



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2024 – 01:21 PM EST

PDB ID : 5J8B
Title : Crystal structure of Elongation Factor 4 (EF-4/LepA) in complex with GDCPCP bound to the Thermus thermophilus 70S ribosome
Authors : Gagnon, M.G.; Lin, J.; Steitz, T.A.
Deposited on : 2016-04-07
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

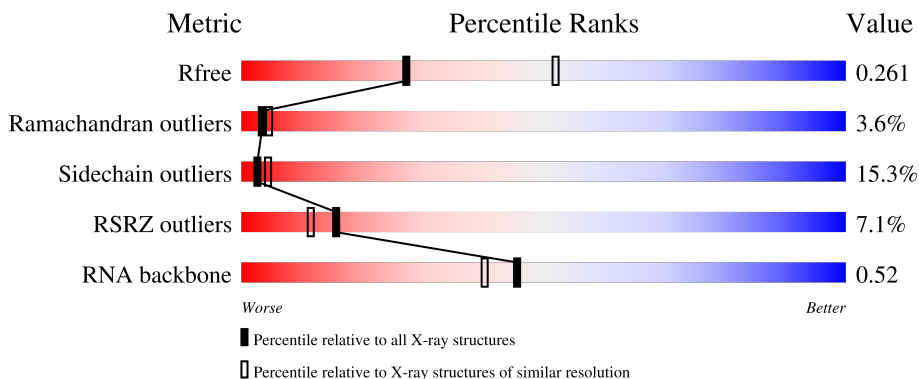
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



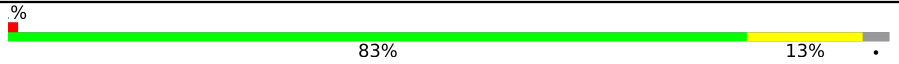

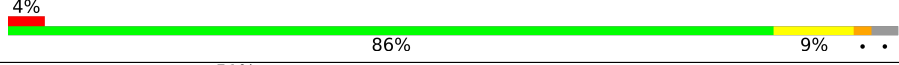
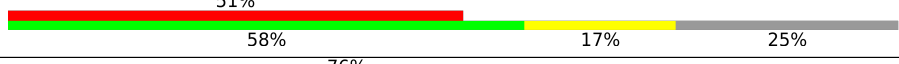

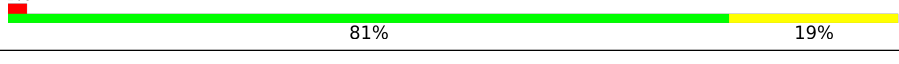
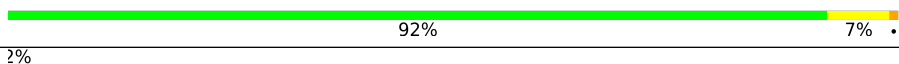
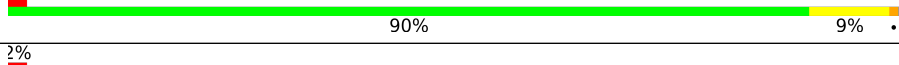
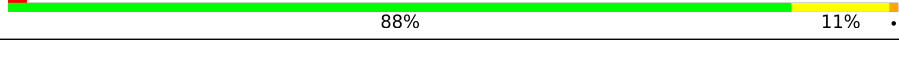

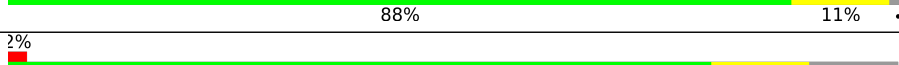
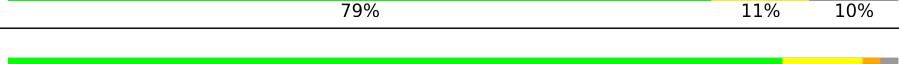
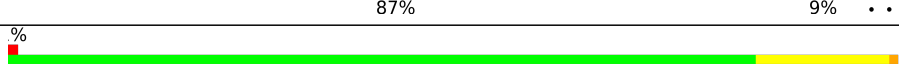
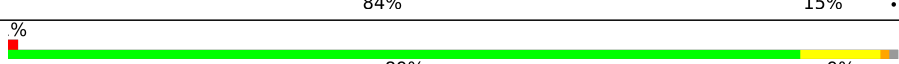
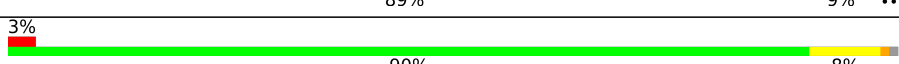
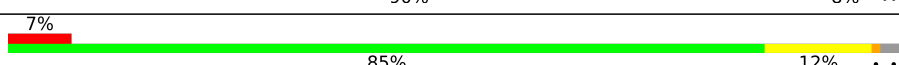

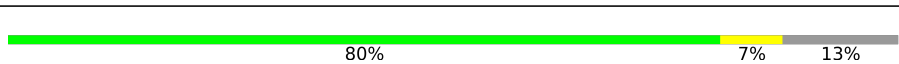
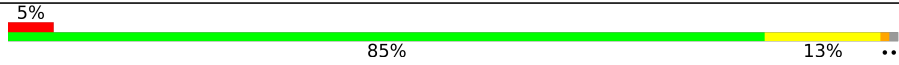


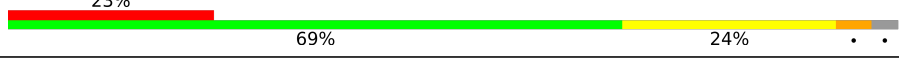
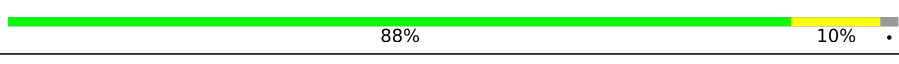
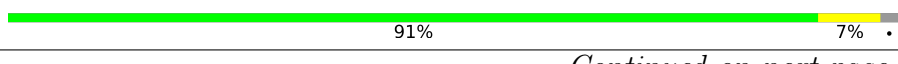

