G:N2 | 2.41 | 0.54 |
| 26:A:2636:C:O2' | 29:D:45:TYR:OH | 2.25 | 0.54 |
| 35:J:36:LEU:HD11 | 35:J:54:ILE:HG12 | 1.88 | 0.54 |
| 40:O:66:GLY:O | 40:O:102:ARG:NH2 | 2.41 | 0.54 |
| 29:D:131:ASP:O | 29:D:136:ASN:ND2 | 2.41 | 0.54 |
| 26:A:2532:G:O2' | 26:A:2657:A:N1 | 2.41 | 0.53 |
| 32:G:82:PHE:O | 32:G:133:LYS:HA | 2.08 | 0.53 |
| 26:A:111:A:O2' | 50:Y:58:ASN:ND2 | 2.35 | 0.53 |
| 35:J:16:TYR:HB2 | 35:J:54:ILE:HG22 | 1.89 | 0.53 |
| 26:A:2336:A:H61 | 48:W:39:THR:HG21 | 1.74 | 0.53 |
| 26:A:2136:G:N2 | 26:A:2156:G:O2' | 2.42 | 0.53 |
| 30:E:105:LEU:HD11 | 30:E:200:LEU:HD21 | 1.90 | 0.53 |
| 26:A:910:A:H62 | 38:M:12:MET:HA | 1.72 | 0.53 |
| 26:A:792:A:O2' | 26:A:794:A:N7 | 15.01 | 0.53 |
| 27:B:27:C:OP1 | 40:O:34:HIS:NE2 | 2.41 | 0.53 |
| 40:O:92:PHE:HB2 | 40:O:117:PHE:HD2 | 1.72 | 0.53 |
| 26:A:2107:G:N2 | 26:A:2182:U:O2' | 2.41 | 0.53 |
| 26:A:2773:C:OP1 | 29:D:169:ARG:NH2 | 2.41 | 0.53 |
| 30:E:120:VAL:HG12 | 30:E:188:MET:HB2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:J:80:HIS:O | 35:J:82:GLY:N | 2.41 | 0.53 |
| 26:A:415:A:O2' | 26:A:1866:A:OP1 | 2.25 | 0.53 |
| 26:A:1682:G:OP2 | 26:A:1699:G:N2 | 2.42 | 0.53 |
| 26:A:1796:U:H2' | 26:A:1797:G:H8 | 1.72 | 0.53 |
| 26:A:304:U:H3 | 26:A:313:G:H1 | 1.54 | 0.53 |
| 26:A:1223:G:N2 | 26:A:1226:A:OP2 | 2.33 | 0.53 |
| 26:A:1942:C:OP2 | 26:A:1943:U:O2' | 2.26 | 0.53 |
| 26:A:2481:G:HO2' | 26:A:2482:A:H8 | 1.55 | 0.53 |
| 26:A:571:U:O2' | 26:A:573:U:OP2 | 2.27 | 0.53 |
| 34:H:27:ARG:NH2 | 49:X:59:ASP:OD2 | 2.42 | 0.53 |
| 26:A:1802:A:H2' | 26:A:1803:A:C8 | 2.44 | 0.52 |
| 26:A:1138:G:O2' | 35:J:104:ALA:O | 2.28 | 0.52 |
| 32:G:29:ASN:OD1 | 32:G:30:GLY:N | 2.40 | 0.52 |
| 26:A:1065:U:O2 | 26:A:1066:U:O2' | 2.22 | 0.52 |
| 26:A:2144:G:O2' | 26:A:2147:A:N6 | 2.42 | 0.52 |
| 31:F:37:MET:HG3 | 31:F:56:LEU:HD12 | 1.91 | 0.52 |
| 26:A:2140:G:N2 | 26:A:2152:G:N7 | 2.58 | 0.52 |
| 29:D:109:VAL:HG12 | 29:D:203:VAL:HG12 | 1.90 | 0.52 |
| 26:A:2353:G:O2' | 48:W:29:ALA:O | 2.20 | 0.52 |
| 26:A:489:G:N2 | 26:A:1321:A:OP1 | 2.42 | 0.52 |
| 26:A:349:U:H2' | 26:A:350:G:H8 | 1.75 | 0.52 |
| 30:E:159:LEU:HA | 30:E:162:ARG:HE | 1.74 | 0.52 |
| 26:A:1614:A:N6 | 44:S:88:ARG:H | 2.08 | 0.52 |
| 26:A:1998:A:OP2 | 29:D:141:ARG:NH1 | 2.40 | 0.52 |
| 26:A:2755:C:OP1 | 56:4:19:ARG:NH2 | 2.42 | 0.52 |
| 27:B:31:C:O2' | 27:B:53:A:N1 | 2.36 | 0.52 |
| 51:Z:16:LEU:HD12 | 51:Z:17:PRO:HD2 | 1.91 | 0.52 |
| 26:A:253:C:OP2 | 55:3:4:LYS:NZ | 2.36 | 0.52 |
| 27:B:95:U:OP2 | 47:V:19:ARG:NH2 | 2.43 | 0.52 |
| 32:G:87:GLN:HA | 32:G:129:GLU:HA | 1.90 | 0.52 |
| 26:A:1437:C:O2' | 26:A:1516:G:O2' | 2.25 | 0.52 |
| 31:F:46:LYS:HB2 | 31:F:47:LYS:HD2 | 1.91 | 0.52 |
| 38:M:47:GLU:OE1 | 38:M:51:ARG:NH1 | 2.43 | 0.52 |
| 44:S:25:ARG:NH2 | 44:S:74:ILE:O | 2.41 | 0.52 |
| 26:A:1601:G:OP1 | 45:T:64:LYS:NZ | 2.43 | 0.52 |
| 38:M:40:ARG:HG2 | 38:M:95:LEU:HA | 1.91 | 0.52 |
| 26:A:1496:A:N3 | 26:A:1577:C:O2' | 2.39 | 0.52 |
| 29:D:148:GLN:HB2 | 29:D:152:PRO:HG2 | 1.92 | 0.52 |
| 44:S:3:THR:HG21 | 44:S:58:ALA:HB2 | 1.90 | 0.51 |
| 48:W:66:GLU:HB3 | 48:W:68:LYS:HG2 | 1.91 | 0.51 |
| 26:A:1063:G:O6 | 26:A:1076:C:O2' | 2.20 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:A:566:U:H5'' | 37:L:29:LYS:HE3 | 1.92 | 0.51 |
| 26:A:187:G:N2 | 26:A:190:A:OP2 | 11.77 | 0.51 |
| 26:A:2817:U:OP1 | 39:N:42:LYS:NZ | 2.39 | 0.51 |
| 28:C:153:LEU:HD23 | 28:C:175:LEU:HD21 | 1.92 | 0.51 |
| 28:C:128:THR:HA | 28:C:189:ALA:O | 2.11 | 0.51 |
| 26:A:1071:G:N3 | 26:A:1089:A:O2' | 2.36 | 0.51 |
| 46:U:8:ASP:H | 46:U:24:VAL:HG22 | 1.74 | 0.51 |
| 48:W:16:ARG:O | 48:W:35:ARG:NH1 | 2.44 | 0.51 |
| 26:A:2202:U:O2' | 26:A:2204:G:OP1 | 2.24 | 0.51 |
| 26:A:77:G:OP1 | 50:Y:52:ARG:NH2 | 2.41 | 0.51 |
| 26:A:1019:U:OP1 | 26:A:1035:U:O2' | 2.21 | 0.51 |
| 45:T:19:LYS:NZ | 45:T:84:TYR:OH | 2.40 | 0.51 |
| 26:A:2233:U:H2' | 26:A:2234:G:C8 | 2.46 | 0.51 |
| 26:A:2857:G:N2 | 26:A:2860:A:OP2 | 2.36 | 0.51 |
| 33:I:74:PRO:HG2 | 33:I:77:VAL:HG22 | 1.93 | 0.51 |
| 44:S:30:SER:OG | 44:S:31:GLN:OE1 | 2.29 | 0.51 |
| 37:L:77:ILE:HD13 | 37:L:101:ILE:HD11 | 1.93 | 0.51 |
| 46:U:13:LEU:N | 46:U:68:ASN:O | 2.32 | 0.51 |
| 56:4:11:CYS:SG | 56:4:14:CYS:N | 2.85 | 0.50 |
| 26:A:28:A:O2' | 42:Q:10:ARG:NH2 | 2.44 | 0.50 |
| 38:M:71:LYS:HB3 | 38:M:93:VAL:O | 2.11 | 0.50 |
| 26:A:77:G:H5'' | 50:Y:2:LYS:HE2 | 1.94 | 0.50 |
| 53:1:41:VAL:HG13 | 53:1:42:VAL:HG23 | 1.93 | 0.50 |
| 26:A:2258:C:O2' | 26:A:2427:C:OP2 | 2.22 | 0.50 |
| 26:A:2645:G:N2 | 26:A:2645:G:OP2 | 2.43 | 0.50 |
| 31:F:72:SER:OG | 31:F:80:GLN:N | 2.44 | 0.50 |
| 34:H:3:VAL:HA | 34:H:38:PRO:HA | 1.93 | 0.50 |
| 37:L:74:THR:HG22 | 37:L:107:PHE:HB2 | 1.93 | 0.50 |
| 45:T:65:GLY:O | 45:T:76:ARG:NH1 | 2.43 | 0.50 |
| 53:1:24:LYS:NZ | 53:1:50:GLU:OE1 | 2.42 | 0.50 |
| 26:A:1961:C:H2' | 26:A:1962:5MC:C2 | 2.46 | 0.50 |
| 26:A:200:U:OP1 | 49:X:22:ASN:ND2 | 2.44 | 0.50 |
| 26:A:2024:G:O3' | 29:D:154:LYS:NZ | 2.40 | 0.50 |
| 26:A:2282:G:N2 | 26:A:2390:U:O2 | 2.43 | 0.50 |
| 31:F:43:ILE:HG12 | 31:F:78:ILE:HG22 | 1.93 | 0.50 |
| 26:A:329:G:H1 | 46:U:16:LYS:HZ3 | 1.59 | 0.50 |
| 26:A:564:C:O4' | 42:Q:36:GLN:NE2 | 2.44 | 0.50 |
| 26:A:2045:C:O2 | 52:0:18:HIS:NE2 | 2.45 | 0.50 |
| 26:A:1183:U:O3' | 51:Z:29:ARG:NH2 | 2.44 | 0.50 |
| 56:4:9:LYS:HG3 | 56:4:14:CYS:HB2 | 1.94 | 0.50 |
| 26:A:2199:A:O4' | 34:H:28:ASN:ND2 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:D:124:ARG:NH2 | 29:D:161:MET:O | 2.41 | 0.50 |
| 29:D:10:GLY:H | 29:D:197:THR:HG23 | 1.76 | 0.50 |
| 26:A:1011:G:OP1 | 42:Q:74:SER:OG | 2.29 | 0.50 |
| 46:U:15:GLY:O | 46:U:18:LYS:NZ | 2.39 | 0.50 |
| 26:A:1664:A:H61 | 26:A:1996:C:H42 | 1.58 | 0.50 |
| 26:A:411:G:OP2 | 26:A:2406:A:O2' | 2.26 | 0.50 |
| 36:K:7:MET:HA | 36:K:19:VAL:O | 2.12 | 0.50 |
| 41:P:24:THR:HG22 | 41:P:87:ARG:HB3 | 1.94 | 0.50 |
| 26:A:1478:G:H1 | 26:A:1513:U:H3 | 1.59 | 0.50 |
| 26:A:2108:A:H2' | 26:A:2109:U:C6 | 2.46 | 0.50 |
| 29:D:4:LEU:HB2 | 29:D:32:ASN:HD22 | 1.76 | 0.50 |
| 39:N:56:LYS:NZ | 39:N:87:PHE:O | 2.44 | 0.50 |
| 40:O:35:ILE:HG22 | 40:O:66:GLY:HA2 | 1.93 | 0.50 |
| 55:3:31:ILE:O | 55:3:35:LYS:NZ | 2.34 | 0.49 |
| 26:A:581:C:H2' | 26:A:582:A:H8 | 1.77 | 0.49 |
| 38:M:69:PRO:HA | 38:M:94:ALA:HB2 | 1.94 | 0.49 |
| 50:Y:24:GLU:HB3 | 50:Y:46:VAL:HG21 | 1.94 | 0.49 |
| 26:A:1128:G:N3 | 26:A:2516:A:O2' | 2.37 | 0.49 |
| 26:A:882:G:N3 | 26:A:896:A:N6 | 2.59 | 0.49 |
| 54:2:34:ARG:NE | 54:2:42:LEU:O | 2.45 | 0.49 |
| 37:L:128:THR:HG23 | 37:L:131:ALA:H | 1.75 | 0.49 |
| 26:A:1493:C:OP1 | 26:A:1495:A:N6 | 2.45 | 0.49 |
| 26:A:578:G:OP1 | 26:A:1255:U:O2' | 2.30 | 0.49 |
| 26:A:2600:A:H62 | 28:C:235:GLU:HG3 | 1.77 | 0.49 |
| 43:R:68:ARG:NH1 | 43:R:90:ARG:O | 2.45 | 0.49 |
| 26:A:2178:C:O2' | 26:A:2180:U:OP2 | 2.29 | 0.49 |
| 28:C:141:HIS:ND1 | 28:C:192:GLY:O | 2.40 | 0.49 |
| 29:D:5:VAL:HG22 | 29:D:202:ILE:HG22 | 1.94 | 0.49 |
| 47:V:30:ILE:HG12 | 47:V:91:PHE:HB2 | 1.95 | 0.49 |
| 26:A:1021:A:O2' | 26:A:1123:C:OP1 | 2.28 | 0.49 |
| 26:A:2119:A:H61 | 26:A:2169:A:N6 | 2.10 | 0.49 |
| 53:1:7:LYS:HA | 53:1:23:THR:HA | 1.94 | 0.49 |
| 31:F:25:MET:HG3 | 31:F:26:GLN:HE21 | 1.78 | 0.49 |
| 32:G:18:ILE:HD11 | 32:G:42:VAL:HG13 | 1.95 | 0.49 |
| 26:A:2031:A:N3 | 26:A:2455:G:O2' | 2.41 | 0.49 |
| 26:A:1636:U:H2' | 26:A:1637:A:C8 | 2.48 | 0.49 |
| 26:A:249:C:OP2 | 26:A:2394:C:O2' | 2.27 | 0.49 |
| 26:A:355:U:H2' | 26:A:356:G:H8 | 1.78 | 0.49 |
| 26:A:478:A:N6 | 26:A:500:G:O2' | 2.46 | 0.49 |
| 29:D:101:PHE:HB2 | 29:D:180:VAL:HG23 | 1.94 | 0.49 |
| 26:A:688:U:H2' | 26:A:689:A:H8 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:E:148:ILE:HB | 30:E:169:VAL:HG22 | 1.95 | 0.49 |
| 30:E:95:LYS:NZ | 30:E:97:ASN:OD1 | 2.46 | 0.49 |
| 32:G:132:LEU:HD13 | 32:G:143:VAL:HG23 | 1.94 | 0.49 |
| 26:A:1527:G:N1 | 26:A:1544:A:OP2 | 2.38 | 0.48 |
| 26:A:2482:A:H61 | 38:M:55:ARG:HH12 | 1.59 | 0.48 |
| 26:A:1085:A:H2' | 26:A:1086:A:O4' | 2.13 | 0.48 |
| 45:T:12:ARG:HA | 50:Y:29:ARG:HH22 | 1.78 | 0.48 |
| 26:A:1011:G:OP2 | 42:Q:65:ASN:ND2 | 2.47 | 0.48 |
| 34:H:100:ALA:HB2 | 34:H:112:LYS:HD3 | 1.95 | 0.48 |
| 37:L:95:LEU:HD22 | 37:L:100:ILE:HD11 | 1.95 | 0.48 |
| 38:M:17:ASN:OD1 | 38:M:97:GLN:NE2 | 2.46 | 0.48 |
| 26:A:1681:G:H21 | 26:A:1762:A:H3' | 1.78 | 0.48 |
| 26:A:195:A:H2' | 26:A:196:A:C4 | 9.89 | 0.48 |
| 28:C:132:ARG:O | 28:C:166:ARG:NH1 | 2.41 | 0.48 |
| 26:A:1244:A:HO2' | 30:E:29:HIS:HE2 | 1.58 | 0.48 |
| 31:F:28:PRO:HB2 | 31:F:168:LEU:HD22 | 1.96 | 0.48 |
| 32:G:86:LEU:HD22 | 32:G:130:ILE:HD11 | 1.95 | 0.48 |
| 38:M:30:SER:N | 38:M:106:ASP:OD1 | 2.45 | 0.48 |
| 26:A:2579:C:O3' | 29:D:137:SER:OG | 2.30 | 0.48 |
| 34:H:30:LEU:HD23 | 34:H:36:ALA:HB3 | 1.96 | 0.48 |
| 37:L:75:ALA:O | 37:L:108:ALA:HA | 2.14 | 0.48 |
| 26:A:1386:C:H2' | 26:A:1387:A:H8 | 1.79 | 0.48 |
| 26:A:488:G:O2' | 26:A:491:G:O6 | 2.32 | 0.48 |
| 30:E:112:LEU:HB3 | 30:E:118:LEU:HB2 | 1.96 | 0.48 |
| 26:A:2199:A:OP1 | 49:X:36:ARG:NH2 | 2.47 | 0.48 |
| 26:A:1673:G:N2 | 26:A:1675:C:O4' | 2.47 | 0.48 |
| 26:A:1259:G:H2' | 26:A:1260:A:H8 | 1.79 | 0.47 |
| 26:A:2759:G:H1' | 32:G:34:ARG:HH22 | 1.79 | 0.47 |
| 26:A:2849:U:OP1 | 41:P:92:ARG:NH2 | 2.47 | 0.47 |
| 26:A:1070:A:OP2 | 26:A:1077:A:N6 | 2.40 | 0.47 |
| 26:A:1079:C:N3 | 33:I:131:THR:OG1 | 2.48 | 0.47 |
| 26:A:196:A:H61 | 26:A:831:G:H21 | 1.62 | 0.47 |
| 46:U:46:LYS:HD2 | 46:U:47:PRO:HD2 | 1.96 | 0.47 |
| 26:A:1323:C:N4 | 26:A:1324:G:O6 | 2.48 | 0.47 |
| 45:T:51:PHE:O | 45:T:92:ASN:ND2 | 2.47 | 0.47 |
| 26:A:1312:U:O2' | 26:A:1314:C:N4 | 2.46 | 0.47 |
| 26:A:1818:U:O2' | 28:C:152:GLN:O | 2.28 | 0.47 |
| 45:T:54:GLU:HG3 | 45:T:88:LYS:HE2 | 1.96 | 0.47 |
| 26:A:1915:3TD:H3' | 26:A:1916:A:H8 | 1.80 | 0.47 |
| 26:A:32:C:N4 | 26:A:447:A:OP2 | 2.47 | 0.47 |
| 41:P:1:SER:OG | 41:P:2:ASN:N | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:W:33:ILE:HG22 | 48:W:34:VAL:HG23 | 1.96 | 0.47 |
| 26:A:1796:U:H2' | 26:A:1797:G:C8 | 2.50 | 0.47 |
| 26:A:1799:G:OP2 | 26:A:1819:A:N6 | 2.44 | 0.47 |
| 26:A:2052:A:O2' | 29:D:149:ASN:O | 2.31 | 0.47 |
| 26:A:2796:U:O2' | 26:A:2798:U:OP2 | 2.33 | 0.47 |
| 26:A:577:G:H2' | 26:A:578:G:C8 | 2.50 | 0.47 |
| 26:A:1715:G:O2' | 26:A:1743:G:O6 | 2.28 | 0.47 |
| 26:A:1995:U:O2 | 36:K:32:TYR:OH | 2.31 | 0.47 |
| 26:A:1057:A:H2 | 33:I:117:THR:HG21 | 1.79 | 0.47 |
| 35:J:8:PRO:HG3 | 35:J:48:VAL:HG23 | 1.96 | 0.47 |
| 26:A:1853:A:N3 | 26:A:2233:U:O2' | 2.40 | 0.47 |
| 26:A:2032:G:O2' | 29:D:150:GLN:NE2 | 2.48 | 0.47 |
| 28:C:184:GLU:HG3 | 28:C:186:ASP:H | 1.80 | 0.47 |
| 29:D:4:LEU:HB2 | 29:D:32:ASN:ND2 | 2.30 | 0.47 |
| 30:E:112:LEU:O | 30:E:118:LEU:N | 2.44 | 0.47 |
| 45:T:11:LEU:O | 50:Y:29:ARG:NH1 | 2.38 | 0.47 |
| 46:U:35:VAL:HB | 46:U:38:ILE:HG13 | 1.97 | 0.47 |
| 26:A:818:G:H21 | 26:A:1189:A:H62 | 1.62 | 0.47 |
| 26:A:355:U:H2' | 26:A:356:G:C8 | 2.50 | 0.47 |
| 26:A:776:G:N2 | 26:A:802:A:OP2 | 23.62 | 0.47 |
| 32:G:88:LEU:HA | 32:G:161:VAL:HA | 1.96 | 0.47 |
| 26:A:405:U:H3' | 29:D:4:LEU:HD21 | 167.58 | 0.47 |
| 26:A:927:A:H2' | 26:A:928:A:C8 | 2.49 | 0.47 |
| 28:C:179:GLU:HG3 | 28:C:269:ARG:HA | 1.97 | 0.47 |
| 53:1:10:LEU:HG | 53:1:48:TYR:HB3 | 1.97 | 0.46 |
| 26:A:2899:A:H2' | 26:A:2900:A:C8 | 2.50 | 0.46 |
| 26:A:1715:G:H1' | 26:A:1716:U:H5 | 1.81 | 0.46 |
| 26:A:1266:G:O2' | 26:A:2012:G:O6 | 2.32 | 0.46 |
| 26:A:572:A:OP2 | 43:R:80:ARG:NH1 | 2.46 | 0.46 |
| 30:E:118:LEU:HD11 | 30:E:188:MET:HG2 | 1.97 | 0.46 |
| 43:R:38:VAL:HG13 | 43:R:54:VAL:HG12 | 1.97 | 0.46 |
| 26:A:558:U:H2' | 26:A:559:G:C8 | 2.51 | 0.46 |
| 26:A:861:A:N3 | 27:B:79:G:O2' | 2.43 | 0.46 |
| 31:F:16:MET:HE2 | 31:F:27:VAL:HG13 | 1.97 | 0.46 |
| 36:K:68:GLY:HA2 | 36:K:77:ILE:O | 2.15 | 0.46 |
| 51:Z:17:PRO:HA | 51:Z:20:LYS:HG2 | 1.96 | 0.46 |
| 26:A:488:G:N1 | 26:A:491:G:OP2 | 2.48 | 0.46 |
| 26:A:570:G:O3' | 26:A:819:A:O2' | 21.16 | 0.46 |
| 26:A:2246:G:H2' | 26:A:2247:A:H8 | 1.81 | 0.46 |
| 26:A:2500:U:O2' | 26:A:2504:PSU:OP1 | 2.33 | 0.46 |
| 26:A:1227:G:OP2 | 42:Q:15:LYS:NZ | 2.43 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:A:265:A:N1 | 26:A:427:U:O2' | 2.40 | 0.46 |
| 26:A:1469:A:H2' | 26:A:1470:A:H8 | 1.80 | 0.46 |
| 26:A:629:G:N3 | 26:A:639:U:O2' | 2.47 | 0.46 |
| 26:A:6:A:H2' | 26:A:7:G:H8 | 1.81 | 0.46 |
| 28:C:169:ALA:O | 28:C:185:ALA:N | 2.46 | 0.46 |
| 34:H:99:ILE:HD11 | 34:H:144:VAL:HG21 | 1.97 | 0.46 |
| 26:A:2022:U:O2 | 26:A:2616:C:O2' | 2.33 | 0.46 |
| 26:A:881:G:N2 | 26:A:896:A:N7 | 2.64 | 0.46 |
| 26:A:1615:C:OP2 | 26:A:1617:C:N4 | 2.37 | 0.46 |
| 26:A:581:C:H2' | 26:A:582:A:C8 | 2.50 | 0.46 |
| 46:U:24:VAL:HA | 46:U:35:VAL:HG22 | 1.97 | 0.46 |
| 46:U:95:PHE:HB2 | 46:U:99:SER:HA | 1.98 | 0.46 |
| 26:A:1907:G:O6 | 26:A:1924:C:N4 | 2.49 | 0.45 |
| 36:K:1:MET:HA | 36:K:32:TYR:HB3 | 1.98 | 0.45 |
| 26:A:1469:A:H2' | 26:A:1470:A:C8 | 2.51 | 0.45 |
| 26:A:155:A:H2' | 26:A:156:A:H8 | 1.81 | 0.45 |
| 26:A:177:G:OP2 | 26:A:177:G:N2 | 2.34 | 0.45 |
| 26:A:2229:U:H2' | 26:A:2230:G:H8 | 1.81 | 0.45 |
| 26:A:2446:G:N7 | 26:A:2501:C:O2' | 2.48 | 0.45 |
| 26:A:279:A:H62 | 26:A:361:G:N2 | 2.13 | 0.45 |
| 26:A:594:U:H2' | 26:A:595:C:C6 | 2.51 | 0.45 |
| 26:A:200:U:H5' | 49:X:22:ASN:HD22 | 1.81 | 0.45 |
| 26:A:993:G:H1' | 43:R:91:GLN:HE21 | 1.81 | 0.45 |
| 29:D:49:GLN:HB3 | 29:D:81:GLU:HB3 | 1.99 | 0.45 |
| 43:R:60:LYS:HB2 | 43:R:99:THR:O | 2.16 | 0.45 |
| 26:A:850:U:H5'' | 51:Z:18:LYS:HG3 | 1.99 | 0.45 |
| 26:A:819:A:OP2 | 26:A:1187:G:N2 | 2.42 | 0.45 |
| 26:A:832:U:H2' | 26:A:833:A:C8 | 2.52 | 0.45 |
| 33:I:38:CYS:SG | 33:I:39:LYS:N | 2.89 | 0.45 |
| 38:M:17:ASN:ND2 | 38:M:96:ILE:O | 2.44 | 0.45 |
| 51:Z:39:ASP:OD2 | 51:Z:44:ARG:NH1 | 2.49 | 0.45 |
| 36:K:24:VAL:HA | 36:K:39:ILE:HG22 | 1.99 | 0.45 |
| 37:L:63:LYS:HA | 55:3:12:ARG:HG2 | 1.97 | 0.45 |
| 26:A:1068:G:HO2' | 26:A:1070:A:H62 | 1.59 | 0.45 |
| 26:A:1047:G:N2 | 26:A:1110:G:O2' | 2.48 | 0.45 |
| 26:A:1316:U:H2' | 26:A:1317:G:C8 | 2.52 | 0.45 |
| 26:A:1506:U:H2' | 26:A:1507:C:C6 | 2.52 | 0.45 |
| 26:A:1264:A:N6 | 26:A:2014:A:OP2 | 2.46 | 0.45 |
| 26:A:2519:U:O4' | 26:A:2542:A:N6 | 2.50 | 0.45 |
| 26:A:546:U:H1' | 26:A:548:G:C6 | 2.51 | 0.45 |
| 31:F:57:ALA:HB2 | 31:F:64:PRO:HD3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:A:971:G:OP1 | 26:A:989:G:N1 | 2.43 | 0.45 |
| 27:B:43:C:OP1 | 57:6:2:LYS:N | 2.44 | 0.45 |
| 36:K:64:ARG:HB2 | 36:K:83:ALA:HB3 | 1.99 | 0.45 |
| 38:M:42:THR:HA | 38:M:93:VAL:HA | 1.99 | 0.45 |
| 26:A:1769:U:H2' | 26:A:1770:G:H8 | 1.82 | 0.45 |
| 26:A:2250:G:H21 | 26:A:2497:A:P | 2.40 | 0.45 |
| 31:F:64:PRO:HA | 31:F:88:VAL:HG23 | 1.98 | 0.45 |
| 41:P:24:THR:HA | 41:P:45:VAL:HA | 1.99 | 0.45 |
| 26:A:2140:G:H2' | 26:A:2141:G:C8 | 2.52 | 0.45 |
| 26:A:2375:G:N2 | 26:A:2378:A:OP2 | 2.45 | 0.45 |
| 45:T:92:ASN:OD1 | 45:T:93:LEU:N | 2.49 | 0.45 |
| 26:A:1278:C:H2' | 26:A:1279:G:H8 | 1.82 | 0.45 |
| 26:A:13:A:O2' | 26:A:15:G:N7 | 2.46 | 0.45 |
| 26:A:1934:C:H2' | 26:A:1935:G:C8 | 2.51 | 0.45 |
| 26:A:1935:G:N2 | 26:A:1964:G:O4' | 2.49 | 0.45 |
| 39:N:49:GLU:HA | 39:N:52:ILE:HG22 | 1.98 | 0.45 |
| 46:U:11:ILE:HG22 | 46:U:21:ARG:HB3 | 1.99 | 0.45 |
| 55:3:31:ILE:HG21 | 55:3:34:LYS:HD3 | 1.99 | 0.44 |
| 32:G:153:PRO:HB2 | 32:G:168:VAL:HG11 | 1.99 | 0.44 |
| 32:G:3:VAL:HG22 | 32:G:68:ARG:HH21 | 1.81 | 0.44 |
| 33:I:102:ARG:NH2 | 33:I:141:ASP:OD1 | 2.40 | 0.44 |
| 27:B:9:G:OP2 | 40:O:15:ARG:NH2 | 2.49 | 0.44 |
| 26:A:2595:G:N2 | 26:A:2598:A:OP2 | 2.45 | 0.44 |
| 29:D:121:THR:HG21 | 29:D:143:PRO:HB3 | 1.99 | 0.44 |
| 30:E:146:VAL:HG12 | 30:E:185:LYS:HB2 | 1.99 | 0.44 |
| 45:T:6:ARG:NH2 | 45:T:37:ASP:OD2 | 2.50 | 0.44 |
| 47:V:35:GLU:HB2 | 47:V:93:ARG:NH2 | 2.32 | 0.44 |
| 26:A:2291:U:H2' | 26:A:2292:U:C6 | 2.53 | 0.44 |
| 26:A:2581:G:H22 | 26:A:2610:C:H2' | 1.82 | 0.44 |
| 26:A:281:C:H2' | 26:A:282:A:C8 | 2.53 | 0.44 |
| 26:A:833:A:H2' | 26:A:834:G:C8 | 2.53 | 0.44 |
| 46:U:82:VAL:O | 46:U:96:LYS:NZ | 2.50 | 0.44 |
| 26:A:1395:A:O2' | 26:A:1397:U:OP2 | 2.35 | 0.44 |
| 26:A:1432:G:H2' | 26:A:1433:A:C8 | 2.51 | 0.44 |
| 26:A:1704:C:H2' | 26:A:1705:A:H8 | 1.82 | 0.44 |
| 26:A:345:A:O2' | 26:A:347:A:N6 | 2.42 | 0.44 |
| 26:A:833:A:H2' | 26:A:834:G:H8 | 1.82 | 0.44 |
| 26:A:848:C:H2' | 26:A:849:A:H8 | 1.82 | 0.44 |
| 38:M:29:GLY:H | 38:M:104:GLU:HG3 | 1.82 | 0.44 |
| 26:A:1023:U:OP2 | 26:A:1025:G:O2' | 2.36 | 0.44 |
| 26:A:1167:C:H2' | 26:A:1168:G:C8 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:A:1434:A:H2' | 26:A:1435:G:C8 | 2.52 | 0.44 |
| 26:A:1563:U:H2' | 26:A:1564:C:C6 | 2.52 | 0.44 |
| 29:D:179:ARG:HB3 | 29:D:188:LEU:HB2 | 2.00 | 0.44 |
| 36:K:43:ILE:HD11 | 36:K:54:LYS:HA | 1.99 | 0.44 |
| 26:A:516:C:O2' | 26:A:1261:C:O2' | 2.31 | 0.44 |
| 26:A:2057:G:H2' | 26:A:2058:A:H8 | 1.81 | 0.44 |
| 26:A:2443:C:H2' | 26:A:2444:G:H8 | 1.83 | 0.44 |
| 26:A:834:G:O2' | 26:A:2358:A:O2' | 2.23 | 0.44 |
| 26:A:918:A:N3 | 27:B:80:U:O2' | 2.46 | 0.44 |
| 26:A:2303:G:O2' | 31:F:128:SER:OG | 2.23 | 0.44 |
| 35:J:37:ARG:HD3 | 35:J:39:LYS:HD2 | 1.98 | 0.44 |
| 50:Y:8:GLU:OE1 | 50:Y:12:GLU:HB2 | 2.18 | 0.44 |
| 28:C:268:ARG:NH2 | 28:C:271:SER:OG | 2.50 | 0.44 |
| 28:C:76:VAL:HG12 | 28:C:114:GLN:HG3 | 1.99 | 0.44 |
| 32:G:89:VAL:HG21 | 32:G:162:ARG:NH1 | 2.33 | 0.44 |
| 39:N:79:LEU:HA | 39:N:83:LEU:HB2 | 1.99 | 0.44 |
| 27:B:12:C:O2' | 48:W:70:PRO:O | 2.34 | 0.44 |
| 26:A:1571:A:H2' | 26:A:1572:A:C8 | 2.53 | 0.44 |
| 26:A:514:A:N3 | 26:A:581:C:O2' | 2.49 | 0.44 |
| 26:A:151:C:H2' | 26:A:152:A:H8 | 1.82 | 0.44 |
| 26:A:745:1MG:HM11 | 26:A:745:1MG:HN21 | 1.70 | 0.44 |
| 33:I:100:ILE:HG22 | 33:I:101:SER:H | 1.82 | 0.44 |
| 36:K:113:MET:HA | 36:K:116:ILE:HG22 | 2.00 | 0.44 |
| 54:2:25:LYS:O | 54:2:28:ARG:N | 2.50 | 0.43 |
| 26:A:1311:G:H21 | 26:A:1603:A:N6 | 2.13 | 0.43 |
| 26:A:926:G:H2' | 26:A:927:A:C8 | 2.53 | 0.43 |
| 34:H:58:LEU:HA | 34:H:61:VAL:HG22 | 1.99 | 0.43 |
| 26:A:1167:C:H2' | 26:A:1168:G:H8 | 1.83 | 0.43 |
| 26:A:1802:A:H2' | 26:A:1803:A:H8 | 1.83 | 0.43 |
| 28:C:24:HIS:CG | 28:C:79:ARG:HD2 | 2.52 | 0.43 |
| 31:F:115:GLY:HA3 | 31:F:177:ARG:HA | 2.00 | 0.43 |
| 26:A:1654:A:OP2 | 39:N:1:MET:N | 2.40 | 0.43 |
| 26:A:1667:G:O2' | 26:A:1991:U:O4 | 2.34 | 0.43 |
| 26:A:2176:A:O2' | 26:A:2177:C:O5' | 2.30 | 0.43 |
| 26:A:1638:C:O2 | 26:A:2698:U:O2' | 2.35 | 0.43 |
| 26:A:280:U:H2' | 26:A:281:C:C6 | 2.54 | 0.43 |
| 26:A:2850:A:N7 | 26:A:2868:A:O2' | 2.39 | 0.43 |
| 26:A:2885:G:N7 | 52:O:39:ARG:NH1 | 2.65 | 0.43 |
| 26:A:1013:C:H2' | 26:A:1014:A:H8 | 1.82 | 0.43 |
| 26:A:1114:C:H2' | 26:A:1115:G:C8 | 2.52 | 0.43 |
| 26:A:1229:C:H2' | 26:A:1230:A:C8 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:E:119:ILE:O | 30:E:187:VAL:HA | 2.18 | 0.43 |
| 26:A:2249:U:O2' | 26:A:2252:G:OP2 | 2.37 | 0.43 |
| 26:A:372:G:H1' | 26:A:373:U:H5 | 1.84 | 0.43 |
| 41:P:30:TRP:HE3 | 41:P:37:LYS:HG2 | 1.83 | 0.43 |
| 26:A:1538:G:H2' | 26:A:1539:U:C6 | 2.53 | 0.43 |
| 26:A:1652:A:H62 | 39:N:11:ASN:HD21 | 1.66 | 0.43 |
| 26:A:1716:U:H2' | 26:A:1717:A:H8 | 1.83 | 0.43 |
| 26:A:2485:G:OP1 | 38:M:45:GLN:NE2 | 2.51 | 0.43 |
| 26:A:476:G:O2' | 26:A:502:A:N6 | 2.38 | 0.43 |
| 27:B:80:U:H2' | 27:B:81:G:H8 | 1.83 | 0.43 |
| 35:J:64:VAL:HB | 35:J:68:LYS:HD2 | 2.00 | 0.43 |
| 42:Q:59:LEU:HD11 | 42:Q:63:ARG:HH21 | 1.84 | 0.43 |
| 56:4:14:CYS:SG | 56:4:27:CYS:HB2 | 2.59 | 0.43 |
| 26:A:1028:A:H2' | 26:A:1029:A:C8 | 2.54 | 0.43 |
| 26:A:1149:G:H2' | 26:A:1150:C:C6 | 2.54 | 0.43 |
| 26:A:149:A:N1 | 26:A:172:A:N6 | 15.47 | 0.43 |
| 26:A:2183:A:H2' | 26:A:2184:A:H8 | 1.82 | 0.43 |
| 26:A:2818:U:H2' | 26:A:2819:G:C8 | 2.54 | 0.43 |
| 26:A:721:A:H2' | 26:A:722:A:C8 | 2.54 | 0.43 |
| 26:A:1322:A:H2 | 26:A:1333:G:HO2' | 1.65 | 0.43 |
| 26:A:742:A:H2' | 26:A:743:A:C8 | 2.54 | 0.43 |
| 26:A:796:C:H2' | 26:A:797:G:H8 | 1.84 | 0.43 |
| 26:A:96:C:OP1 | 50:Y:39:GLN:NE2 | 2.52 | 0.43 |
| 29:D:109:VAL:HG22 | 29:D:175:LEU:HD21 | 2.00 | 0.43 |
| 26:A:2529:G:H4' | 32:G:174:LYS:HD3 | 2.01 | 0.43 |
| 34:H:55:GLU:HA | 34:H:58:LEU:HG | 2.00 | 0.43 |
| 37:L:70:LYS:HG3 | 37:L:73:ILE:HD11 | 2.00 | 0.43 |
| 27:B:52:A:H2' | 40:O:33:ARG:HH22 | 1.82 | 0.43 |
| 56:4:3:VAL:HG12 | 56:4:36:ARG:HD3 | 2.01 | 0.43 |
| 26:A:1103:A:OP2 | 26:A:1104:C:N4 | 2.44 | 0.43 |
| 26:A:1727:C:H2' | 26:A:1728:C:C6 | 2.54 | 0.43 |
| 26:A:2070:A:H2' | 26:A:2071:A:H8 | 1.84 | 0.43 |
| 26:A:227:A:O2' | 26:A:2407:A:O2' | 2.30 | 0.43 |
| 26:A:892:A:H2' | 26:A:893:C:H6 | 1.84 | 0.43 |
| 26:A:1081:U:H5' | 33:I:126:ARG:HE | 1.84 | 0.43 |
| 26:A:1278:C:H2' | 26:A:1279:G:C8 | 2.53 | 0.43 |
| 26:A:558:U:H2' | 26:A:559:G:H8 | 1.83 | 0.43 |
| 34:H:23:ALA:HB1 | 34:H:27:ARG:HH21 | 1.83 | 0.43 |
| 44:S:72:THR:OG1 | 44:S:73:LYS:N | 2.51 | 0.43 |
| 26:A:1934:C:H2' | 26:A:1935:G:H8 | 1.84 | 0.42 |
| 30:E:153:LEU:HD12 | 30:E:158:PHE:HE2 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:T:40:LYS:HB2 | 45:T:58:VAL:HG23 | 2.01 | 0.42 |