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 3163 (2.60-2.60) |
| Ramachandran outliers | 138981 | 3455 (2.60-2.60) |
| Sidechain outliers | 138945 | 3455 (2.60-2.60) |
| RSRZ outliers | 127900 | 3104 (2.60-2.60) |
| RNA backbone | 3102 | 1040 (2.90-2.30) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 2915 | 5% (Poor fit) 78% (0 outliers), 18% (1 outlier), 1% (2 outliers), 1% (3+ outliers) |
| 2 | B | 121 | 87% (0 outliers), 12% (1 outlier), 1% (2 outliers), 1% (3+ outliers) |
| 3 | C | 228 | 26% (Poor fit), 45% (0 outliers), 14% (1 outlier), 15% (2 outliers), 1% (3+ outliers), 40% (Not modelled) |
| 4 | D | 276 | 88% (0 outliers), 11% (1 outlier), 1% (2 outliers), 1% (3+ outliers) |
| 5 | E | 206 | 2% (Poor fit), 85% (0 outliers), 13% (1 outlier), 1% (2 outliers), 1% (3+ outliers) |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 6 | F | 210 |  % 83% 13% |
| 7 | G | 182 |  5% 81% 17% |
| 8 | H | 180 |  4% 86% 9% |
| 9 | J | 173 |  51% 58% 17% 25% |
| 10 | K | 147 |  76% 60% 31% 5% |
| 11 | N | 140 |  2% 81% 19% |
| 12 | O | 122 |  92% 7% |
| 13 | P | 150 |  2% 90% 9% |
| 14 | Q | 141 |  2% 88% 11% |
| 15 | R | 118 |  86% 14% |
| 16 | S | 112 |  % 88% 11% |
| 17 | T | 146 |  2% 79% 11% 10% |
| 18 | U | 118 |  87% 9% |
| 19 | V | 101 |  % 84% 15% |
| 20 | W | 113 |  % 89% 9% |
| 21 | X | 96 |  3% 90% 8% |
| 22 | Y | 110 |  7% 85% 12% |
| 23 | Z | 206 |  2% 40% 5% 54% |
| 24 | 0 | 85 |  80% 7% 13% |
| 25 | 1 | 98 |  5% 85% 13% |
| 26 | 2 | 72 |  3% 79% 18% |
| 27 | 3 | 60 |  8% 87% 10% |
| 28 | 4 | 71 |  23% 69% 24% |
| 29 | 5 | 60 |  88% 10% |
| 30 | 6 | 54 |  91% 7% |




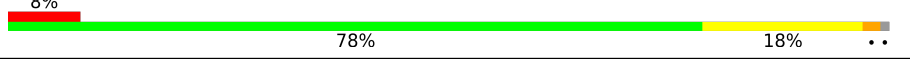
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-------------------------|
| 31 | 7 | 49 | 4% 82% 16% . |
| 32 | 8 | 65 | 91% 8% |
| 33 | 9 | 37 | 5% 86% 14% |
| 34 | a | 1521 | 5% 79% 17% . . |
| 35 | b | 256 | 12% 71% 17% . 10% |
| 36 | c | 239 | 3% 78% 8% 14% |
| 37 | d | 209 | 3% 86% 13% |
| 38 | e | 162 | 2% 79% 12% . 9% |
| 39 | f | 101 | 7% 82% 16% . . |
| 40 | g | 156 | 8% 84% 15% . |
| 41 | h | 138 | % 88% 10% . . |
| 42 | i | 128 | 2% 81% 18% . |
| 43 | j | 105 | 17% 72% 18% . 9% |
| 44 | k | 129 | 2% 81% 7% 12% |
| 45 | l | 132 | % 83% 8% . 8% |
| 46 | m | 126 | 10% 81% 12% . 6% |
| 47 | n | 61 | 85% 11% . . |
| 48 | o | 89 | 2% 89% 9% . . |
| 49 | p | 88 | 6% 81% 13% 7% |
| 50 | q | 105 | 80% 12% . 6% |
| 51 | r | 88 | 3% 67% 10% 23% |
| 52 | s | 93 | 8% 73% 14% . 11% |
| 53 | t | 106 | % 78% 10% . 9% |
| 54 | u | 27 | 78% 7% 15% |
| 55 | v | 24 | 4% 46% 8% 46% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 56 | w | 76 |  |
| 57 | x | 77 |  |
| 58 | y | 76 |  |
| 59 | z | 679 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | 5MU | w | 54 | - | - | - | X |
| 60 | MG | A | 3004 | - | - | - | X |
| 60 | MG | A | 3050 | - | - | - | X |
| 60 | MG | A | 3094 | - | - | - | X |
| 60 | MG | A | 3100 | - | - | - | X |
| 60 | MG | A | 3144 | - | - | - | X |
| 60 | MG | A | 3157 | - | - | - | X |
| 60 | MG | A | 3169 | - | - | - | X |
| 60 | MG | A | 3217 | - | - | - | X |
| 60 | MG | A | 3223 | - | - | - | X |
| 60 | MG | A | 3234 | - | - | - | X |
| 60 | MG | A | 3236 | - | - | - | X |
| 60 | MG | A | 3237 | - | - | - | X |
| 60 | MG | A | 3242 | - | - | - | X |
| 60 | MG | A | 3267 | - | - | - | X |
| 60 | MG | A | 3277 | - | - | - | X |
| 60 | MG | A | 3283 | - | - | - | X |
| 60 | MG | A | 3391 | - | - | - | X |
| 60 | MG | A | 3573 | - | - | - | X |
| 60 | MG | A | 3577 | - | - | - | X |
| 60 | MG | A | 3586 | - | - | - | X |
| 60 | MG | A | 3624 | - | - | - | X |
| 60 | MG | B | 201 | - | - | - | X |
| 60 | MG | V | 202 | - | - | - | X |
| 60 | MG | a | 1614 | - | - | - | X |
| 60 | MG | a | 1615 | - | - | - | X |
| 60 | MG | a | 1620 | - | - | - | X |
| 60 | MG | a | 1636 | - | - | - | X |
| 60 | MG | a | 1638 | - | - | - | X |
| 60 | MG | a | 1643 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 60 | MG | a | 1665 | - | - | - | X |
| 60 | MG | a | 1666 | - | - | - | X |
| 60 | MG | a | 1718 | - | - | - | X |
| 60 | MG | a | 1785 | - | - | - | X |
| 60 | MG | x | 106 | - | - | - | X |

2 Entry composition [i](#)

There are 64 unique types of molecules in this entry. The entry contains 155465 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | A | 2874 | 61902 | 27550 | 11582 | 19897 | 2873 | 11 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 2 | B | 120 | 2573 | 1146 | 476 | 832 | 119 | 0 | 0 | 0 |

- Molecule 3 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | C | 136 | 1024 | 644 | 190 | 189 | 1 | 1 | 0 | 0 |

- Molecule 4 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 4 | D | 275 | 2136 | 1349 | 423 | 361 | 3 | 0 | 0 | 0 |

- Molecule 5 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 5 | E | 204 | 1559 | 985 | 298 | 270 | 6 | 0 | 0 | 0 |

- Molecule 6 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 6 | F | 203 | 1584 | 1009 | 298 | 275 | 2 | 0 | 0 | 1 |

- Molecule 7 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 7 | G | 181 | 1425 | 914 | 256 | 251 | 4 | 0 | 0 | 0 |

- Molecule 8 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 8 | H | 174 | 1330 | 845 | 248 | 236 | 1 | 1 | 0 | 0 |

- Molecule 9 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 9 | J | 130 | 641 | 381 | 130 | 130 | 0 | 0 | 0 |