| 47:V:30:ILE:HG13 | 47:V:40:ILE:HG13 | 2.00 | 0.42 |
| 47:V:6:ALA:HB3 | 47:V:65:VAL:HG22 | 2.01 | 0.42 |
| 26:A:1486:U:H2' | 26:A:1487:U:C6 | 2.54 | 0.42 |
| 26:A:2246:G:H2' | 26:A:2247:A:C8 | 2.54 | 0.42 |
| 26:A:680:C:H2' | 26:A:681:G:C8 | 2.54 | 0.42 |
| 27:B:65:U:O4 | 27:B:108:A:O2' | 2.31 | 0.42 |
| 26:A:2393:U:O2' | 37:L:59:ARG:O | 2.33 | 0.42 |
| 51:Z:31:ILE:HG21 | 51:Z:31:ILE:HD13 | 1.91 | 0.42 |
| 52:O:27:LEU:HD12 | 52:O:36:LYS:HE3 | 2.01 | 0.42 |
| 26:A:1681:G:OP2 | 26:A:1757:A:N6 | 2.52 | 0.42 |
| 26:A:568:U:H1' | 26:A:2030:6MZ:H9C1 | 2.01 | 0.42 |
| 26:A:706:A:OP1 | 28:C:6:LYS:NZ | 2.52 | 0.42 |
| 41:P:88:ARG:NH1 | 41:P:114:ASN:OD1 | 2.52 | 0.42 |
| 26:A:1798:U:OP2 | 28:C:269:ARG:NH2 | 2.53 | 0.42 |
| 26:A:6:A:H2' | 26:A:7:G:C8 | 2.54 | 0.42 |
| 29:D:177:VAL:HG22 | 29:D:189:VAL:HG12 | 2.01 | 0.42 |
| 37:L:85:VAL:HG11 | 37:L:90:VAL:HG12 | 2.01 | 0.42 |
| 39:N:103:ARG:HG2 | 39:N:105:GLY:H | 1.85 | 0.42 |
| 41:P:29:VAL:HG12 | 41:P:80:VAL:HG22 | 2.00 | 0.42 |
| 26:A:1409:U:H2' | 26:A:1410:G:H8 | 1.84 | 0.42 |
| 26:A:2141:G:H2' | 26:A:2142:A:C8 | 2.55 | 0.42 |
| 28:C:146:LYS:HB3 | 28:C:149:LYS:HE2 | 2.02 | 0.42 |
| 32:G:83:THR:HA | 32:G:132:LEU:O | 2.20 | 0.42 |
| 26:A:2684:U:O2' | 36:K:78:ARG:NH2 | 2.52 | 0.42 |
| 36:K:90:ASN:OD1 | 36:K:91:SER:N | 2.50 | 0.42 |
| 41:P:47:ILE:HG22 | 41:P:99:LEU:HD21 | 2.01 | 0.42 |
| 26:A:1273:U:O2' | 26:A:1275:A:OP1 | 2.37 | 0.42 |
| 26:A:2109:U:H3 | 26:A:2180:U:H3 | 1.68 | 0.42 |
| 26:A:680:C:H2' | 26:A:681:G:H8 | 1.84 | 0.42 |
| 27:B:93:C:H2' | 27:B:94:A:H8 | 1.85 | 0.42 |
| 33:I:102:ARG:O | 33:I:106:GLN:HB3 | 2.20 | 0.42 |
| 37:L:77:ILE:HG13 | 37:L:78:ARG:H | 1.85 | 0.42 |
| 26:A:1664:A:H61 | 26:A:1996:C:N4 | 2.17 | 0.42 |
| 26:A:2135:A:H61 | 26:A:2156:G:H2' | 1.85 | 0.42 |
| 26:A:784:G:N2 | 26:A:792:A:O4' | 2.53 | 0.42 |
| 27:B:111:U:H2' | 27:B:112:G:H8 | 1.85 | 0.42 |
| 32:G:37:ASN:OD1 | 32:G:38:ASP:N | 2.53 | 0.42 |
| 45:T:56:GLU:HB2 | 45:T:86:THR:HG23 | 2.01 | 0.42 |
| 26:A:2037:A:H2' | 26:A:2038:G:C8 | 2.55 | 0.42 |
| 26:A:2698:U:H2' | 26:A:2699:C:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:D:9:VAL:O | 29:D:26:VAL:HB | 2.20 | 0.42 |
| 26:A:1614:A:H61 | 44:S:88:ARG:H | 1.67 | 0.42 |
| 26:A:1252:G:OP2 | 42:Q:13:HIS:NE2 | 2.50 | 0.42 |
| 26:A:2107:G:H2' | 26:A:2108:A:C4 | 2.55 | 0.42 |
| 26:A:2567:G:H2' | 26:A:2568:U:C6 | 2.55 | 0.42 |
| 26:A:2899:A:H2' | 26:A:2900:A:H8 | 1.84 | 0.42 |
| 26:A:479:A:N3 | 26:A:481:G:H5'' | 2.35 | 0.42 |
| 26:A:657:U:H2' | 26:A:658:U:C6 | 2.54 | 0.42 |
| 26:A:793:A:OP2 | 26:A:2071:A:O2' | 2.29 | 0.42 |
| 27:B:49:C:H2' | 27:B:50:A:C8 | 2.54 | 0.42 |
| 31:F:125:GLY:O | 31:F:157:THR:OG1 | 2.37 | 0.42 |
| 37:L:19:LEU:HD23 | 37:L:27:LEU:HD13 | 2.02 | 0.42 |
| 46:U:32:LYS:HE3 | 46:U:63:ALA:HB3 | 2.02 | 0.42 |
| 57:6:11:GLU:OE1 | 57:6:25:ARG:NH1 | 2.46 | 0.42 |
| 26:A:1485:U:H5' | 26:A:1961:C:H5'' | 99.22 | 0.42 |
| 26:A:1754:A:O3' | 41:P:102:ARG:NH2 | 2.51 | 0.42 |
| 26:A:406:G:H5' | 29:D:4:LEU:HG | 164.06 | 0.42 |
| 30:E:128:ALA:HB3 | 30:E:133:LEU:HD21 | 2.02 | 0.42 |
| 32:G:36:LEU:HD21 | 32:G:70:LEU:HD11 | 2.02 | 0.42 |
| 34:H:70:GLU:HB2 | 34:H:134:VAL:HG11 | 2.01 | 0.42 |
| 43:R:4:VAL:HG23 | 43:R:39:LEU:HB2 | 2.01 | 0.42 |
| 26:A:1353:A:H2' | 26:A:1354:A:H8 | 1.84 | 0.41 |
| 26:A:1386:C:H2' | 26:A:1387:A:C8 | 2.55 | 0.41 |
| 26:A:1737:G:O2' | 26:A:1738:G:N3 | 2.53 | 0.41 |
| 26:A:2183:A:H2' | 26:A:2184:A:C8 | 2.55 | 0.41 |
| 26:A:2514:U:H2' | 26:A:2515:C:C6 | 2.55 | 0.41 |
| 26:A:596:U:H2' | 26:A:597:G:H8 | 1.84 | 0.41 |
| 28:C:36:ASN:HB2 | 28:C:61:TYR:HB2 | 2.02 | 0.41 |
| 32:G:4:ALA:HB2 | 32:G:65:GLY:HA2 | 2.02 | 0.41 |
| 39:N:79:LEU:O | 39:N:84:GLY:N | 2.49 | 0.41 |
| 26:A:1503:A:H2' | 26:A:1504:A:H8 | 1.85 | 0.41 |
| 26:A:20:C:H2' | 26:A:21:A:H8 | 1.85 | 0.41 |
| 26:A:576:U:H2' | 26:A:577:G:C8 | 2.54 | 0.41 |
| 34:H:5:LEU:HB2 | 34:H:16:GLY:H | 1.85 | 0.41 |
| 37:L:80:SER:OG | 37:L:115:GLU:OE2 | 2.38 | 0.41 |
| 39:N:56:LYS:NZ | 39:N:90:ARG:O | 2.51 | 0.41 |
| 46:U:52:ASN:OD1 | 46:U:53:GLN:N | 2.52 | 0.41 |
| 26:A:466:A:OP1 | 54:2:34:ARG:NH1 | 2.54 | 0.41 |
| 26:A:1039:A:H61 | 26:A:1116:G:H1 | 1.68 | 0.41 |
| 26:A:1190:G:OP1 | 37:L:30:THR:OG1 | 2.28 | 0.41 |
| 26:A:1693:U:O4 | 26:A:1976:U:O2' | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:A:298:G:O2' | 26:A:322:A:N1 | 2.38 | 0.41 |
| 32:G:51:PHE:HE2 | 32:G:68:ARG:HA | 1.85 | 0.41 |
| 33:I:9:LYS:HB3 | 33:I:55:PRO:HB2 | 2.03 | 0.41 |
| 51:Z:16:LEU:HB3 | 51:Z:19:HIS:ND1 | 2.35 | 0.41 |
| 26:A:1028:A:OP2 | 26:A:1126:A:N6 | 2.36 | 0.41 |
| 26:A:1197:G:N2 | 26:A:1249:U:O2' | 2.54 | 0.41 |
| 33:I:82:ALA:HB1 | 33:I:108:ILE:HD13 | 2.02 | 0.41 |
| 33:I:2:LYS:HE2 | 33:I:61:TYR:CD1 | 2.55 | 0.41 |
| 35:J:45:THR:HB | 35:J:48:VAL:HG12 | 2.01 | 0.41 |
| 26:A:1250:G:P | 37:L:21:ARG:HE | 2.42 | 0.41 |
| 57:6:16:CYS:SG | 57:6:18:CYS:HB2 | 2.60 | 0.41 |
| 26:A:1751:U:H2' | 26:A:1752:C:C6 | 2.55 | 0.41 |
| 26:A:2047:C:H2' | 26:A:2048:G:H8 | 1.85 | 0.41 |
| 26:A:2428:G:H21 | 37:L:60:ARG:HH22 | 1.69 | 0.41 |
| 39:N:59:SER:OG | 39:N:62:ASN:OD1 | 2.27 | 0.41 |
| 57:6:41:HIS:HD2 | 57:6:43:PHE:HB2 | 1.85 | 0.41 |
| 26:A:1078:U:H5' | 26:A:1079:C:H5'' | 2.02 | 0.41 |
| 26:A:2295:C:OP1 | 40:O:10:ARG:NH1 | 2.51 | 0.41 |
| 26:A:796:C:H2' | 26:A:797:G:C8 | 2.55 | 0.41 |
| 47:V:35:GLU:HB2 | 47:V:93:ARG:HH22 | 1.86 | 0.41 |
| 26:A:1171:G:H2' | 26:A:1172:C:O4' | 2.20 | 0.41 |
| 26:A:154:U:H2' | 26:A:155:A:C8 | 2.69 | 0.41 |
| 26:A:569:U:O2' | 26:A:971:G:N2 | 2.48 | 0.41 |
| 26:A:882:G:H2' | 26:A:883:G:C8 | 2.55 | 0.41 |
| 31:F:37:MET:HB2 | 31:F:86:CYS:SG | 2.60 | 0.41 |
| 34:H:96:THR:O | 34:H:99:ILE:HG22 | 2.21 | 0.41 |
| 42:Q:78:PHE:CE1 | 42:Q:109:VAL:HG22 | 2.55 | 0.41 |
| 26:A:1601:G:H5'' | 45:T:64:LYS:HZ3 | 1.85 | 0.41 |
| 26:A:1927:A:H2' | 26:A:1928:A:C8 | 2.56 | 0.41 |
| 26:A:242:G:H1' | 26:A:243:U:H5 | 1.85 | 0.41 |
| 26:A:2530:A:N7 | 32:G:171:LYS:NZ | 2.51 | 0.41 |
| 26:A:935:C:H2' | 26:A:936:A:H8 | 1.85 | 0.41 |
| 32:G:42:VAL:HG23 | 32:G:51:PHE:CE1 | 2.55 | 0.41 |
| 47:V:40:ILE:HG23 | 47:V:40:ILE:HD12 | 1.87 | 0.41 |
| 26:A:922:C:H1' | 48:W:22:PHE:CD2 | 2.55 | 0.41 |
| 26:A:1244:A:O2' | 30:E:29:HIS:NE2 | 2.42 | 0.41 |
| 26:A:679:C:H2' | 26:A:680:C:C6 | 2.56 | 0.41 |
| 32:G:86:LEU:HG | 32:G:163:TYR:HD1 | 1.85 | 0.41 |
| 46:U:7:ASP:HB2 | 46:U:23:LYS:HB2 | 2.02 | 0.41 |
| 26:A:213:A:H2' | 26:A:214:G:C8 | 2.56 | 0.41 |
| 26:A:514:A:H2' | 26:A:515:A:C8 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:C:171:VAL:O | 28:C:182:LYS:HA | 2.20 | 0.41 |
| 57:6:14:ALA:HB1 | 57:6:34:LEU:HD11 | 2.03 | 0.41 |
| 26:A:1475:G:O2' | 26:A:1514:G:O6 | 2.39 | 0.41 |
| 26:A:1808:A:O2' | 26:A:1809:A:O4' | 2.35 | 0.41 |
| 26:A:2012:G:N7 | 44:S:16:LYS:NZ | 2.69 | 0.41 |
| 26:A:2591:C:H2' | 26:A:2592:G:C8 | 2.55 | 0.41 |
| 26:A:1939:5MU:OP1 | 26:A:2604:PSU:O2' | 2.39 | 0.41 |
| 26:A:285:G:C6 | 26:A:356:G:C6 | 3.08 | 0.41 |
| 26:A:589:U:H2' | 26:A:590:A:H8 | 1.86 | 0.41 |
| 26:A:191:A:O2' | 26:A:678:C:O2 | 2.36 | 0.41 |
| 27:B:57:A:H1' | 31:F:26:GLN:HG3 | 2.03 | 0.41 |
| 48:W:42:HIS:CD2 | 48:W:73:ARG:HD3 | 2.56 | 0.41 |
| 26:A:48:G:O2' | 26:A:118:A:N1 | 2.40 | 0.40 |
| 26:A:1274:A:OP1 | 26:A:1646:C:N4 | 2.45 | 0.40 |
| 26:A:2086:U:H2' | 26:A:2087:G:C8 | 2.56 | 0.40 |
| 30:E:133:LEU:HA | 30:E:136:GLN:HG2 | 2.02 | 0.40 |
| 31:F:12:VAL:HG12 | 31:F:27:VAL:HG21 | 2.02 | 0.40 |
| 41:P:19:PHE:HE2 | 41:P:46:VAL:HG11 | 1.87 | 0.40 |
| 57:6:7:PRO:HB2 | 57:6:27:THR:HG23 | 2.03 | 0.40 |
| 26:A:1265:A:H61 | 26:A:2013:A:H5'' | 1.87 | 0.40 |
| 26:A:1687:G:N1 | 26:A:1700:A:OP1 | 2.44 | 0.40 |
| 26:A:2229:U:H2' | 26:A:2230:G:C8 | 2.57 | 0.40 |
| 26:A:924:G:H2' | 26:A:925:A:C8 | 2.56 | 0.40 |
| 26:A:1972:G:OP2 | 28:C:237:ARG:NH1 | 2.54 | 0.40 |
| 29:D:110:THR:HB | 29:D:202:ILE:HG13 | 2.04 | 0.40 |
| 35:J:91:GLU:HG3 | 35:J:95:ARG:HH22 | 1.86 | 0.40 |
| 38:M:57:VAL:HG12 | 38:M:112:LEU:HG | 2.03 | 0.40 |
| 52:0:32:THR:OG1 | 52:0:33:SER:N | 2.55 | 0.40 |
| 26:A:83:A:N6 | 26:A:101:A:O2' | 2.49 | 0.40 |
| 26:A:1857:G:H22 | 26:A:1884:G:H2' | 1.86 | 0.40 |
| 26:A:1899:A:H4' | 26:A:1901:A:H5'' | 2.03 | 0.40 |
| 26:A:1997:C:H2' | 26:A:1998:A:H8 | 1.86 | 0.40 |
| 26:A:2185:U:H2' | 26:A:2186:G:C8 | 2.56 | 0.40 |
| 26:A:744:U:H2' | 26:A:745:1MG:O4' | 2.21 | 0.40 |
| 27:B:13:G:N2 | 27:B:16:G:N3 | 2.69 | 0.40 |
| 32:G:3:VAL:HG22 | 32:G:68:ARG:NH2 | 2.37 | 0.40 |
| 47:V:21:ARG:NH1 | 47:V:87:GLN:O | 2.46 | 0.40 |
| 26:A:2041:U:H2' | 26:A:2042:A:C8 | 2.56 | 0.40 |
| 26:A:2699:C:H2' | 26:A:2700:A:C8 | 2.57 | 0.40 |
| 26:A:500:G:N1 | 26:A:503:A:OP2 | 2.50 | 0.40 |
| 26:A:697:G:H2' | 26:A:698:C:C6 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 27:B:49:C:H2' | 27:B:50:A:H8 | 1.87 | 0.40 |
| 37:L:89:VAL:HG13 | 37:L:123:ARG:NH1 | 2.37 | 0.40 |
| 39:N:33:ILE:HB | 39:N:114:GLU:HG3 | 2.03 | 0.40 |
| 26:A:1151:A:H4' | 42:Q:80:ASN:ND2 | 2.37 | 0.40 |
| 46:U:70:ALA:HB3 | 46:U:79:ALA:HB1 | 2.03 | 0.40 |
| 48:W:19:VAL:HA | 48:W:34:VAL:HG22 | 2.03 | 0.40 |
| 26:A:1123:C:H2' | 26:A:1124:G:C8 | 2.56 | 0.40 |
| 26:A:2022:U:H3 | 52:O:5:ASN:ND2 | 2.20 | 0.40 |
| 26:A:2087:G:H2' | 26:A:2088:A:H8 | 1.86 | 0.40 |
| 28:C:175:LEU:HD23 | 28:C:175:LEU:HA | 1.84 | 0.40 |
| 37:L:123:ARG:NH2 | 37:L:143:GLU:OE2 | 2.55 | 0.40 |
| 40:O:31:THR:HG23 | 40:O:33:ARG:O | 2.22 | 0.40 |
| 43:R:98:ILE:HD12 | 43:R:98:ILE:HA | 1.92 | 0.40 |
| 47:V:77:VAL:HG23 | 47:V:89:ILE:HG22 | 2.02 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | b | 216/218 (99%) | 188 (87%) | 24 (11%) | 4 (2%) | 9 | 48 |
| 3 | c | 204/206 (99%) | 191 (94%) | 10 (5%) | 3 (2%) | 12 | 53 |
| 4 | d | 203/205 (99%) | 190 (94%) | 8 (4%) | 5 (2%) | 6 | 42 |
| 5 | e | 155/157 (99%) | 142 (92%) | 6 (4%) | 7 (4%) | 3 | 29 |
| 6 | f | 98/100 (98%) | 81 (83%) | 13 (13%) | 4 (4%) | 3 | 31 |
| 7 | g | 149/151 (99%) | 139 (93%) | 7 (5%) | 3 (2%) | 9 | 47 |
| 8 | h | 127/129 (98%) | 115 (91%) | 11 (9%) | 1 (1%) | 22 | 66 |
| 9 | i | 125/127 (98%) | 108 (86%) | 13 (10%) | 4 (3%) | 5 | 37 |
| 10 | j | 96/98 (98%) | 83 (86%) | 7 (7%) | 6 (6%) | 1 | 22 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 11 | k | 114/116 (98%) | 104 (91%) | 8 (7%) | 2 (2%) | 10 | 49 |
| 12 | l | 121/123 (98%) | 110 (91%) | 7 (6%) | 4 (3%) | 4 | 36 |
| 13 | m | 112/114 (98%) | 101 (90%) | 8 (7%) | 3 (3%) | 6 | 41 |
| 14 | n | 98/100 (98%) | 85 (87%) | 13 (13%) | 0 | 100 | 100 |
| 15 | o | 86/88 (98%) | 76 (88%) | 7 (8%) | 3 (4%) | 4 | 35 |
| 16 | p | 80/82 (98%) | 72 (90%) | 5 (6%) | 3 (4%) | 4 | 33 |
| 17 | q | 78/80 (98%) | 70 (90%) | 5 (6%) | 3 (4%) | 4 | 33 |
| 18 | r | 63/65 (97%) | 57 (90%) | 3 (5%) | 3 (5%) | 2 | 28 |
| 19 | s | 77/79 (98%) | 69 (90%) | 8 (10%) | 0 | 100 | 100 |
| 20 | t | 83/85 (98%) | 77 (93%) | 5 (6%) | 1 (1%) | 15 | 58 |
| 21 | u | 63/65 (97%) | 53 (84%) | 7 (11%) | 3 (5%) | 2 | 28 |
| 25 | z | 613/614 (100%) | 587 (96%) | 20 (3%) | 6 (1%) | 18 | 61 |
| 28 | C | 269/271 (99%) | 254 (94%) | 13 (5%) | 2 (1%) | 25 | 68 |
| 29 | D | 207/209 (99%) | 197 (95%) | 8 (4%) | 2 (1%) | 18 | 61 |
| 30 | E | 199/201 (99%) | 189 (95%) | 8 (4%) | 2 (1%) | 18 | 61 |
| 31 | F | 175/177 (99%) | 163 (93%) | 9 (5%) | 3 (2%) | 11 | 51 |
| 32 | G | 174/176 (99%) | 162 (93%) | 7 (4%) | 5 (3%) | 5 | 39 |
| 33 | I | 139/141 (99%) | 121 (87%) | 14 (10%) | 4 (3%) | 5 | 39 |
| 34 | H | 147/149 (99%) | 130 (88%) | 12 (8%) | 5 (3%) | 4 | 36 |
| 35 | J | 140/142 (99%) | 136 (97%) | 3 (2%) | 1 (1%) | 25 | 68 |
| 36 | K | 120/122 (98%) | 116 (97%) | 2 (2%) | 2 (2%) | 11 | 51 |
| 37 | L | 141/143 (99%) | 131 (93%) | 8 (6%) | 2 (1%) | 13 | 54 |
| 38 | M | 134/136 (98%) | 127 (95%) | 5 (4%) | 2 (2%) | 12 | 53 |
| 39 | N | 118/120 (98%) | 108 (92%) | 9 (8%) | 1 (1%) | 22 | 66 |
| 40 | O | 114/116 (98%) | 103 (90%) | 10 (9%) | 1 (1%) | 20 | 63 |
| 41 | P | 112/114 (98%) | 108 (96%) | 4 (4%) | 0 | 100 | 100 |
| 42 | Q | 115/117 (98%) | 110 (96%) | 5 (4%) | 0 | 100 | 100 |
| 43 | R | 101/103 (98%) | 93 (92%) | 6 (6%) | 2 (2%) | 9 | 47 |
| 44 | S | 108/110 (98%) | 102 (94%) | 4 (4%) | 2 (2%) | 9 | 48 |
| 45 | T | 91/93 (98%) | 79 (87%) | 11 (12%) | 1 (1%) | 17 | 60 |
| 46 | U | 100/102 (98%) | 89 (89%) | 5 (5%) | 6 (6%) | 2 | 22 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 47 | V | 92/94 (98%) | 88 (96%) | 4 (4%) | 0 | 100 | 100 |
| 48 | W | 73/75 (97%) | 69 (94%) | 4 (6%) | 0 | 100 | 100 |
| 49 | X | 75/77 (97%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 50 | Y | 61/63 (97%) | 56 (92%) | 4 (7%) | 1 (2%) | 11 | 52 |
| 51 | Z | 56/58 (97%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 52 | 0 | 54/56 (96%) | 51 (94%) | 2 (4%) | 1 (2%) | 9 | 48 |
| 53 | 1 | 48/50 (96%) | 46 (96%) | 1 (2%) | 1 (2%) | 8 | 46 |
| 54 | 2 | 44/46 (96%) | 42 (96%) | 1 (2%) | 1 (2%) | 7 | 44 |
| 55 | 3 | 62/64 (97%) | 57 (92%) | 4 (6%) | 1 (2%) | 11 | 52 |
| 56 | 4 | 36/38 (95%) | 33 (92%) | 3 (8%) | 0 | 100 | 100 |
| 57 | 6 | 64/66 (97%) | 57 (89%) | 5 (8%) | 2 (3%) | 5 | 37 |
| All | All | 6330/6431 (98%) | 5844 (92%) | 368 (6%) | 118 (2%) | 14 | 48 |

All (118) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | b | 18 | GLN |
| 2 | b | 151 | LYS |
| 5 | e | 89 | THR |
| 6 | f | 94 | HIS |
| 9 | i | 57 | VAL |
| 9 | i | 125 | GLN |
| 10 | j | 34 | ALA |
| 10 | j | 57 | VAL |
| 10 | j | 92 | LEU |
| 11 | k | 92 | ARG |
| 12 | l | 101 | LEU |
| 13 | m | 4 | ALA |
| 13 | m | 6 | ILE |
| 15 | o | 46 | LYS |
| 15 | o | 87 | ARG |
| 16 | p | 44 | SER |
| 17 | q | 16 | MET |
| 17 | q | 49 | ASN |
| 25 | z | 191 | VAL |
| 25 | z | 301 | GLU |
| 25 | z | 328 | ALA |
| 28 | C | 121 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | E | 83 | VAL |
| 32 | G | 174 | LYS |
| 32 | G | 175 | LYS |
| 33 | I | 64 | ARG |
| 34 | H | 9 | VAL |
| 35 | J | 81 | ILE |
| 37 | L | 36 | LYS |
| 38 | M | 58 | LYS |
| 44 | S | 64 | ALA |
| 46 | U | 51 | LEU |
| 46 | U | 88 | ASP |
| 52 | 0 | 2 | VAL |
| 53 | 1 | 4 | ILE |
| 55 | 3 | 31 | ILE |
| 3 | c | 60 | ALA |
| 3 | c | 79 | LYS |
| 4 | d | 165 | GLU |
| 4 | d | 191 | SER |
| 5 | e | 77 | ASN |
| 5 | e | 93 | VAL |
| 8 | h | 44 | PHE |
| 9 | i | 107 | ALA |
| 10 | j | 42 | LEU |
| 11 | k | 91 | GLY |
| 12 | l | 25 | ALA |
| 18 | r | 11 | ARG |
| 18 | r | 18 | GLN |
| 21 | u | 25 | ALA |
| 25 | z | 487 | PHE |
| 32 | G | 108 | PHE |
| 33 | I | 24 | GLY |
| 34 | H | 3 | VAL |
| 34 | H | 41 | LYS |
| 36 | K | 35 | VAL |
| 39 | N | 117 | ASP |
| 43 | R | 52 | PRO |
| 43 | R | 53 | PHE |
| 46 | U | 6 | ARG |
| 46 | U | 18 | LYS |
| 57 | 6 | 40 | CYS |
| 57 | 6 | 43 | PHE |
| 4 | d | 47 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | e | 23 | THR |
| 6 | f | 99 | ALA |
| 7 | g | 129 | ASN |
| 9 | i | 12 | LYS |
| 15 | o | 2 | LEU |
| 16 | p | 43 | ALA |
| 21 | u | 24 | LYS |
| 21 | u | 34 | ARG |
| 28 | C | 204 | LEU |
| 29 | D | 140 | HIS |
| 29 | D | 149 | ASN |
| 32 | G | 118 | ALA |
| 33 | I | 69 | VAL |
| 34 | H | 15 | LEU |
| 37 | L | 29 | LYS |
| 2 | b | 17 | HIS |
| 3 | c | 156 | LEU |
| 5 | e | 122 | VAL |
| 7 | g | 57 | GLU |
| 10 | j | 58 | ASN |
| 12 | l | 2 | THR |
| 12 | l | 46 | SER |
| 17 | q | 72 | TRP |
| 20 | t | 26 | MET |
| 31 | F | 20 | ASN |
| 32 | G | 173 | ALA |
| 34 | H | 89 | LYS |
| 44 | S | 3 | THR |
| 45 | T | 88 | LYS |
| 54 | 2 | 40 | ALA |
| 2 | b | 120 | SER |
| 4 | d | 150 | LYS |
| 5 | e | 158 | LYS |
| 6 | f | 92 | THR |
| 7 | g | 56 | SER |
| 10 | j | 75 | ASP |
| 25 | z | 345 | ARG |
| 30 | E | 122 | GLU |
| 31 | F | 149 | ARG |
| 36 | K | 92 | GLU |
| 40 | O | 101 | GLY |
| 46 | U | 97 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | U | 98 | ASN |
| 50 | Y | 24 | GLU |
| 4 | d | 4 | LEU |
| 13 | m | 11 | HIS |
| 38 | M | 69 | PRO |
| 5 | e | 24 | VAL |
| 16 | p | 49 | GLY |
| 18 | r | 17 | VAL |
| 25 | z | 600 | GLY |
| 31 | F | 135 | ILE |
| 6 | f | 19 | PRO |
| 33 | I | 12 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2 | b | 180/180 (100%) | 180 (100%) | 0 | 100 | 100 |
| 3 | c | 170/170 (100%) | 170 (100%) | 0 | 100 | 100 |
| 4 | d | 172/172 (100%) | 172 (100%) | 0 | 100 | 100 |
| 5 | e | 119/119 (100%) | 119 (100%) | 0 | 100 | 100 |
| 6 | f | 87/87 (100%) | 87 (100%) | 0 | 100 | 100 |
| 7 | g | 124/124 (100%) | 124 (100%) | 0 | 100 | 100 |
| 8 | h | 104/104 (100%) | 104 (100%) | 0 | 100 | 100 |
| 9 | i | 105/105 (100%) | 105 (100%) | 0 | 100 | 100 |
| 10 | j | 86/86 (100%) | 86 (100%) | 0 | 100 | 100 |
| 11 | k | 89/89 (100%) | 89 (100%) | 0 | 100 | 100 |
| 12 | l | 103/103 (100%) | 102 (99%) | 1 (1%) | 80 | 90 |
| 13 | m | 92/92 (100%) | 92 (100%) | 0 | 100 | 100 |
| 14 | n | 79/83 (95%) | 79 (100%) | 0 | 100 | 100 |
| 15 | o | 76/76 (100%) | 76 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 16 | p | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 17 | q | 74/74 (100%) | 74 (100%) | 0 | 100 | 100 |
| 18 | r | 48/56 (86%) | 48 (100%) | 0 | 100 | 100 |
| 19 | s | 70/70 (100%) | 70 (100%) | 0 | 100 | 100 |
| 20 | t | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 21 | u | 44/55 (80%) | 44 (100%) | 0 | 100 | 100 |
| 25 | z | 502/501 (100%) | 502 (100%) | 0 | 100 | 100 |
| 28 | C | 216/216 (100%) | 216 (100%) | 0 | 100 | 100 |
| 29 | D | 164/164 (100%) | 164 (100%) | 0 | 100 | 100 |
| 30 | E | 165/165 (100%) | 165 (100%) | 0 | 100 | 100 |
| 31 | F | 148/148 (100%) | 148 (100%) | 0 | 100 | 100 |
| 32 | G | 137/137 (100%) | 137 (100%) | 0 | 100 | 100 |
| 33 | I | 109/109 (100%) | 109 (100%) | 0 | 100 | 100 |
| 34 | H | 114/114 (100%) | 114 (100%) | 0 | 100 | 100 |
| 35 | J | 116/116 (100%) | 116 (100%) | 0 | 100 | 100 |
| 36 | K | 103/103 (100%) | 103 (100%) | 0 | 100 | 100 |
| 37 | L | 102/102 (100%) | 102 (100%) | 0 | 100 | 100 |
| 38 | M | 109/109 (100%) | 109 (100%) | 0 | 100 | 100 |
| 39 | N | 100/100 (100%) | 100 (100%) | 0 | 100 | 100 |
| 40 | O | 86/86 (100%) | 86 (100%) | 0 | 100 | 100 |
| 41 | P | 99/99 (100%) | 99 (100%) | 0 | 100 | 100 |
| 42 | Q | 89/89 (100%) | 89 (100%) | 0 | 100 | 100 |
| 43 | R | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 44 | S | 93/93 (100%) | 93 (100%) | 0 | 100 | 100 |
| 45 | T | 80/80 (100%) | 80 (100%) | 0 | 100 | 100 |
| 46 | U | 83/83 (100%) | 83 (100%) | 0 | 100 | 100 |
| 47 | V | 78/78 (100%) | 78 (100%) | 0 | 100 | 100 |
| 48 | W | 57/57 (100%) | 57 (100%) | 0 | 100 | 100 |
| 49 | X | 67/67 (100%) | 67 (100%) | 0 | 100 | 100 |
| 50 | Y | 55/55 (100%) | 55 (100%) | 0 | 100 | 100 |
| 51 | Z | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 52 | 0 | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 53 | 1 | 45/45 (100%) | 45 (100%) | 0 | 100 | 100 |
| 54 | 2 | 38/38 (100%) | 38 (100%) | 0 | 100 | 100 |
| 55 | 3 | 51/51 (100%) | 51 (100%) | 0 | 100 | 100 |
| 56 | 4 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 57 | 6 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| All | All | 5230/5252 (100%) | 5229 (100%) | 1 (0%) | 100 | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | l | 23 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | c | 138 | GLN |
| 5 | e | 121 | ASN |
| 9 | i | 4 | GLN |
| 9 | i | 109 | GLN |
| 9 | i | 125 | GLN |
| 14 | n | 42 | ASN |
| 15 | o | 36 | ASN |
| 15 | o | 45 | HIS |
| 17 | q | 44 | HIS |
| 18 | r | 51 | GLN |
| 19 | s | 51 | HIS |
| 19 | s | 56 | HIS |
| 25 | z | 47 | GLN |
| 25 | z | 292 | HIS |
| 25 | z | 388 | GLN |
| 25 | z | 483 | HIS |
| 25 | z | 529 | GLN |
| 28 | C | 85 | ASN |
| 28 | C | 89 | ASN |
| 28 | C | 250 | GLN |
| 29 | D | 150 | GLN |
| 30 | E | 90 | GLN |
| 31 | F | 26 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | G | 114 | HIS |
| 32 | G | 138 | GLN |
| 34 | H | 2 | GLN |
| 34 | H | 18 | GLN |
| 36 | K | 29 | HIS |
| 37 | L | 35 | HIS |
| 41 | P | 55 | HIS |
| 43 | R | 91 | GLN |
| 44 | S | 102 | HIS |
| 46 | U | 73 | ASN |
| 50 | Y | 58 | ASN |
| 52 | 0 | 5 | ASN |
| 56 | 4 | 33 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | a | 1535/1539 (99%) | 197 (12%) | 0 |
| 22 | v | 76/77 (98%) | 10 (13%) | 0 |
| 23 | x | 47/48 (97%) | 29 (61%) | 0 |
| 24 | y | 93/95 (97%) | 23 (24%) | 0 |
| 26 | A | 2898/2903 (99%) | 414 (14%) | 5 (0%) |
| 27 | B | 119/120 (99%) | 11 (9%) | 0 |
| 58 | w | 2/3 (66%) | 0 | 0 |
| All | All | 4770/4785 (99%) | 684 (14%) | 5 (0%) |

All (684) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | a | 8 | A |
| 1 | a | 9 | G |
| 1 | a | 22 | G |
| 1 | a | 32 | A |
| 1 | a | 39 | G |
| 1 | a | 47 | C |
| 1 | a | 48 | C |
| 1 | a | 49 | U |
| 1 | a | 50 | A |
| 1 | a | 51 | A |
| 1 | a | 86 | G |
| 1 | a | 94 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | a | 95 | C |