- Molecule 10 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 10 | K | 139 | 1025 | 653 | 181 | 186 | 5 | 0 | 0 | 0 |

- Molecule 11 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 11 | N | 140 | 1117 | 719 | 207 | 187 | 4 | 0 | 0 | 0 |

- Molecule 12 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 12 | O | 122 | 933 | 588 | 171 | 170 | 4 | 0 | 0 | 0 |

- Molecule 13 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 13 | P | 149 | 1135 | 706 | 230 | 196 | 3 | 0 | 0 | 0 |

- Molecule 14 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 14 | Q | 141 | 1122 | 715 | 212 | 188 | 7 | 0 | 0 | 0 |

- Molecule 15 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 15 | R | 118 | 968 | 604 | 203 | 160 | 1 | 0 | 0 | 0 |

- Molecule 16 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 16 | S | 110 | 877 | 553 | 175 | 149 | 0 | 0 | 0 |

- Molecule 17 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 17 | T | 131 | 1091 | 680 | 225 | 185 | 1 | 0 | 0 | 0 |

- Molecule 18 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 18 | U | 116 | 959 | 608 | 201 | 149 | 1 | 0 | 0 | 0 |

- Molecule 19 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 19 | V | 101 | 771 | 495 | 140 | 135 | 1 | 0 | 0 | 0 |

- Molecule 20 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 20 | W | 112 | 886 | 557 | 174 | 153 | 2 | 0 | 0 | 0 |

- Molecule 21 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 21 | X | 95 | 750 | 488 | 135 | 126 | 1 | 0 | 0 | 0 |

- Molecule 22 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 22 | Y | 107 | 806 | 517 | 152 | 131 | 6 | 1 | 0 | 0 |

- Molecule 23 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 23 | Z | 94 | 784 | 499 | 150 | 134 | 1 | 0 | 0 | 0 |

- Molecule 24 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 24 | 0 | 74 | 591 | 366 | 126 | 98 | 1 | 0 | 0 | 0 |

- Molecule 25 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 25 | 1 | 97 | 755 | 475 | 148 | 131 | 1 | 0 | 0 | 0 |

- Molecule 26 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 26 | 2 | 70 | 588 | 365 | 118 | 103 | 2 | 0 | 0 | 0 |

- Molecule 27 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 27 | 3 | 59 | 469 | 298 | 90 | 81 | 0 | 0 | 0 |

- Molecule 28 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | 4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 557 | 350 | 101 | 101 | 5 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | 5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | 6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 31 | 7 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 263 | 108 | 57 | 2 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 32 | 8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 511 | 328 | 99 | 82 | 2 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 33 | 9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 34 | a | 1498 | Total | C | N | O | P | 4 | 0 | 0 |
| | | | 32207 | 14334 | 5973 | 10402 | 1498 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 35 | b | 231 | 1850 | 1181 | 331 | 333 | 5 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 36 | c | 206 | 1550 | 974 | 302 | 273 | 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 37 | d | 208 | 1655 | 1038 | 326 | 284 | 7 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 38 | e | 148 | 1129 | 714 | 213 | 198 | 4 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 39 | f | 100 | 806 | 511 | 143 | 149 | 3 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 40 | g | 155 | 1227 | 764 | 242 | 215 | 6 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 41 | h | 137 | 1088 | 689 | 206 | 191 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 42 | i | 127 | 983 | 623 | 193 | 167 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 43 | j | 96 | 698 | 434 | 134 | 130 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 44 | k | 114 | 829 | 516 | 155 | 155 | 3 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 45 | l | 122 | 930 | 585 | 185 | 159 | 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 46 | m | 119 | 924 | 570 | 192 | 160 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 47 | n | 60 | 492 | 312 | 104 | 72 | 4 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 48 | o | 88 | 728 | 456 | 144 | 126 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 49 | p | 82 | 681 | 433 | 134 | 113 | 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 50 | q | 99 | 823 | 528 | 151 | 142 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 51 | r | 68 | 555 | 355 | 108 | 92 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 52 | s | 83 | 650 | 415 | 120 | 113 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 53 | t | 96 | 724 | 443 | 155 | 124 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 54 | u | 23 | 199 | 122 | 48 | 29 | 0 | 0 | 0 |

- Molecule 55 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 55 | v | 13 | 277 | 125 | 51 | 88 | 13 | 0 | 0 | 0 |

- Molecule 56 is a RNA chain called A-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 56 | w | 74 | Total | C | N | O | P | S | 1 | 0 | 0 |
| | | | 1586 | 713 | 285 | 513 | 73 | 2 | | | |

- Molecule 57 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 57 | x | 77 | Total | C | N | O | P | S | 3 | 0 | 0 |
| | | | 1645 | 734 | 297 | 536 | 77 | 1 | | | |

- Molecule 58 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 58 | y | 74 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1580 | 706 | 285 | 515 | 73 | 1 | | | |

- Molecule 59 is a protein called GDPCP fused to the N-terminus of the ribosomal protein L9,Elongation factor 4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 59 | z | 671 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5200 | 3333 | 897 | 961 | 9 | | | |

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 60 | A | 644 | Total | Mg | 0 | 0 |
| | | | 644 | 644 | | |
| 60 | B | 18 | Total | Mg | 0 | 0 |
| | | | 18 | 18 | | |
| 60 | D | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |
| 60 | E | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 60 | F | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |
| 60 | G | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 60 | H | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | N | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | O | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 60 | P | 3 | Total Mg 3 3 | 0 | 0 |
| 60 | Q | 2 | Total Mg 2 2 | 0 | 0 |
| 60 | R | 2 | Total Mg 2 2 | 0 | 0 |
| 60 | U | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | V | 2 | Total Mg 2 2 | 0 | 0 |
| 60 | W | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | X | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | Z | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | 0 | 4 | Total Mg 4 4 | 0 | 0 |
| 60 | 5 | 2 | Total Mg 2 2 | 0 | 0 |
| 60 | 6 | 2 | Total Mg 2 2 | 0 | 0 |
| 60 | 7 | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | 8 | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | 9 | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | a | 188 | Total Mg 188 188 | 0 | 0 |
| 60 | d | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | e | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | f | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | l | 1 | Total Mg 1 1 | 0 | 0 |
| 60 | m | 2 | Total Mg 2 2 | 0 | 0 |
| 60 | n | 3 | Total Mg 3 3 | 0 | 0 |