| 1 | a | 96 | U |
| 1 | a | 121 | U |
| 1 | a | 127 | G |
| 1 | a | 131 | A |
| 1 | a | 141 | G |
| 1 | a | 164 | G |
| 1 | a | 173 | U |
| 1 | a | 177 | G |
| 1 | a | 183 | C |
| 1 | a | 197 | A |
| 1 | a | 209 | U |
| 1 | a | 210 | C |
| 1 | a | 211 | G |
| 1 | a | 212 | G |
| 1 | a | 226 | G |
| 1 | a | 237 | G |
| 1 | a | 245 | U |
| 1 | a | 247 | G |
| 1 | a | 251 | G |
| 1 | a | 254 | G |
| 1 | a | 266 | G |
| 1 | a | 267 | C |
| 1 | a | 289 | G |
| 1 | a | 298 | A |
| 1 | a | 316 | C |
| 1 | a | 319 | G |
| 1 | a | 328 | C |
| 1 | a | 330 | C |
| 1 | a | 347 | G |
| 1 | a | 352 | C |
| 1 | a | 354 | G |
| 1 | a | 356 | A |
| 1 | a | 367 | U |
| 1 | a | 368 | U |
| 1 | a | 372 | C |
| 1 | a | 392 | C |
| 1 | a | 406 | G |
| 1 | a | 407 | U |
| 1 | a | 411 | A |
| 1 | a | 412 | A |
| 1 | a | 414 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | a | 420 | U |
| 1 | a | 426 | U |
| 1 | a | 429 | U |
| 1 | a | 430 | A |
| 1 | a | 436 | C |
| 1 | a | 438 | U |
| 1 | a | 439 | U |
| 1 | a | 467 | U |
| 1 | a | 481 | G |
| 1 | a | 482 | A |
| 1 | a | 491 | G |
| 1 | a | 497 | G |
| 1 | a | 499 | A |
| 1 | a | 509 | A |
| 1 | a | 511 | C |
| 1 | a | 512 | U |
| 1 | a | 517 | G |
| 1 | a | 518 | C |
| 1 | a | 524 | G |
| 1 | a | 527 | G7M |
| 1 | a | 528 | C |
| 1 | a | 531 | U |
| 1 | a | 532 | A |
| 1 | a | 546 | A |
| 1 | a | 547 | A |
| 1 | a | 551 | U |
| 1 | a | 562 | U |
| 1 | a | 564 | C |
| 1 | a | 572 | A |
| 1 | a | 575 | G |
| 1 | a | 576 | C |
| 1 | a | 577 | G |
| 1 | a | 633 | G |
| 1 | a | 642 | A |
| 1 | a | 653 | U |
| 1 | a | 661 | G |
| 1 | a | 665 | A |
| 1 | a | 686 | U |
| 1 | a | 723 | U |
| 1 | a | 724 | G |
| 1 | a | 733 | G |
| 1 | a | 748 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | a | 777 | A |
| 1 | a | 793 | U |
| 1 | a | 794 | A |
| 1 | a | 815 | A |
| 1 | a | 816 | A |
| 1 | a | 817 | C |
| 1 | a | 819 | A |
| 1 | a | 832 | G |
| 1 | a | 841 | C |
| 1 | a | 842 | U |
| 1 | a | 843 | U |
| 1 | a | 844 | G |
| 1 | a | 845 | A |
| 1 | a | 876 | C |
| 1 | a | 878 | A |
| 1 | a | 889 | A |
| 1 | a | 890 | G |
| 1 | a | 926 | G |
| 1 | a | 934 | C |
| 1 | a | 935 | A |
| 1 | a | 942 | G |
| 1 | a | 960 | U |
| 1 | a | 966 | 2MG |
| 1 | a | 968 | A |
| 1 | a | 969 | A |
| 1 | a | 974 | A |
| 1 | a | 975 | A |
| 1 | a | 976 | G |
| 1 | a | 977 | A |
| 1 | a | 991 | U |
| 1 | a | 993 | G |
| 1 | a | 1004 | A |
| 1 | a | 1020 | G |
| 1 | a | 1032 | G |
| 1 | a | 1034 | G |
| 1 | a | 1043 | G |
| 1 | a | 1065 | U |
| 1 | a | 1085 | U |
| 1 | a | 1089 | G |
| 1 | a | 1094 | G |
| 1 | a | 1095 | U |
| 1 | a | 1101 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | a | 1105 | A |
| 1 | a | 1134 | G |
| 1 | a | 1135 | U |
| 1 | a | 1136 | C |
| 1 | a | 1137 | C |
| 1 | a | 1138 | G |
| 1 | a | 1139 | G |
| 1 | a | 1140 | C |
| 1 | a | 1158 | C |
| 1 | a | 1159 | U |
| 1 | a | 1160 | G |
| 1 | a | 1168 | U |
| 1 | a | 1169 | A |
| 1 | a | 1182 | G |
| 1 | a | 1196 | A |
| 1 | a | 1197 | A |
| 1 | a | 1213 | A |
| 1 | a | 1227 | A |
| 1 | a | 1238 | A |
| 1 | a | 1240 | U |
| 1 | a | 1241 | G |
| 1 | a | 1260 | G |
| 1 | a | 1278 | G |
| 1 | a | 1280 | A |
| 1 | a | 1287 | A |
| 1 | a | 1297 | G |
| 1 | a | 1300 | G |
| 1 | a | 1302 | C |
| 1 | a | 1305 | G |
| 1 | a | 1317 | C |
| 1 | a | 1320 | C |
| 1 | a | 1338 | G |
| 1 | a | 1345 | U |
| 1 | a | 1346 | A |
| 1 | a | 1363 | A |
| 1 | a | 1364 | U |
| 1 | a | 1394 | A |
| 1 | a | 1396 | A |
| 1 | a | 1397 | C |
| 1 | a | 1398 | A |
| 1 | a | 1406 | U |
| 1 | a | 1419 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | a | 1429 | A |
| 1 | a | 1441 | A |
| 1 | a | 1491 | G |
| 1 | a | 1492 | A |
| 1 | a | 1493 | A |
| 1 | a | 1497 | G |
| 1 | a | 1503 | A |
| 1 | a | 1506 | U |
| 1 | a | 1507 | A |
| 1 | a | 1517 | G |
| 1 | a | 1520 | C |
| 1 | a | 1529 | G |
| 1 | a | 1530 | G |
| 1 | a | 1533 | C |
| 1 | a | 1534 | A |
| 1 | a | 1536 | C |
| 1 | a | 1537 | U |
| 22 | v | 9 | G |
| 22 | v | 18 | G |
| 22 | v | 20 | H2U |
| 22 | v | 21 | A |
| 22 | v | 22 | G |
| 22 | v | 31 | G |
| 22 | v | 52 | G |
| 22 | v | 54 | 5MU |
| 22 | v | 59 | A |
| 22 | v | 75 | C |
| 23 | x | 88 | A |
| 23 | x | 90 | G |
| 23 | x | 96 | C |
| 23 | x | 98 | U |
| 23 | x | 104 | U |
| 23 | x | 108 | A |
| 23 | x | 109 | C |
| 23 | x | 110 | G |
| 23 | x | 111 | G |
| 23 | x | 112 | C |
| 23 | x | 113 | C |
| 23 | x | 114 | C |
| 23 | x | 115 | A |
| 23 | x | 116 | U |
| 23 | x | 117 | C |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 23 | x | 118 | G |
| 23 | x | 119 | G |
| 23 | x | 120 | U |
| 23 | x | 121 | U |
| 23 | x | 123 | C |
| 23 | x | 125 | G |
| 23 | x | 126 | G |
| 23 | x | 127 | U |
| 23 | x | 128 | C |
| 23 | x | 129 | U |
| 23 | x | 130 | G |
| 23 | x | 131 | C |
| 23 | x | 133 | C |
| 23 | x | 134 | C |
| 24 | y | 8 | G |
| 24 | y | 15 | C |
| 24 | y | 18 | G |
| 24 | y | 20 | G |
| 24 | y | 29 | G |
| 24 | y | 31 | A |
| 24 | y | 40 | C |
| 24 | y | 45 | U |
| 24 | y | 46 | G |
| 24 | y | 47(F) | C |
| 24 | y | 47(G) | C |
| 24 | y | 47(H) | A |
| 24 | y | 47(I) | G |
| 24 | y | 47(J) | C |
| 24 | y | 49 | G |
| 24 | y | 54 | 5MU |
| 24 | y | 55 | PSU |
| 24 | y | 56 | C |
| 24 | y | 60 | U |
| 24 | y | 61 | C |
| 24 | y | 64 | G |
| 24 | y | 66 | G |
| 24 | y | 73 | G |
| 26 | A | 10 | A |
| 26 | A | 15 | G |
| 26 | A | 23 | G |
| 26 | A | 27 | G |
| 26 | A | 34 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | A | 60 | G |
| 26 | A | 63 | A |
| 26 | A | 71 | A |
| 26 | A | 74 | A |
| 26 | A | 75 | G |
| 26 | A | 91 | A |
| 26 | A | 101 | A |
| 26 | A | 102 | U |
| 26 | A | 118 | A |
| 26 | A | 120 | U |
| 26 | A | 125 | A |
| 26 | A | 131 | A |
| 26 | A | 138 | U |
| 26 | A | 139 | U |
| 26 | A | 142 | A |
| 26 | A | 181 | A |
| 26 | A | 196 | A |
| 26 | A | 199 | A |
| 26 | A | 204 | A |
| 26 | A | 205 | G |
| 26 | A | 216 | A |
| 26 | A | 222 | A |
| 26 | A | 228 | C |
| 26 | A | 230 | G |
| 26 | A | 232 | G |
| 26 | A | 248 | G |
| 26 | A | 255 | A |
| 26 | A | 277 | G |
| 26 | A | 278 | A |
| 26 | A | 279 | A |
| 26 | A | 285 | G |
| 26 | A | 311 | A |
| 26 | A | 322 | A |
| 26 | A | 329 | G |
| 26 | A | 330 | A |
| 26 | A | 362 | A |
| 26 | A | 367 | G |
| 26 | A | 372 | G |
| 26 | A | 386 | G |
| 26 | A | 396 | G |
| 26 | A | 404 | A |
| 26 | A | 405 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | A | 411 | G |
| 26 | A | 448 | U |
| 26 | A | 451 | U |
| 26 | A | 456 | C |
| 26 | A | 473 | G |
| 26 | A | 479 | A |
| 26 | A | 480 | A |
| 26 | A | 481 | G |
| 26 | A | 490 | C |
| 26 | A | 491 | G |
| 26 | A | 504 | A |
| 26 | A | 505 | A |
| 26 | A | 508 | A |
| 26 | A | 509 | C |
| 26 | A | 529 | A |
| 26 | A | 530 | G |
| 26 | A | 531 | C |
| 26 | A | 532 | A |
| 26 | A | 533 | G |
| 26 | A | 549 | G |
| 26 | A | 562 | U |
| 26 | A | 563 | A |
| 26 | A | 573 | U |
| 26 | A | 603 | A |
| 26 | A | 614 | A |
| 26 | A | 615 | U |
| 26 | A | 616 | A |
| 26 | A | 622 | G |
| 26 | A | 637 | A |
| 26 | A | 646 | U |
| 26 | A | 647 | G |
| 26 | A | 655 | A |
| 26 | A | 664 | G |
| 26 | A | 668 | A |
| 26 | A | 675 | A |
| 26 | A | 686 | U |
| 26 | A | 695 | G |
| 26 | A | 711 | G |
| 26 | A | 717 | C |
| 26 | A | 726 | G |
| 26 | A | 730 | A |
| 26 | A | 747 | 5MU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | A | 748 | G |
| 26 | A | 765 | C |
| 26 | A | 775 | G |
| 26 | A | 782 | A |
| 26 | A | 784 | G |
| 26 | A | 789 | A |
| 26 | A | 805 | G |
| 26 | A | 812 | C |
| 26 | A | 819 | A |
| 26 | A | 827 | U |
| 26 | A | 830 | G |
| 26 | A | 846 | U |
| 26 | A | 859 | G |
| 26 | A | 869 | G |
| 26 | A | 885 | C |
| 26 | A | 887 | U |
| 26 | A | 888 | C |
| 26 | A | 889 | C |
| 26 | A | 890 | C |
| 26 | A | 910 | A |
| 26 | A | 932 | U |
| 26 | A | 941 | A |
| 26 | A | 946 | C |
| 26 | A | 959 | A |
| 26 | A | 961 | C |
| 26 | A | 965 | C |
| 26 | A | 973 | A |
| 26 | A | 974 | G |
| 26 | A | 983 | A |
| 26 | A | 990 | A |
| 26 | A | 1009 | A |
| 26 | A | 1012 | U |
| 26 | A | 1013 | C |
| 26 | A | 1022 | G |
| 26 | A | 1023 | U |
| 26 | A | 1026 | G |
| 26 | A | 1033 | U |
| 26 | A | 1040 | A |
| 26 | A | 1042 | G |
| 26 | A | 1043 | C |
| 26 | A | 1045 | C |
| 26 | A | 1046 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | A | 1047 | G |
| 26 | A | 1057 | A |
| 26 | A | 1058 | U |
| 26 | A | 1059 | G |
| 26 | A | 1061 | U |
| 26 | A | 1062 | G |
| 26 | A | 1064 | C |
| 26 | A | 1065 | U |
| 26 | A | 1066 | U |
| 26 | A | 1067 | A |
| 26 | A | 1068 | G |
| 26 | A | 1069 | A |
| 26 | A | 1070 | A |
| 26 | A | 1071 | G |
| 26 | A | 1073 | A |
| 26 | A | 1076 | C |
| 26 | A | 1077 | A |
| 26 | A | 1078 | U |
| 26 | A | 1079 | C |
| 26 | A | 1084 | A |
| 26 | A | 1088 | A |
| 26 | A | 1092 | C |
| 26 | A | 1094 | U |
| 26 | A | 1100 | C |
| 26 | A | 1101 | U |
| 26 | A | 1110 | G |
| 26 | A | 1112 | G |
| 26 | A | 1119 | U |
| 26 | A | 1132 | U |
| 26 | A | 1133 | A |
| 26 | A | 1134 | A |
| 26 | A | 1135 | C |
| 26 | A | 1142 | A |
| 26 | A | 1143 | A |
| 26 | A | 1157 | G |
| 26 | A | 1171 | G |
| 26 | A | 1175 | A |
| 26 | A | 1178 | C |
| 26 | A | 1180 | U |
| 26 | A | 1206 | G |
| 26 | A | 1210 | G |
| 26 | A | 1211 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | A | 1236 | G |
| 26 | A | 1248 | G |
| 26 | A | 1253 | A |
| 26 | A | 1255 | U |
| 26 | A | 1256 | G |
| 26 | A | 1271 | G |
| 26 | A | 1272 | A |
| 26 | A | 1273 | U |
| 26 | A | 1300 | G |
| 26 | A | 1301 | A |
| 26 | A | 1311 | G |
| 26 | A | 1314 | C |
| 26 | A | 1325 | U |
| 26 | A | 1329 | U |
| 26 | A | 1345 | C |
| 26 | A | 1359 | A |
| 26 | A | 1365 | A |
| 26 | A | 1378 | A |
| 26 | A | 1379 | U |
| 26 | A | 1383 | A |
| 26 | A | 1392 | A |
| 26 | A | 1394 | U |
| 26 | A | 1395 | A |
| 26 | A | 1401 | G |
| 26 | A | 1403 | A |
| 26 | A | 1407 | G |
| 26 | A | 1416 | G |
| 26 | A | 1417 | C |
| 26 | A | 1420 | A |
| 26 | A | 1428 | C |
| 26 | A | 1437 | C |
| 26 | A | 1452 | G |
| 26 | A | 1455 | G |
| 26 | A | 1458 | U |
| 26 | A | 1460 | U |
| 26 | A | 1468 | U |
| 26 | A | 1482 | G |
| 26 | A | 1490 | A |
| 26 | A | 1493 | C |
| 26 | A | 1497 | U |
| 26 | A | 1509 | A |
| 26 | A | 1515 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | A | 1532 | A |