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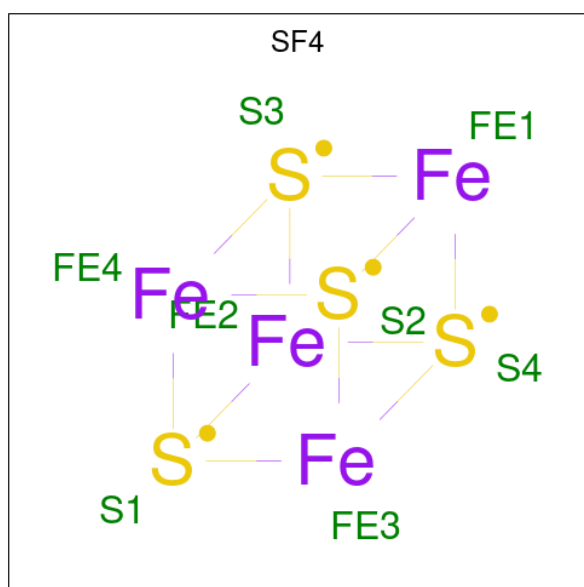
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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 60 | v | 2 | Total Mg 2 2 | 0 | 0 |
| 60 | x | 9 | Total Mg 9 9 | 0 | 0 |
| 60 | z | 2 | Total Mg 2 2 | 0 | 0 |

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

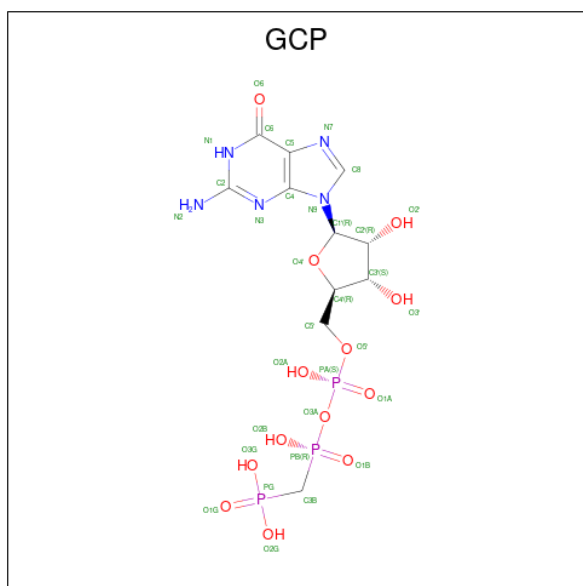
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|-----|-------|----------|-----------------|---------|---------|
| 61 | Y | 1 | Total Zn 1 1 | 0 | 0 |
| 61 | 4 | 1 | Total Zn 1 1 | 0 | 0 |
| 61 | 5 | 1 | Total Zn 1 1 | 0 | 0 |
| 61 | 6 | 1 | Total Zn 1 1 | 0 | 0 |
| 61 | 9 | 1 | Total Zn 1 1 | 0 | 0 |
| 61 | n | 1 | Total Zn 1 1 | 0 | 0 |

- Molecule 62 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 62 | d | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 63 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 63 | z | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 32 | 11 | 5 | 13 | 3 | | |

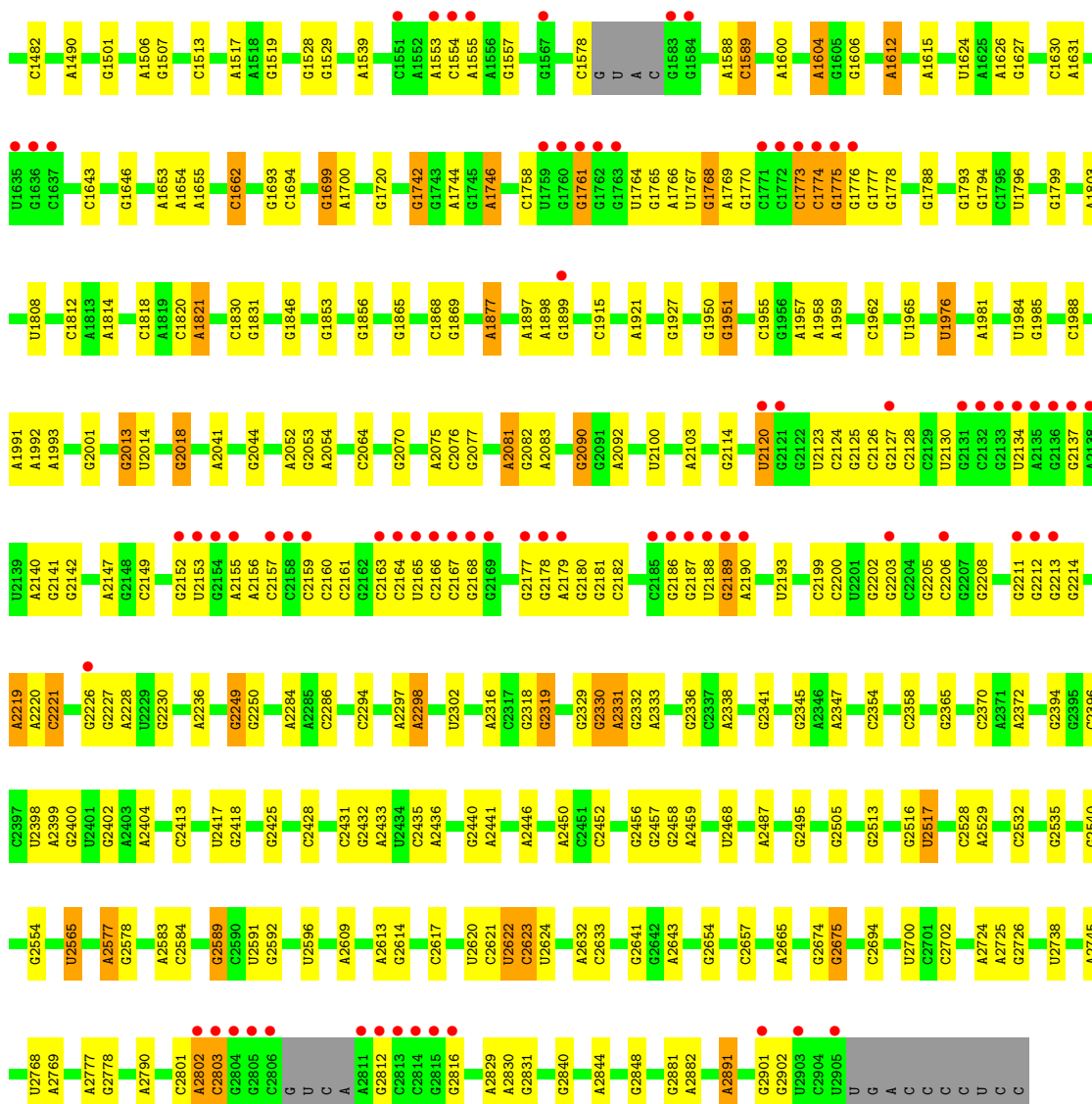
- Molecule 64 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 64 | A | 715 | Total | O | 0 | 0 |
| | | | 715 | 715 | | |
| 64 | B | 32 | Total | O | 0 | 0 |
| | | | 32 | 32 | | |
| 64 | D | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 64 | E | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 64 | F | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 64 | H | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 64 | N | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