| 26 | A | 1534 | U |
| 26 | A | 1535 | A |
| 26 | A | 1536 | C |
| 26 | A | 1537 | G |
| 26 | A | 1566 | A |
| 26 | A | 1569 | A |
| 26 | A | 1578 | U |
| 26 | A | 1583 | A |
| 26 | A | 1608 | A |
| 26 | A | 1609 | A |
| 26 | A | 1619 | G |
| 26 | A | 1639 | C |
| 26 | A | 1646 | C |
| 26 | A | 1648 | U |
| 26 | A | 1649 | G |
| 26 | A | 1654 | A |
| 26 | A | 1660 | G |
| 26 | A | 1674 | G |
| 26 | A | 1675 | C |
| 26 | A | 1715 | G |
| 26 | A | 1738 | G |
| 26 | A | 1758 | U |
| 26 | A | 1764 | C |
| 26 | A | 1773 | A |
| 26 | A | 1784 | A |
| 26 | A | 1791 | A |
| 26 | A | 1799 | G |
| 26 | A | 1800 | C |
| 26 | A | 1801 | A |
| 26 | A | 1808 | A |
| 26 | A | 1816 | C |
| 26 | A | 1829 | A |
| 26 | A | 1833 | C |
| 26 | A | 1847 | A |
| 26 | A | 1870 | C |
| 26 | A | 1871 | A |
| 26 | A | 1876 | A |
| 26 | A | 1906 | G |
| 26 | A | 1913 | A |
| 26 | A | 1927 | A |
| 26 | A | 1929 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | A | 1930 | G |
| 26 | A | 1937 | A |
| 26 | A | 1941 | C |
| 26 | A | 1955 | U |
| 26 | A | 1960 | A |
| 26 | A | 1962 | 5MC |
| 26 | A | 1963 | U |
| 26 | A | 1964 | G |
| 26 | A | 1967 | C |
| 26 | A | 1971 | U |
| 26 | A | 1972 | G |
| 26 | A | 1991 | U |
| 26 | A | 1992 | G |
| 26 | A | 1993 | U |
| 26 | A | 1997 | C |
| 26 | A | 2002 | G |
| 26 | A | 2021 | C |
| 26 | A | 2022 | U |
| 26 | A | 2023 | C |
| 26 | A | 2031 | A |
| 26 | A | 2032 | G |
| 26 | A | 2043 | C |
| 26 | A | 2051 | A |
| 26 | A | 2052 | A |
| 26 | A | 2055 | C |
| 26 | A | 2056 | G |
| 26 | A | 2060 | A |
| 26 | A | 2061 | G |
| 26 | A | 2062 | A |
| 26 | A | 2069 | G7M |
| 26 | A | 2070 | A |
| 26 | A | 2080 | A |
| 26 | A | 2100 | G |
| 26 | A | 2105 | U |
| 26 | A | 2107 | G |
| 26 | A | 2110 | G |
| 26 | A | 2111 | U |
| 26 | A | 2112 | G |
| 26 | A | 2113 | U |
| 26 | A | 2116 | G |
| 26 | A | 2118 | U |
| 26 | A | 2119 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | A | 2120 | G |
| 26 | A | 2125 | G |
| 26 | A | 2127 | G |
| 26 | A | 2129 | C |
| 26 | A | 2131 | U |
| 26 | A | 2132 | U |
| 26 | A | 2133 | G |
| 26 | A | 2134 | A |
| 26 | A | 2146 | C |
| 26 | A | 2147 | A |
| 26 | A | 2157 | G |
| 26 | A | 2159 | G |
| 26 | A | 2160 | C |
| 26 | A | 2162 | G |
| 26 | A | 2168 | G |
| 26 | A | 2171 | A |
| 26 | A | 2172 | U |
| 26 | A | 2173 | A |
| 26 | A | 2177 | C |
| 26 | A | 2178 | C |
| 26 | A | 2179 | C |
| 26 | A | 2182 | U |
| 26 | A | 2198 | A |
| 26 | A | 2204 | G |
| 26 | A | 2210 | U |
| 26 | A | 2211 | A |
| 26 | A | 2212 | A |
| 26 | A | 2225 | A |
| 26 | A | 2238 | G |
| 26 | A | 2239 | G |
| 26 | A | 2250 | G |
| 26 | A | 2251 | OMG |
| 26 | A | 2268 | A |
| 26 | A | 2278 | A |
| 26 | A | 2283 | C |
| 26 | A | 2287 | A |
| 26 | A | 2305 | U |
| 26 | A | 2308 | G |
| 26 | A | 2310 | C |
| 26 | A | 2312 | U |
| 26 | A | 2319 | G |
| 26 | A | 2322 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | A | 2333 | A |
| 26 | A | 2334 | U |
| 26 | A | 2335 | A |
| 26 | A | 2336 | A |
| 26 | A | 2342 | C |
| 26 | A | 2347 | C |
| 26 | A | 2350 | C |
| 26 | A | 2354 | C |
| 26 | A | 2357 | G |
| 26 | A | 2383 | G |
| 26 | A | 2385 | C |
| 26 | A | 2402 | U |
| 26 | A | 2403 | C |
| 26 | A | 2428 | G |
| 26 | A | 2429 | G |
| 26 | A | 2430 | A |
| 26 | A | 2434 | A |
| 26 | A | 2436 | G |
| 26 | A | 2441 | U |
| 26 | A | 2445 | 2MG |
| 26 | A | 2447 | G |
| 26 | A | 2448 | A |
| 26 | A | 2470 | G |
| 26 | A | 2476 | A |
| 26 | A | 2478 | A |
| 26 | A | 2480 | C |
| 26 | A | 2484 | G |
| 26 | A | 2494 | G |
| 26 | A | 2502 | G |
| 26 | A | 2504 | PSU |
| 26 | A | 2505 | G |
| 26 | A | 2506 | U |
| 26 | A | 2513 | A |
| 26 | A | 2518 | A |
| 26 | A | 2520 | C |
| 26 | A | 2525 | G |
| 26 | A | 2529 | G |
| 26 | A | 2547 | A |
| 26 | A | 2554 | U |
| 26 | A | 2567 | G |
| 26 | A | 2581 | G |
| 26 | A | 2582 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | A | 2585 | U |
| 26 | A | 2602 | A |
| 26 | A | 2609 | U |
| 26 | A | 2613 | U |
| 26 | A | 2629 | U |
| 26 | A | 2630 | G |
| 26 | A | 2639 | A |
| 26 | A | 2663 | G |
| 26 | A | 2689 | U |
| 26 | A | 2690 | U |
| 26 | A | 2714 | G |
| 26 | A | 2718 | G |
| 26 | A | 2726 | A |
| 26 | A | 2733 | A |
| 26 | A | 2744 | G |
| 26 | A | 2755 | C |
| 26 | A | 2758 | A |
| 26 | A | 2764 | A |
| 26 | A | 2765 | A |
| 26 | A | 2778 | A |
| 26 | A | 2791 | G |
| 26 | A | 2793 | C |
| 26 | A | 2797 | U |
| 26 | A | 2809 | A |
| 26 | A | 2818 | U |
| 26 | A | 2821 | A |
| 26 | A | 2833 | U |
| 26 | A | 2849 | U |
| 26 | A | 2872 | A |
| 26 | A | 2879 | A |
| 26 | A | 2884 | U |
| 27 | B | 24 | G |
| 27 | B | 26 | C |
| 27 | B | 35 | C |
| 27 | B | 38 | C |
| 27 | B | 42 | C |
| 27 | B | 45 | A |
| 27 | B | 57 | A |
| 27 | B | 87 | U |
| 27 | B | 90 | C |
| 27 | B | 108 | A |
| 27 | B | 109 | A |

All (5) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | A | 818 | G |
| 26 | A | 960 | A |
| 26 | A | 1042 | G |
| 26 | A | 1358 | G |
| 26 | A | 1875 | G |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | 6MZ | A | 1618 | 26 | 18,25,26 | 1.09 | 1 (5%) | 16,36,39 | 2.89 | 4 (25%) |
| 26 | 2MG | A | 1835 | 26 | 19,26,27 | 1.28 | 2 (10%) | 20,38,41 | 2.63 | 8 (40%) |
| 26 | PSU | A | 1911 | 26 | 16,21,22 | 1.27 | 3 (18%) | 20,30,33 | 3.31 | 5 (25%) |
| 26 | 3TD | A | 1915 | 26 | 16,22,23 | 3.16 | 7 (43%) | 19,32,35 | 2.11 | 5 (26%) |
| 26 | PSU | A | 1917 | 26 | 16,21,22 | 1.16 | 2 (12%) | 20,30,33 | 3.68 | 6 (30%) |
| 26 | 5MU | A | 1939 | 26 | 14,22,23 | 0.69 | 0 | 16,32,35 | 2.22 | 3 (18%) |
| 26 | 5MC | A | 1962 | 26 | 15,22,23 | 1.24 | 1 (6%) | 17,32,35 | 1.65 | 2 (11%) |
| 26 | 6MZ | A | 2030 | 26 | 18,25,26 | 1.12 | 1 (5%) | 16,36,39 | 2.08 | 5 (31%) |
| 26 | G7M | A | 2069 | 26 | 19,26,27 | 1.43 | 4 (21%) | 19,39,42 | 2.53 | 9 (47%) |
| 26 | OMG | A | 2251 | 26,22 | 18,26,27 | 1.37 | 3 (16%) | 22,38,41 | 2.17 | 6 (27%) |
| 26 | 2MG | A | 2445 | 26 | 19,26,27 | 1.29 | 2 (10%) | 20,38,41 | 2.32 | 6 (30%) |
| 26 | H2U | A | 2449 | 26 | 17,21,22 | 1.25 | 3 (17%) | 21,30,33 | 1.98 | 3 (14%) |
| 26 | PSU | A | 2457 | 26 | 16,21,22 | 1.43 | 2 (12%) | 20,30,33 | 3.50 | 7 (35%) |
| 26 | OMC | A | 2498 | 26 | 15,22,23 | 0.78 | 0 | 19,31,34 | 0.89 | 1 (5%) |
| 26 | 2MA | A | 2503 | 26 | 18,25,26 | 1.75 | 3 (16%) | 17,37,40 | 1.87 | 2 (11%) |
| 26 | PSU | A | 2504 | 26 | 16,21,22 | 1.17 | 2 (12%) | 20,30,33 | 3.50 | 7 (35%) |
| 26 | OMU | A | 2552 | 26 | 14,22,23 | 0.81 | 1 (7%) | 18,31,34 | 2.16 | 1 (5%) |
| 26 | PSU | A | 2580 | 26 | 16,21,22 | 1.44 | 2 (12%) | 20,30,33 | 3.53 | 6 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | PSU | A | 2604 | 26 | 16,21,22 | 1.19 | 2 (12%) | 20,30,33 | 3.37 | 6 (30%) |
| 26 | PSU | A | 2605 | 26 | 16,21,22 | 1.44 | 3 (18%) | 20,30,33 | 3.41 | 6 (30%) |
| 26 | 1MG | A | 745 | 26 | 18,26,27 | 1.61 | 3 (16%) | 18,39,42 | 2.16 | 5 (27%) |
| 26 | PSU | A | 746 | 26 | 16,21,22 | 1.63 | 1 (6%) | 20,30,33 | 3.59 | 7 (35%) |
| 26 | 5MU | A | 747 | 26 | 14,22,23 | 0.75 | 0 | 16,32,35 | 2.40 | 2 (12%) |
| 26 | PSU | A | 955 | 26 | 16,21,22 | 1.28 | 2 (12%) | 20,30,33 | 3.46 | 6 (30%) |
| 1 | 2MG | a | 1207 | 1 | 19,26,27 | 1.26 | 2 (10%) | 20,38,41 | 2.28 | 7 (35%) |
| 1 | 4OC | a | 1402 | 1 | 16,23,24 | 0.72 | 0 | 19,32,35 | 1.19 | 1 (5%) |
| 1 | 5MC | a | 1407 | 1 | 15,22,23 | 1.45 | 1 (6%) | 17,32,35 | 0.93 | 0 |
| 1 | UR3 | a | 1498 | 1 | 14,22,23 | 0.76 | 0 | 16,32,35 | 0.89 | 1 (6%) |
| 1 | 2MG | a | 1516 | 1 | 19,26,27 | 1.31 | 2 (10%) | 20,38,41 | 2.24 | 7 (35%) |
| 1 | MA6 | a | 1518 | 1 | 16,26,27 | 0.99 | 1 (6%) | 18,38,41 | 2.78 | 7 (38%) |
| 1 | MA6 | a | 1519 | 1 | 16,26,27 | 1.00 | 1 (6%) | 18,38,41 | 2.71 | 5 (27%) |
| 1 | PSU | a | 516 | 1 | 16,21,22 | 1.18 | 1 (6%) | 20,30,33 | 3.52 | 6 (30%) |
| 1 | G7M | a | 527 | 1 | 19,26,27 | 1.36 | 3 (15%) | 19,39,42 | 2.82 | 10 (52%) |
| 1 | 2MG | a | 966 | 1 | 19,26,27 | 1.24 | 2 (10%) | 20,38,41 | 2.21 | 7 (35%) |
| 1 | 5MC | a | 967 | 1 | 15,22,23 | 1.44 | 1 (6%) | 17,32,35 | 0.97 | 1 (5%) |
| 22 | H2U | v | 20 | 22 | 17,21,22 | 1.08 | 2 (11%) | 21,30,33 | 1.79 | 3 (14%) |
| 22 | 5MU | v | 54 | 22 | 14,22,23 | 0.84 | 1 (7%) | 16,32,35 | 2.38 | 2 (12%) |
| 22 | PSU | v | 55 | 22 | 16,21,22 | 1.32 | 3 (18%) | 20,30,33 | 3.49 | 8 (40%) |
| 22 | 4SU | v | 8 | 22 | 14,21,22 | 1.32 | 1 (7%) | 15,30,33 | 1.50 | 2 (13%) |
| 24 | H2U | y | 19 | 24 | 17,21,22 | 1.32 | 3 (17%) | 21,30,33 | 3.17 | 5 (23%) |
| 24 | 6IA | y | 37 | 24 | 21,29,30 | 0.99 | 1 (4%) | 21,41,44 | 2.96 | 3 (14%) |
| 24 | 5MU | y | 54 | 24 | 14,22,23 | 0.70 | 0 | 16,32,35 | 2.36 | 3 (18%) |
| 24 | PSU | y | 55 | 24 | 16,21,22 | 1.64 | 3 (18%) | 20,30,33 | 3.72 | 8 (40%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 26 | 6MZ | A | 1618 | 26 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | 2MG | A | 1835 | 26 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | PSU | A | 1911 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | 3TD | A | 1915 | 26 | - | 1/7/25/26 | 0/2/2/2 |
| 26 | PSU | A | 1917 | 26 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|-----------|---------|
| 26 | 5MU | A | 1939 | 26 | - | 0/3/25/26 | 0/2/2/2 |
| 26 | 5MC | A | 1962 | 26 | - | 0/3/25/26 | 0/2/2/2 |
| 26 | 6MZ | A | 2030 | 26 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | G7M | A | 2069 | 26 | 2/2/5/5 | 0/3/25/26 | 0/3/3/3 |
| 26 | OMG | A | 2251 | 26,22 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | 2MG | A | 2445 | 26 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | H2U | A | 2449 | 26 | - | 0/7/38/39 | 0/2/2/2 |
| 26 | PSU | A | 2457 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | OMC | A | 2498 | 26 | - | 0/5/27/28 | 0/2/2/2 |
| 26 | 2MA | A | 2503 | 26 | - | 0/3/25/26 | 0/3/3/3 |
| 26 | PSU | A | 2504 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | OMU | A | 2552 | 26 | - | 0/5/27/28 | 0/2/2/2 |
| 26 | PSU | A | 2580 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | PSU | A | 2604 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | PSU | A | 2605 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | 1MG | A | 745 | 26 | - | 0/3/25/26 | 0/3/3/3 |