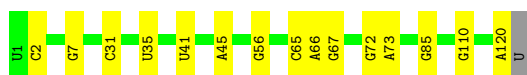
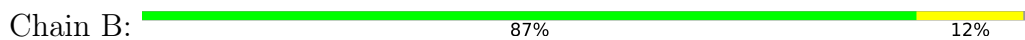
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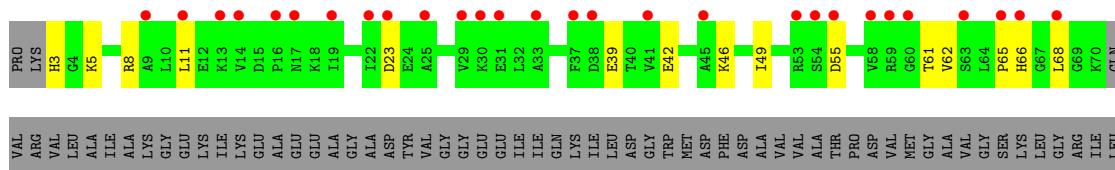
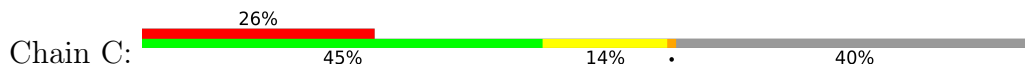
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 64 | O | 3 | Total O 3 3 | 0 | 0 |
| 64 | P | 8 | Total O 8 8 | 0 | 0 |
| 64 | Q | 3 | Total O 3 3 | 0 | 0 |
| 64 | T | 2 | Total O 2 2 | 0 | 0 |
| 64 | U | 3 | Total O 3 3 | 0 | 0 |
| 64 | V | 1 | Total O 1 1 | 0 | 0 |
| 64 | 0 | 3 | Total O 3 3 | 0 | 0 |
| 64 | 1 | 1 | Total O 1 1 | 0 | 0 |
| 64 | 3 | 1 | Total O 1 1 | 0 | 0 |
| 64 | 7 | 1 | Total O 1 1 | 0 | 0 |
| 64 | 8 | 4 | Total O 4 4 | 0 | 0 |
| 64 | a | 165 | Total O 165 165 | 0 | 0 |
| 64 | l | 1 | Total O 1 1 | 0 | 0 |
| 64 | p | 1 | Total O 1 1 | 0 | 0 |
| 64 | v | 3 | Total O 3 3 | 0 | 0 |
| 64 | w | 1 | Total O 1 1 | 0 | 0 |
| 64 | z | 1 | Total O 1 1 | 0 | 0 |

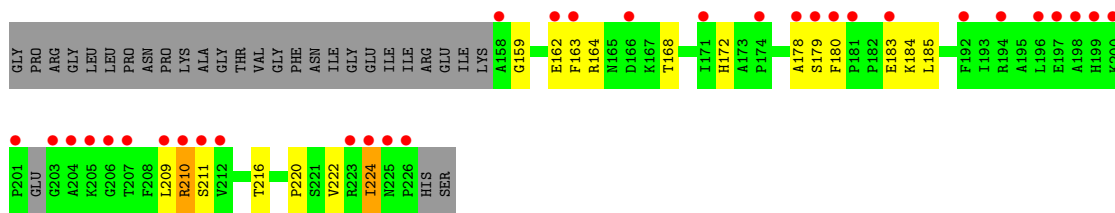


• Molecule 2: 5S Ribosomal RNA

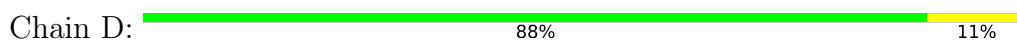


• Molecule 3: 50S ribosomal protein L1

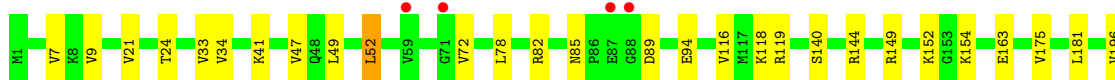
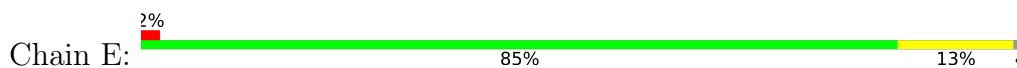




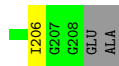
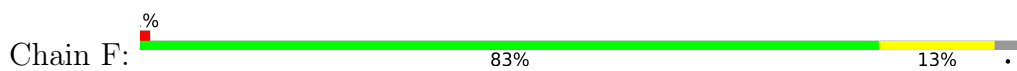
• Molecule 4: 50S ribosomal protein L2