| 26 | PSU | A | 746 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | 5MU | A | 747 | 26 | - | 0/3/25/26 | 0/2/2/2 |
| 26 | PSU | A | 955 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | a | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 4OC | a | 1402 | 1 | - | 0/7/29/30 | 0/2/2/2 |
| 1 | 5MC | a | 1407 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | UR3 | a | 1498 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | 2MG | a | 1516 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | MA6 | a | 1518 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | MA6 | a | 1519 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | PSU | a | 516 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | G7M | a | 527 | 1 | 2/2/5/5 | 0/3/25/26 | 0/3/3/3 |
| 1 | 2MG | a | 966 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 5MC | a | 967 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 22 | H2U | v | 20 | 22 | - | 0/7/38/39 | 0/2/2/2 |
| 22 | 5MU | v | 54 | 22 | - | 0/3/25/26 | 0/2/2/2 |
| 22 | PSU | v | 55 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 4SU | v | 8 | 22 | - | 0/3/25/26 | 0/2/2/2 |
| 24 | H2U | y | 19 | 24 | - | 0/7/38/39 | 0/2/2/2 |
| 24 | 6IA | y | 37 | 24 | - | 0/9/31/32 | 0/3/3/3 |
| 24 | 5MU | y | 54 | 24 | - | 0/3/25/26 | 0/2/2/2 |
| 24 | PSU | y | 55 | 24 | - | 0/7/25/26 | 0/2/2/2 |

All (78) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 26 | A | 746 | PSU | C5-C1' | -5.31 | 1.47 | 1.52 |
| 26 | A | 2457 | PSU | C5-C1' | -4.37 | 1.48 | 1.52 |
| 26 | A | 2580 | PSU | C5-C1' | -4.28 | 1.48 | 1.52 |
| 26 | A | 2605 | PSU | C5-C1' | -4.28 | 1.48 | 1.52 |
| 22 | v | 8 | 4SU | C4-S4 | -4.14 | 1.59 | 1.67 |
| 24 | y | 55 | PSU | C5-C1' | -3.67 | 1.49 | 1.52 |
| 26 | A | 1915 | 3TD | O4-C4 | -3.54 | 1.15 | 1.24 |
| 26 | A | 955 | PSU | C5-C1' | -3.38 | 1.49 | 1.52 |
| 24 | y | 55 | PSU | C2-N1 | -3.36 | 1.31 | 1.38 |
| 24 | y | 19 | H2U | C2-N3 | -3.30 | 1.32 | 1.38 |
| 26 | A | 1911 | PSU | C5-C1' | -3.15 | 1.49 | 1.52 |
| 26 | A | 2604 | PSU | C5-C1' | -3.05 | 1.49 | 1.52 |
| 22 | v | 55 | PSU | C5-C1' | -2.98 | 1.49 | 1.52 |
| 26 | A | 2069 | G7M | O5'-C5' | -2.93 | 1.40 | 1.44 |
| 26 | A | 2449 | H2U | C2-N3 | -2.89 | 1.32 | 1.38 |
| 26 | A | 2449 | H2U | C4-N3 | -2.79 | 1.33 | 1.37 |
| 26 | A | 2504 | PSU | C5-C1' | -2.76 | 1.49 | 1.52 |
| 24 | y | 55 | PSU | C6-C5 | -2.72 | 1.34 | 1.38 |
| 1 | a | 516 | PSU | C5-C1' | -2.63 | 1.50 | 1.52 |
| 1 | a | 527 | G7M | O2'-C2' | -2.62 | 1.36 | 1.43 |
| 26 | A | 2069 | G7M | O2'-C2' | -2.62 | 1.36 | 1.43 |
| 22 | v | 20 | H2U | C2-N3 | -2.60 | 1.33 | 1.38 |
| 22 | v | 20 | H2U | C4-N3 | -2.55 | 1.33 | 1.37 |
| 22 | v | 55 | PSU | C2-N3 | -2.51 | 1.33 | 1.38 |
| 24 | y | 19 | H2U | O4-C4 | -2.47 | 1.18 | 1.23 |
| 24 | y | 19 | H2U | C4-N3 | -2.47 | 1.33 | 1.37 |
| 26 | A | 2251 | OMG | O5'-C5' | -2.36 | 1.41 | 1.44 |
| 26 | A | 1917 | PSU | C5-C1' | -2.34 | 1.50 | 1.52 |
| 26 | A | 2449 | H2U | C2-N1 | -2.28 | 1.32 | 1.35 |
| 26 | A | 2605 | PSU | C2-N3 | -2.17 | 1.33 | 1.38 |
| 22 | v | 55 | PSU | O5'-C5' | -2.16 | 1.41 | 1.44 |
| 26 | A | 2504 | PSU | C2-N3 | -2.14 | 1.33 | 1.38 |
| 26 | A | 1917 | PSU | C2-N1 | -2.12 | 1.34 | 1.38 |
| 26 | A | 1911 | PSU | O4'-C1' | -2.12 | 1.41 | 1.44 |
| 22 | v | 54 | 5MU | O5'-C5' | -2.12 | 1.41 | 1.44 |
| 1 | a | 527 | G7M | O5'-C5' | -2.11 | 1.41 | 1.44 |
| 26 | A | 955 | PSU | C2-N1 | -2.11 | 1.34 | 1.38 |
| 26 | A | 1911 | PSU | C2-N3 | -2.09 | 1.34 | 1.38 |
| 26 | A | 2580 | PSU | O4'-C1' | -2.05 | 1.41 | 1.44 |
| 26 | A | 2604 | PSU | C2-N3 | -2.05 | 1.34 | 1.38 |
| 26 | A | 2552 | OMU | C2-N3 | -2.03 | 1.34 | 1.38 |
| 26 | A | 2605 | PSU | O4'-C1' | -2.02 | 1.41 | 1.44 |
| 26 | A | 1915 | 3TD | O4'-C1' | -2.01 | 1.41 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 26 | A | 2457 | PSU | C2-N3 | -2.00 | 1.34 | 1.38 |
| 26 | A | 1915 | 3TD | C5-C1' | 2.06 | 1.54 | 1.52 |
| 26 | A | 2069 | G7M | C8-N9 | 2.13 | 1.37 | 1.33 |
| 26 | A | 745 | 1MG | C6-N1 | 2.19 | 1.41 | 1.38 |
| 26 | A | 1835 | 2MG | C5-C4 | 3.00 | 1.47 | 1.40 |
| 26 | A | 2251 | OMG | C5-C4 | 3.01 | 1.47 | 1.40 |
| 26 | A | 2445 | 2MG | C5-C4 | 3.09 | 1.47 | 1.40 |
| 1 | a | 1207 | 2MG | C5-C4 | 3.09 | 1.47 | 1.40 |
| 24 | y | 37 | 6IA | C5-C4 | 3.19 | 1.47 | 1.40 |
| 1 | a | 1516 | 2MG | C5-C4 | 3.20 | 1.47 | 1.40 |
| 1 | a | 1519 | MA6 | C5-C4 | 3.23 | 1.47 | 1.40 |
| 1 | a | 966 | 2MG | C5-C4 | 3.28 | 1.47 | 1.40 |
| 1 | a | 1518 | MA6 | C5-C4 | 3.28 | 1.47 | 1.40 |
| 26 | A | 2503 | 2MA | C6-N6 | 3.39 | 1.35 | 1.27 |
| 1 | a | 966 | 2MG | C6-C5 | 3.47 | 1.48 | 1.41 |
| 26 | A | 2503 | 2MA | C5-C4 | 3.57 | 1.48 | 1.40 |
| 26 | A | 2030 | 6MZ | C5-C4 | 3.64 | 1.48 | 1.40 |
| 26 | A | 745 | 1MG | C5-C4 | 3.64 | 1.48 | 1.40 |
| 26 | A | 1618 | 6MZ | C5-C4 | 3.67 | 1.48 | 1.40 |
| 1 | a | 1207 | 2MG | C6-C5 | 3.76 | 1.48 | 1.41 |
| 26 | A | 2069 | G7M | C6-C5 | 3.81 | 1.48 | 1.41 |
| 26 | A | 2251 | OMG | C6-C5 | 3.86 | 1.48 | 1.41 |
| 1 | a | 1516 | 2MG | C6-C5 | 3.95 | 1.48 | 1.41 |
| 26 | A | 1835 | 2MG | C6-C5 | 3.95 | 1.48 | 1.41 |
| 26 | A | 1962 | 5MC | C5-C4 | 3.97 | 1.47 | 1.41 |
| 26 | A | 2445 | 2MG | C6-C5 | 4.01 | 1.49 | 1.41 |
| 1 | a | 527 | G7M | C6-C5 | 4.07 | 1.49 | 1.41 |
| 26 | A | 745 | 1MG | C6-C5 | 4.53 | 1.49 | 1.41 |
| 26 | A | 1915 | 3TD | C4-N3 | 4.65 | 1.45 | 1.38 |
| 1 | a | 1407 | 5MC | C5-C4 | 4.95 | 1.48 | 1.41 |
| 26 | A | 2503 | 2MA | C6-C5 | 5.08 | 1.49 | 1.41 |
| 1 | a | 967 | 5MC | C5-C4 | 5.10 | 1.48 | 1.41 |
| 26 | A | 1915 | 3TD | C6-N1 | 5.45 | 1.46 | 1.34 |
| 26 | A | 1915 | 3TD | C2-N1 | 5.57 | 1.49 | 1.38 |
| 26 | A | 1915 | 3TD | C6-C5 | 7.33 | 1.48 | 1.38 |

All (204) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | a | 516 | PSU | N1-C2-N3 | -9.92 | 121.27 | 128.40 |
| 24 | y | 55 | PSU | N1-C2-N3 | -9.78 | 121.36 | 128.40 |
| 26 | A | 1917 | PSU | C5-C4-N3 | -9.45 | 117.67 | 125.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | A | 1911 | PSU | N1-C2-N3 | -9.38 | 121.65 | 128.40 |
| 26 | A | 1917 | PSU | N1-C2-N3 | -9.22 | 121.76 | 128.40 |
| 26 | A | 746 | PSU | N1-C2-N3 | -9.14 | 121.83 | 128.40 |
| 26 | A | 955 | PSU | C5-C4-N3 | -9.05 | 118.00 | 125.43 |
| 26 | A | 2580 | PSU | C5-C4-N3 | -9.04 | 118.02 | 125.43 |
| 22 | v | 55 | PSU | N1-C2-N3 | -8.95 | 121.97 | 128.40 |
| 26 | A | 2605 | PSU | N1-C2-N3 | -8.92 | 121.98 | 128.40 |
| 26 | A | 2580 | PSU | N1-C2-N3 | -8.92 | 121.98 | 128.40 |
| 26 | A | 2457 | PSU | N1-C2-N3 | -8.87 | 122.02 | 128.40 |
| 26 | A | 2604 | PSU | C5-C4-N3 | -8.83 | 118.18 | 125.43 |
| 26 | A | 2504 | PSU | N1-C2-N3 | -8.61 | 122.20 | 128.40 |
| 26 | A | 2457 | PSU | C5-C4-N3 | -8.57 | 118.40 | 125.43 |
| 26 | A | 746 | PSU | C5-C4-N3 | -8.54 | 118.43 | 125.43 |
| 24 | y | 19 | H2U | C4-N3-C2 | -8.38 | 118.63 | 125.81 |
| 26 | A | 2504 | PSU | C5-C4-N3 | -8.37 | 118.57 | 125.43 |
| 26 | A | 2604 | PSU | N1-C2-N3 | -8.03 | 122.62 | 128.40 |
| 26 | A | 955 | PSU | N1-C2-N3 | -8.02 | 122.63 | 128.40 |
| 1 | a | 516 | PSU | C5-C4-N3 | -7.85 | 118.99 | 125.43 |
| 26 | A | 2605 | PSU | C5-C4-N3 | -7.66 | 119.14 | 125.43 |
| 22 | v | 55 | PSU | C5-C4-N3 | -7.35 | 119.40 | 125.43 |
| 24 | y | 37 | 6IA | N3-C2-N1 | -7.23 | 122.56 | 128.86 |
| 26 | A | 1911 | PSU | C5-C4-N3 | -7.08 | 119.62 | 125.43 |
| 1 | a | 1519 | MA6 | N3-C2-N1 | -6.98 | 122.78 | 128.86 |
| 24 | y | 19 | H2U | C5-C6-N1 | -6.82 | 103.61 | 110.70 |
| 1 | a | 1518 | MA6 | N3-C2-N1 | -6.74 | 122.99 | 128.86 |
| 26 | A | 2449 | H2U | C5-C6-N1 | -6.25 | 104.21 | 110.70 |
| 24 | y | 55 | PSU | C5-C4-N3 | -6.04 | 120.47 | 125.43 |
| 26 | A | 747 | 5MU | C5-C4-N3 | -5.89 | 118.74 | 125.24 |
| 26 | A | 1618 | 6MZ | N3-C2-N1 | -5.84 | 123.78 | 128.86 |
| 22 | v | 54 | 5MU | C5-C4-N3 | -5.57 | 119.09 | 125.24 |
| 1 | a | 527 | G7M | C5-C6-N1 | -5.52 | 115.62 | 123.48 |
| 22 | v | 20 | H2U | C5-C6-N1 | -5.42 | 105.07 | 110.70 |
| 26 | A | 1915 | 3TD | C5-C1'-C2' | -5.37 | 106.29 | 115.55 |
| 26 | A | 2069 | G7M | C5-C6-N1 | -5.31 | 115.92 | 123.48 |
| 26 | A | 1939 | 5MU | C5-C4-N3 | -5.31 | 119.38 | 125.24 |
| 26 | A | 2449 | H2U | C4-N3-C2 | -5.23 | 121.33 | 125.81 |
| 26 | A | 745 | 1MG | C6-C5-C4 | -5.05 | 116.44 | 119.92 |
| 24 | y | 54 | 5MU | C5-C4-N3 | -4.95 | 119.78 | 125.24 |
| 1 | a | 1519 | MA6 | C4-C5-N7 | -4.92 | 104.65 | 109.41 |
| 24 | y | 55 | PSU | C5-C1'-C2' | -4.91 | 107.09 | 115.55 |
| 26 | A | 1835 | 2MG | CM2-N2-C2 | -4.85 | 117.73 | 123.63 |
| 26 | A | 2030 | 6MZ | C4-C5-N7 | -4.85 | 104.73 | 109.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24 | y | 19 | H2U | O4-C4-C5 | -4.56 | 112.36 | 122.08 |
| 26 | A | 746 | PSU | C5-C6-N1 | -4.48 | 118.59 | 124.39 |
| 26 | A | 2445 | 2MG | CM2-N2-C2 | -4.46 | 118.21 | 123.63 |
| 1 | a | 1518 | MA6 | C4-C5-N7 | -4.41 | 105.15 | 109.41 |
| 26 | A | 2457 | PSU | C5-C6-N1 | -4.35 | 118.75 | 124.39 |
| 26 | A | 2605 | PSU | C5-C6-N1 | -4.33 | 118.77 | 124.39 |
| 26 | A | 1618 | 6MZ | C9-N6-C6 | -4.31 | 119.16 | 122.85 |
| 26 | A | 955 | PSU | C5-C1'-C2' | -4.12 | 108.45 | 115.55 |
| 1 | a | 1518 | MA6 | C9-N6-C6 | -4.05 | 107.25 | 119.51 |
| 26 | A | 2251 | OMG | C5-C6-N1 | -4.03 | 117.74 | 123.48 |
| 26 | A | 2030 | 6MZ | N3-C2-N1 | -4.01 | 125.37 | 128.86 |
| 26 | A | 1911 | PSU | C5-C6-N1 | -3.91 | 119.31 | 124.39 |
| 1 | a | 966 | 2MG | C5-C6-N1 | -3.90 | 117.93 | 123.48 |
| 26 | A | 2580 | PSU | C5-C6-N1 | -3.88 | 119.36 | 124.39 |
| 1 | a | 1516 | 2MG | C5-C6-N1 | -3.86 | 117.99 | 123.48 |
| 26 | A | 2604 | PSU | C5-C6-N1 | -3.84 | 119.41 | 124.39 |
| 26 | A | 745 | 1MG | C1'-N9-C4 | -3.83 | 120.02 | 126.64 |
| 22 | v | 20 | H2U | C4-N3-C2 | -3.82 | 122.54 | 125.81 |
| 1 | a | 1402 | 4OC | CM4-N4-C4 | -3.81 | 119.65 | 122.94 |
| 26 | A | 2504 | PSU | C5-C1'-C2' | -3.79 | 109.01 | 115.55 |
| 26 | A | 746 | PSU | C5-C1'-C2' | -3.78 | 109.03 | 115.55 |
| 1 | a | 1519 | MA6 | C10-N6-C6 | -3.77 | 108.10 | 119.51 |
| 1 | a | 1207 | 2MG | C5-C6-N1 | -3.76 | 118.14 | 123.48 |
| 26 | A | 2504 | PSU | C5-C6-N1 | -3.75 | 119.53 | 124.39 |
| 26 | A | 2445 | 2MG | C5-C6-N1 | -3.75 | 118.14 | 123.48 |
| 26 | A | 2251 | OMG | C6-C5-C4 | -3.75 | 117.12 | 120.84 |
| 22 | v | 55 | PSU | C5-C6-N1 | -3.68 | 119.62 | 124.39 |