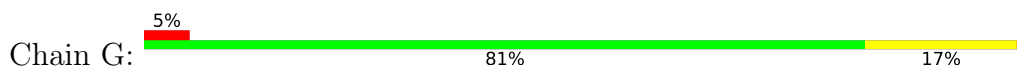
• Molecule 5: 50S ribosomal protein L3



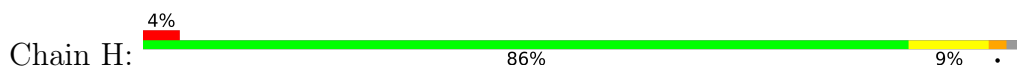
• Molecule 6: 50S ribosomal protein L4

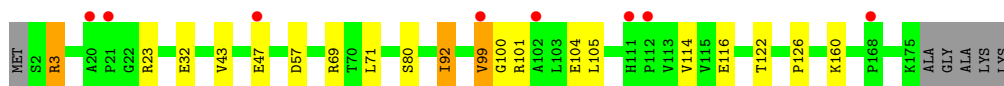


• Molecule 7: 50S ribosomal protein L5

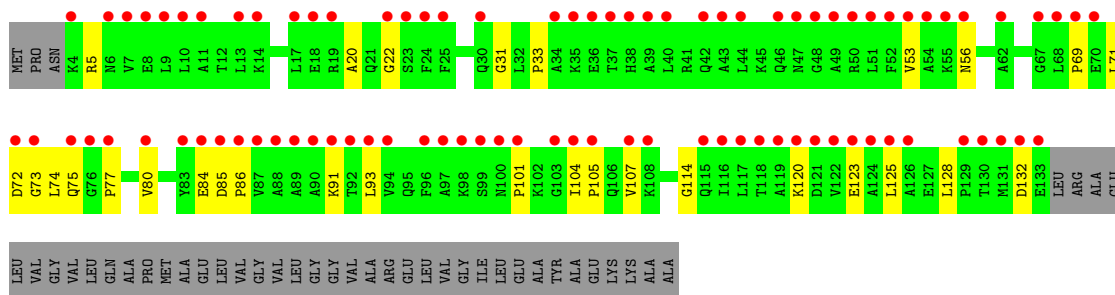


• Molecule 8: 50S ribosomal protein L6

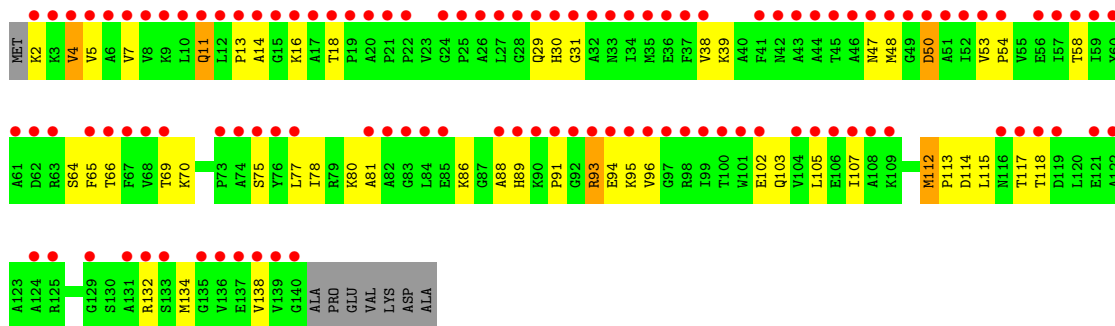
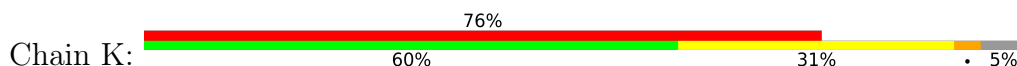




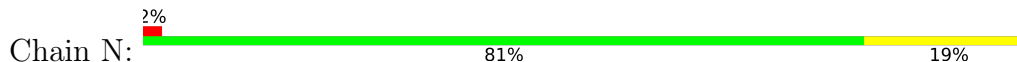
- Molecule 9: 50S ribosomal protein L10



- Molecule 10: 50S ribosomal protein L11



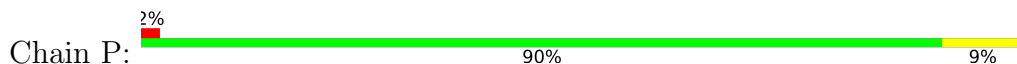
- Molecule 11: 50S ribosomal protein L13



- Molecule 12: 50S ribosomal protein L14

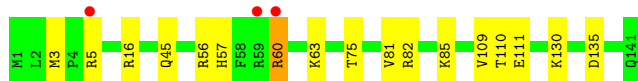
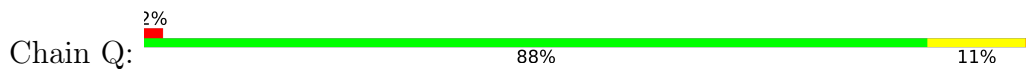


- Molecule 13: 50S ribosomal protein L15

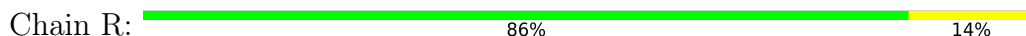




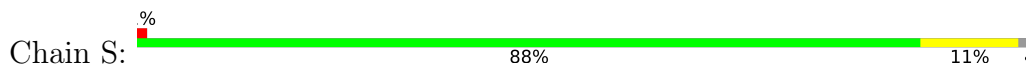
- Molecule 14: 50S ribosomal protein L16



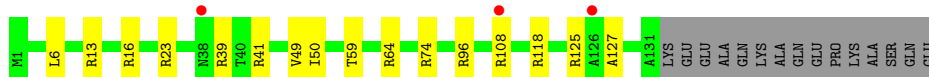
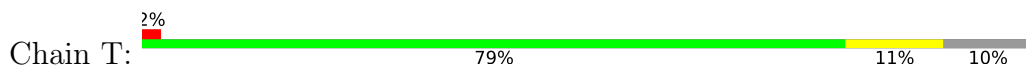
- Molecule 15: 50S ribosomal protein L17



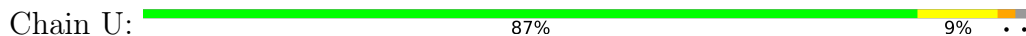
- Molecule 16: 50S ribosomal protein L18



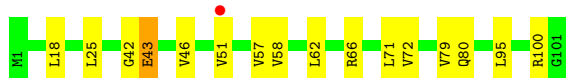
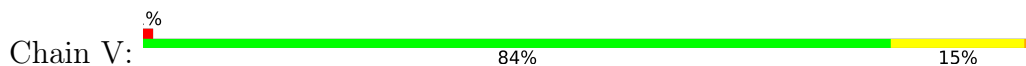
- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20



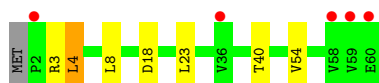
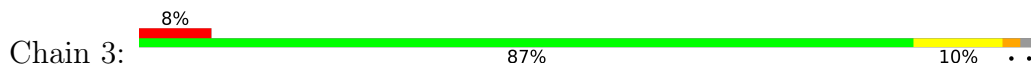
- Molecule 19: 50S ribosomal protein L21



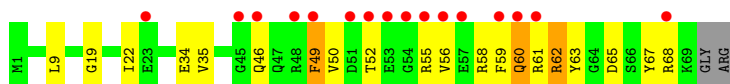
- Molecule 20: 50S ribosomal protein L22



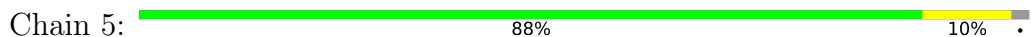
- Molecule 27: 50S ribosomal protein L30



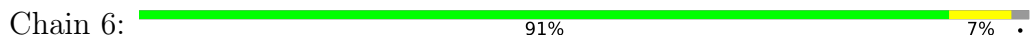
- Molecule 28: 50S ribosomal protein L31



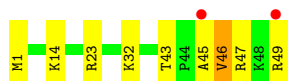
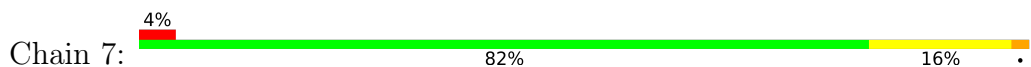
- Molecule 29: 50S ribosomal protein L32



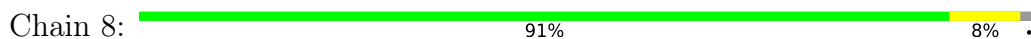
- Molecule 30: 50S ribosomal protein L33



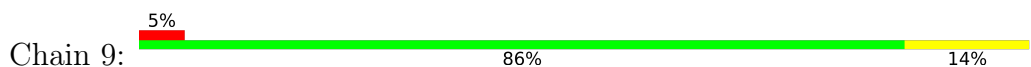
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35

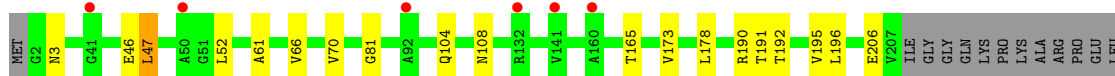
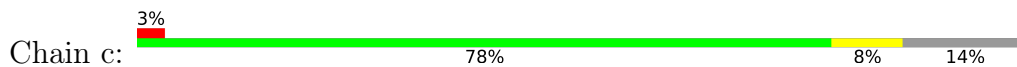


- Molecule 33: 50S ribosomal protein L36



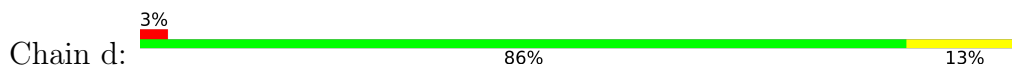
GLU
VAL
GLU
ALA

- Molecule 36: 30S ribosomal protein S3

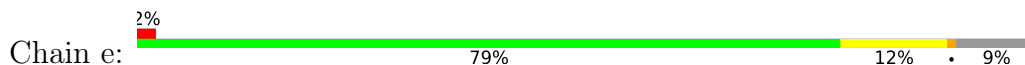


PRO
LYS
ALA
GLU
GLU
ARG
PRO
ARG
ARG
ARG
PRO
ALA
VAL
ARG
VAL
LYS
LYS
GLU
GLU

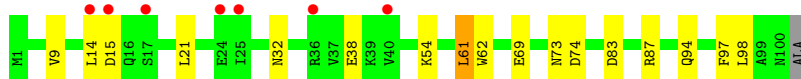
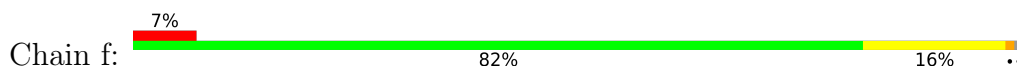
- Molecule 37: 30S ribosomal protein S4



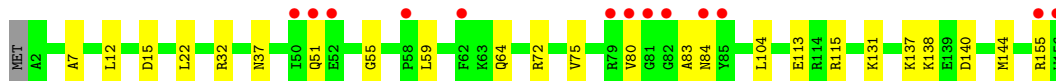
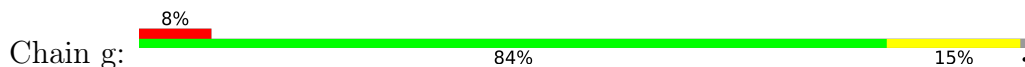
- Molecule 38: 30S ribosomal protein S5



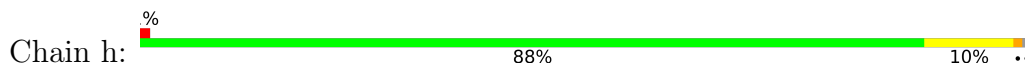
- Molecule 39: 30S ribosomal protein S6



- Molecule 40: 30S ribosomal protein S7

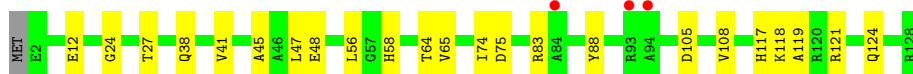
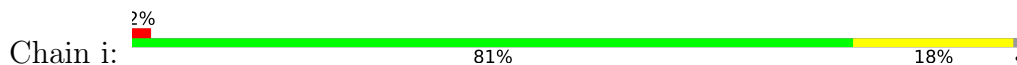


- Molecule 41: 30S ribosomal protein S8





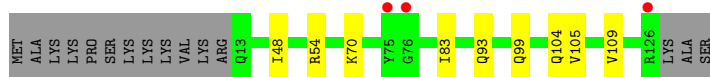
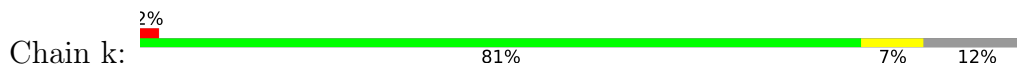
- Molecule 42: 30S ribosomal protein S9



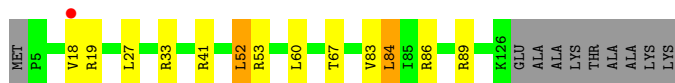
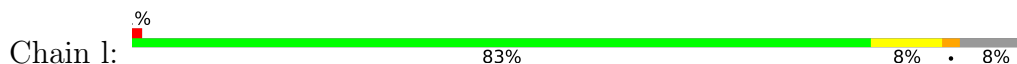
- Molecule 43: 30S ribosomal protein S10



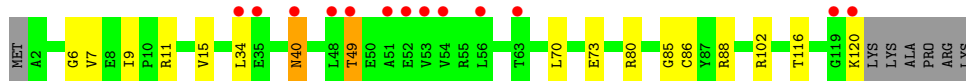
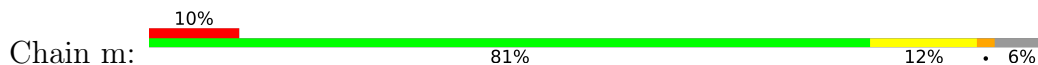
- Molecule 44: 30S ribosomal protein S11



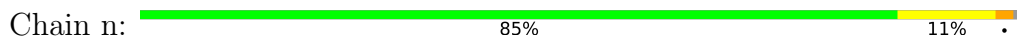
- Molecule 45: 30S ribosomal protein S12



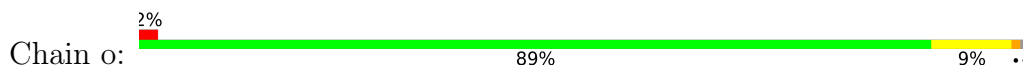
- Molecule 46: 30S ribosomal protein S13



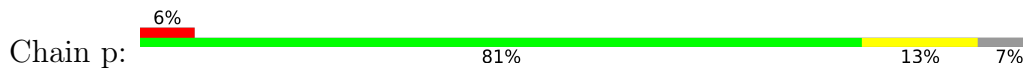
- Molecule 47: 30S ribosomal protein S14 type Z



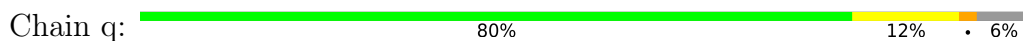
- Molecule 48: 30S ribosomal protein S15



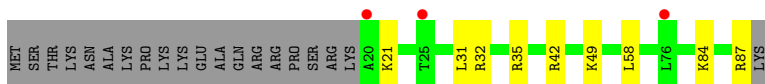
- Molecule 49: 30S ribosomal protein S16



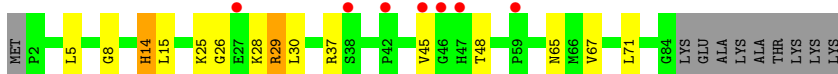
- Molecule 50: 30S ribosomal protein S17