| 1 | a | 1518 | MA6 | N1-C6-N6 | -3.67 | 113.11 | 117.00 |
| 1 | a | 1516 | 2MG | C6-C5-C4 | -3.65 | 117.22 | 120.84 |
| 26 | A | 1835 | 2MG | C6-C5-C4 | -3.60 | 117.26 | 120.84 |
| 26 | A | 1915 | 3TD | C5-C6-N1 | -3.58 | 119.74 | 124.39 |
| 1 | a | 516 | PSU | C5-C6-N1 | -3.55 | 119.79 | 124.39 |
| 26 | A | 2251 | OMG | C4-C5-N7 | -3.50 | 106.03 | 109.41 |
| 1 | a | 1207 | 2MG | C6-C5-C4 | -3.44 | 117.43 | 120.84 |
| 1 | a | 1519 | MA6 | C10-N6-C9 | -3.41 | 105.01 | 116.03 |
| 26 | A | 2605 | PSU | C5-C1'-C2' | -3.36 | 109.75 | 115.55 |
| 26 | A | 2445 | 2MG | C4-C5-N7 | -3.31 | 106.21 | 109.41 |
| 26 | A | 955 | PSU | C5-C6-N1 | -3.27 | 120.14 | 124.39 |
| 26 | A | 1835 | 2MG | C5-C6-N1 | -3.24 | 118.87 | 123.48 |
| 26 | A | 1835 | 2MG | C4-C5-N7 | -3.13 | 106.38 | 109.41 |
| 1 | a | 1207 | 2MG | CM2-N2-C2 | -3.12 | 119.83 | 123.63 |
| 22 | v | 55 | PSU | C5-C1'-C2' | -3.11 | 110.19 | 115.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26 | A | 2251 | OMG | N3-C2-N1 | -3.02 | 123.04 | 127.46 |
| 26 | A | 2445 | 2MG | C6-C5-C4 | -3.00 | 117.86 | 120.84 |
| 1 | a | 1516 | 2MG | CM2-N2-C2 | -2.97 | 120.01 | 123.63 |
| 26 | A | 745 | 1MG | C4-C5-N7 | -2.97 | 106.54 | 109.41 |
| 1 | a | 527 | G7M | C4'-O4'-C1' | -2.92 | 106.67 | 109.77 |
| 26 | A | 2030 | 6MZ | C9-N6-C6 | -2.91 | 120.36 | 122.85 |
| 22 | v | 8 | 4SU | C5-C4-N3 | -2.88 | 120.10 | 123.73 |
| 1 | a | 966 | 2MG | C6-C5-C4 | -2.86 | 118.00 | 120.84 |
| 1 | a | 1207 | 2MG | C4-C5-N7 | -2.86 | 106.64 | 109.41 |
| 24 | y | 37 | 6IA | C4-C5-N7 | -2.85 | 106.65 | 109.41 |
| 26 | A | 1962 | 5MC | C5-C6-N1 | -2.81 | 119.11 | 122.15 |
| 26 | A | 1618 | 6MZ | C4-C5-N7 | -2.77 | 106.73 | 109.41 |
| 26 | A | 2069 | G7M | C4'-O4'-C1' | -2.75 | 106.84 | 109.77 |
| 26 | A | 1917 | PSU | C5-C6-N1 | -2.70 | 120.89 | 124.39 |
| 1 | a | 1516 | 2MG | C4-C5-N7 | -2.69 | 106.81 | 109.41 |
| 26 | A | 1939 | 5MU | C5-C6-N1 | -2.68 | 119.25 | 122.15 |
| 26 | A | 1835 | 2MG | N3-C2-N1 | -2.46 | 122.51 | 126.23 |
| 26 | A | 2503 | 2MA | C4-C5-N7 | -2.39 | 107.10 | 109.41 |
| 26 | A | 2498 | OMC | CM2-O2'-C2' | -2.33 | 108.18 | 114.54 |
| 1 | a | 527 | G7M | N3-C2-N1 | -2.30 | 124.10 | 127.46 |
| 1 | a | 1518 | MA6 | C10-N6-C9 | -2.29 | 108.61 | 116.03 |
| 24 | y | 55 | PSU | O2'-C2'-C1' | -2.28 | 107.05 | 112.21 |
| 1 | a | 1207 | 2MG | N3-C2-N1 | -2.24 | 122.85 | 126.23 |
| 26 | A | 2449 | H2U | O2-C2-N1 | -2.15 | 120.43 | 123.12 |
| 1 | a | 1516 | 2MG | N3-C2-N1 | -2.12 | 123.03 | 126.23 |
| 26 | A | 2069 | G7M | N3-C2-N1 | -2.11 | 124.38 | 127.46 |
| 1 | a | 966 | 2MG | N3-C2-N1 | -2.10 | 123.06 | 126.23 |
| 26 | A | 2457 | PSU | C5-C1'-C2' | -2.09 | 111.95 | 115.55 |
| 26 | A | 2604 | PSU | C5-C1'-C2' | -2.03 | 112.05 | 115.55 |
| 26 | A | 745 | 1MG | O2'-C2'-C1' | -2.02 | 105.30 | 111.61 |
| 1 | a | 967 | 5MC | N4-C4-N3 | 2.01 | 119.97 | 117.00 |
| 22 | v | 55 | PSU | O4'-C1'-C2' | 2.06 | 107.76 | 104.45 |
| 1 | a | 966 | 2MG | C1'-N9-C4 | 2.08 | 130.23 | 126.64 |
| 24 | y | 19 | H2U | O4-C4-N3 | 2.15 | 123.70 | 120.41 |
| 26 | A | 746 | PSU | O4'-C1'-C5 | 2.16 | 113.28 | 109.93 |
| 1 | a | 516 | PSU | O4'-C1'-C2' | 2.18 | 107.95 | 104.45 |
| 26 | A | 2457 | PSU | O4'-C1'-C2' | 2.19 | 107.97 | 104.45 |
| 1 | a | 527 | G7M | O4'-C4'-C5' | 2.25 | 117.01 | 109.40 |
| 22 | v | 20 | H2U | C5-C4-N3 | 2.29 | 119.00 | 116.72 |
| 24 | y | 55 | PSU | O4'-C1'-C2' | 2.29 | 108.13 | 104.45 |
| 26 | A | 1915 | 3TD | O4'-C1'-C5 | 2.30 | 113.50 | 109.93 |
| 26 | A | 2069 | G7M | C5'-C4'-C3' | 2.30 | 124.07 | 115.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 26 | A | 2580 | PSU | O4'-C1'-C2' | 2.31 | 108.16 | 104.45 |
| 1 | a | 1498 | UR3 | C3U-N3-C4 | 2.33 | 121.24 | 118.15 |
| 26 | A | 2069 | G7M | C1'-N9-C4 | 2.34 | 130.68 | 126.64 |
| 24 | y | 54 | 5MU | C5M-C5-C6 | 2.35 | 123.36 | 118.67 |
| 26 | A | 2504 | PSU | O4'-C1'-C5 | 2.41 | 113.66 | 109.93 |
| 26 | A | 2030 | 6MZ | C1'-N9-C4 | 2.43 | 130.84 | 126.64 |
| 1 | a | 527 | G7M | C5'-C4'-C3' | 2.56 | 125.03 | 115.29 |
| 24 | y | 55 | PSU | C6-N1-C2 | 2.57 | 119.47 | 115.36 |
| 26 | A | 1917 | PSU | C4-C5-C1' | 2.67 | 126.32 | 121.15 |
| 26 | A | 2069 | G7M | O3'-C3'-C2' | 2.77 | 120.71 | 111.83 |
| 1 | a | 1518 | MA6 | C5-C6-N6 | 3.12 | 129.55 | 122.58 |
| 1 | a | 527 | G7M | O3'-C3'-C4' | 3.22 | 120.50 | 111.09 |
| 1 | a | 527 | G7M | O3'-C3'-C2' | 3.29 | 122.37 | 111.83 |
| 26 | A | 1915 | 3TD | C6-N1-C2 | 3.35 | 120.72 | 115.36 |
| 26 | A | 1835 | 2MG | C6-N1-C2 | 3.46 | 121.37 | 115.18 |
| 26 | A | 2030 | 6MZ | C2-N1-C6 | 3.46 | 118.79 | 116.53 |
| 26 | A | 2445 | 2MG | C6-N1-C2 | 3.54 | 121.52 | 115.18 |
| 26 | A | 1915 | 3TD | C5-C4-N3 | 3.57 | 121.72 | 118.69 |
| 26 | A | 1835 | 2MG | N2-C2-N1 | 3.57 | 120.42 | 116.95 |
| 1 | a | 966 | 2MG | N2-C2-N3 | 3.66 | 120.51 | 116.95 |
| 26 | A | 955 | PSU | C6-N1-C2 | 3.69 | 121.26 | 115.36 |
| 26 | A | 1917 | PSU | C6-N1-C2 | 3.77 | 121.39 | 115.36 |
| 26 | A | 2069 | G7M | O3'-C3'-C4' | 3.86 | 122.36 | 111.09 |
| 1 | a | 1207 | 2MG | C6-N1-C2 | 3.87 | 122.11 | 115.18 |
| 1 | a | 1516 | 2MG | C6-N1-C2 | 3.96 | 122.27 | 115.18 |
| 26 | A | 2604 | PSU | C6-N1-C2 | 3.97 | 121.72 | 115.36 |
| 26 | A | 2069 | G7M | C2-N3-C4 | 4.01 | 119.85 | 115.16 |
| 1 | a | 966 | 2MG | C6-N1-C2 | 4.05 | 122.44 | 115.18 |
| 22 | v | 55 | PSU | C6-N1-C2 | 4.08 | 121.89 | 115.36 |
| 26 | A | 2580 | PSU | C6-N1-C2 | 4.11 | 121.93 | 115.36 |
| 1 | a | 527 | G7M | C1'-N9-C4 | 4.14 | 133.79 | 126.64 |
| 22 | v | 55 | PSU | O4'-C1'-C5 | 4.16 | 116.38 | 109.93 |
| 26 | A | 2504 | PSU | C6-N1-C2 | 4.18 | 122.05 | 115.36 |
| 26 | A | 746 | PSU | C6-N1-C2 | 4.29 | 122.23 | 115.36 |
| 26 | A | 2251 | OMG | C6-N1-C2 | 4.30 | 122.25 | 116.06 |
| 22 | v | 8 | 4SU | C2-N3-C4 | 4.36 | 121.55 | 115.11 |
| 26 | A | 2457 | PSU | C6-N1-C2 | 4.39 | 122.38 | 115.36 |
| 26 | A | 2605 | PSU | C6-N1-C2 | 4.39 | 122.39 | 115.36 |
| 26 | A | 1911 | PSU | C6-N1-C2 | 4.40 | 122.41 | 115.36 |
| 1 | a | 516 | PSU | C6-N1-C2 | 4.42 | 122.43 | 115.36 |
| 26 | A | 2069 | G7M | C6-N1-C2 | 4.53 | 122.58 | 116.06 |
| 1 | a | 527 | G7M | C6-N1-C2 | 4.62 | 122.70 | 116.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | a | 1518 | MA6 | C2-N1-C6 | 4.66 | 123.25 | 111.82 |
| 26 | A | 1962 | 5MC | N4-C4-N3 | 4.71 | 123.95 | 117.00 |
| 1 | a | 1519 | MA6 | C2-N1-C6 | 4.81 | 123.62 | 111.82 |
| 26 | A | 2251 | OMG | C2-N3-C4 | 4.99 | 120.99 | 115.16 |
| 1 | a | 527 | G7M | C2-N3-C4 | 5.01 | 121.01 | 115.16 |
| 26 | A | 745 | 1MG | C2-N3-C4 | 5.05 | 121.05 | 115.16 |
| 24 | y | 55 | PSU | C4-N3-C2 | 5.09 | 119.61 | 115.16 |
| 1 | a | 1516 | 2MG | C2-N3-C4 | 5.11 | 120.95 | 115.11 |
| 1 | a | 966 | 2MG | C2-N3-C4 | 5.13 | 120.97 | 115.11 |
| 26 | A | 2445 | 2MG | C2-N3-C4 | 5.56 | 121.46 | 115.11 |
| 1 | a | 1207 | 2MG | C2-N3-C4 | 5.59 | 121.49 | 115.11 |
| 26 | A | 2605 | PSU | C4-N3-C2 | 5.74 | 120.18 | 115.16 |
| 26 | A | 1911 | PSU | C4-N3-C2 | 5.92 | 120.33 | 115.16 |
| 26 | A | 1939 | 5MU | C4-N3-C2 | 6.12 | 120.52 | 115.16 |
| 26 | A | 2457 | PSU | C4-N3-C2 | 6.13 | 120.52 | 115.16 |
| 26 | A | 746 | PSU | C4-N3-C2 | 6.14 | 120.53 | 115.16 |
| 26 | A | 2604 | PSU | C4-N3-C2 | 6.27 | 120.64 | 115.16 |
| 26 | A | 2504 | PSU | C4-N3-C2 | 6.37 | 120.73 | 115.16 |
| 22 | v | 55 | PSU | C4-N3-C2 | 6.39 | 120.74 | 115.16 |
| 26 | A | 955 | PSU | C4-N3-C2 | 6.43 | 120.78 | 115.16 |
| 26 | A | 2503 | 2MA | C2-N3-C4 | 6.45 | 120.98 | 115.41 |
| 1 | a | 516 | PSU | C4-N3-C2 | 6.57 | 120.91 | 115.16 |
| 26 | A | 2580 | PSU | C4-N3-C2 | 6.63 | 120.95 | 115.16 |
| 26 | A | 1835 | 2MG | C2-N3-C4 | 6.83 | 122.91 | 115.11 |
| 24 | y | 54 | 5MU | C4-N3-C2 | 6.98 | 121.26 | 115.16 |
| 26 | A | 747 | 5MU | C4-N3-C2 | 7.05 | 121.32 | 115.16 |
| 22 | v | 54 | 5MU | C4-N3-C2 | 7.15 | 121.42 | 115.16 |
| 24 | y | 19 | H2U | C5-C4-N3 | 7.27 | 123.94 | 116.72 |
| 26 | A | 1917 | PSU | C4-N3-C2 | 7.67 | 121.86 | 115.16 |
| 26 | A | 1618 | 6MZ | C2-N1-C6 | 8.38 | 121.99 | 116.53 |
| 24 | y | 55 | PSU | O4'-C1'-C5 | 8.39 | 122.93 | 109.93 |
| 26 | A | 2552 | OMU | C4-N3-C2 | 8.48 | 121.41 | 114.13 |
| 24 | y | 37 | 6IA | C2-N1-C6 | 10.51 | 123.38 | 116.53 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 1 | a | 527 | G7M | C4' |
| 1 | a | 527 | G7M | C3' |
| 26 | A | 2069 | G7M | C4' |
| 26 | A | 2069 | G7M | C3' |

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 26 | A | 1915 | 3TD | O4'-C1'-C5-C4 |

There are no ring outliers.

8 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 26 | A | 1915 | 3TD | 1 | 0 |
| 26 | A | 1939 | 5MU | 1 | 0 |
| 26 | A | 1962 | 5MC | 1 | 0 |
| 26 | A | 2030 | 6MZ | 1 | 0 |
| 26 | A | 2457 | PSU | 1 | 0 |
| 26 | A | 2504 | PSU | 1 | 0 |
| 26 | A | 2604 | PSU | 1 | 0 |
| 26 | A | 745 | 1MG | 2 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 59 | FME | v | 101 | 22 | 9,9,10 | 1.25 | 1 (11%) | 7,9,11 | 1.67 | 2 (28%) |
| 60 | SEC | y | 701 | 24 | 3,5,6 | 0.99 | 0 | 2,5,7 | 1.34 | 0 |
| 61 | GNP | z | 701 | 62 | 27,34,34 | 2.66 | 6 (22%) | 26,54,54 | 1.09 | 4 (15%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 59 | FME | v | 101 | 22 | - | 1/6/9/11 | 0/0/0/0 |
| 60 | SEC | y | 701 | 24 | - | 0/0/4/6 | 0/0/0/0 |
| 61 | GNP | z | 701 | 62 | - | 0/16/38/38 | 0/3/3/3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 61 | z | 701 | GNP | C4-N9 | -10.50 | 1.33 | 1.47 |
| 61 | z | 701 | GNP | C8-N9 | -4.02 | 1.34 | 1.46 |
| 61 | z | 701 | GNP | C5-C6 | -3.34 | 1.47 | 1.53 |
| 61 | z | 701 | GNP | C2-N1 | -2.33 | 1.34 | 1.44 |
| 59 | v | 101 | FME | CA-C | 2.50 | 1.53 | 1.50 |
| 61 | z | 701 | GNP | PG-N3B | 4.01 | 1.74 | 1.63 |
| 61 | z | 701 | GNP | PB-N3B | 4.25 | 1.74 | 1.63 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 59 | v | 101 | FME | CB-CA-C | -2.78 | 107.07 | 111.65 |
| 61 | z | 701 | GNP | O3G-PG-O1G | -2.78 | 106.34 | 113.41 |
| 61 | z | 701 | GNP | C2'-C1'-N9 | -2.17 | 107.72 | 113.34 |
| 61 | z | 701 | GNP | PA-O3A-PB | -2.07 | 125.07 | 132.38 |
| 61 | z | 701 | GNP | C3'-C2'-C1' | 2.15 | 105.56 | 101.43 |
| 59 | v | 101 | FME | CA-N-CN | 2.51 | 126.68 | 122.82 |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 59 | v | 101 | FME | O1-CN-N-CA |

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.