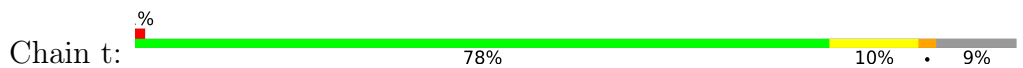
- Molecule 51: 30S ribosomal protein S18



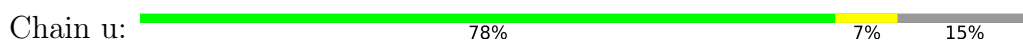
- Molecule 52: 30S ribosomal protein S19



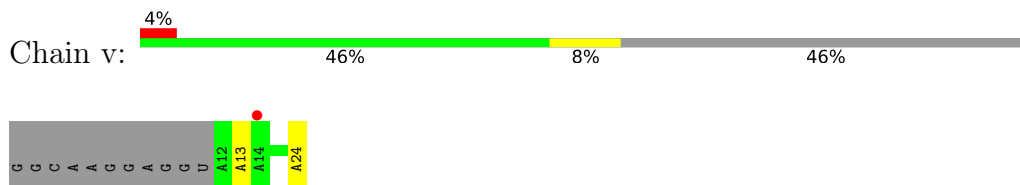
- Molecule 53: 30S ribosomal protein S20



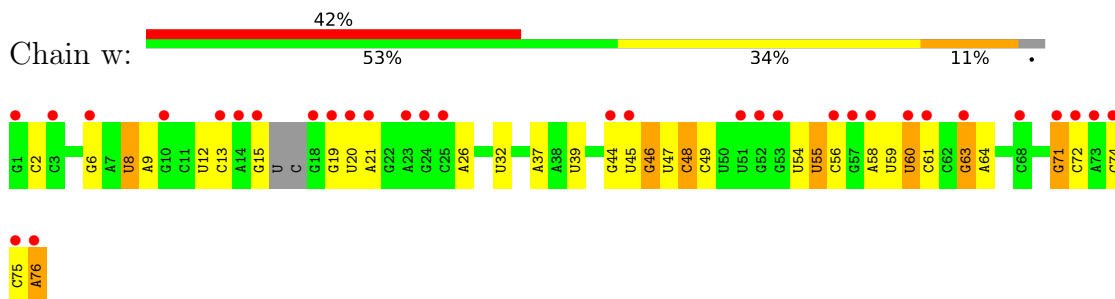
- Molecule 54: 30S ribosomal protein Thx



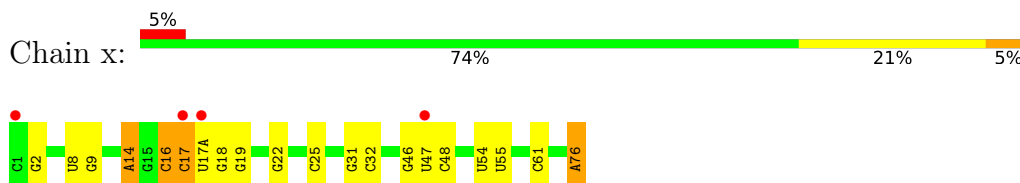
- Molecule 55: mRNA



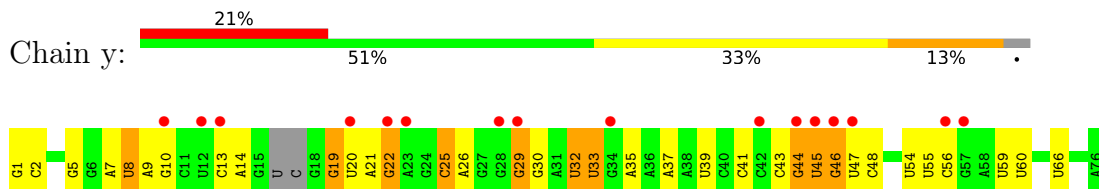
- Molecule 56: A-site tRNA



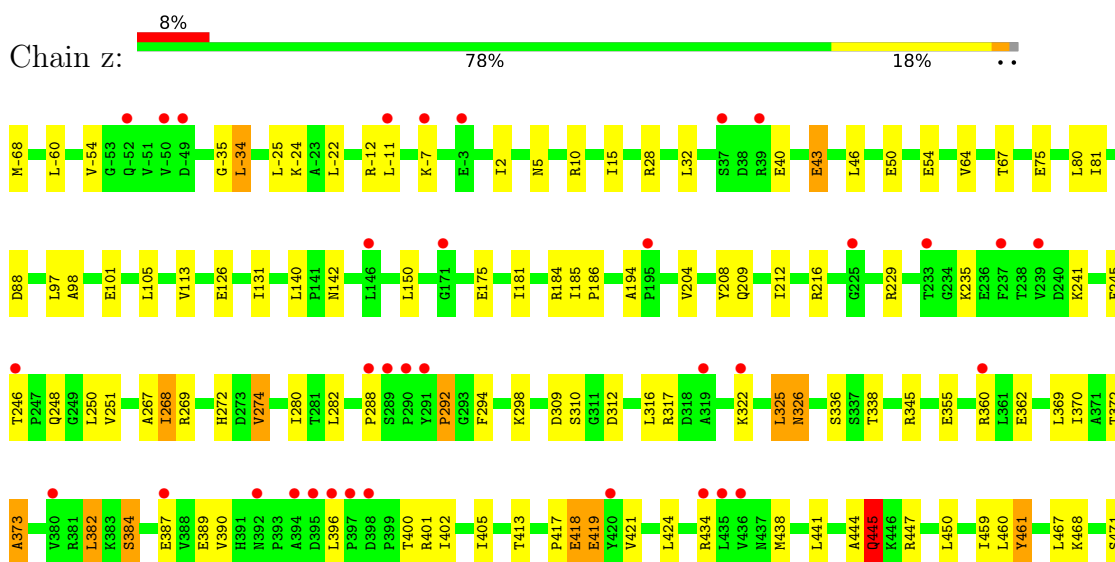
- Molecule 57: P-site tRNA

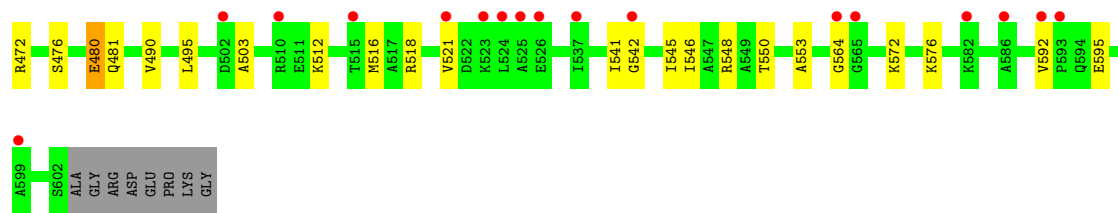


- Molecule 58: E-site tRNA



- Molecule 59: GDPCP fused to the N-terminus of the ribosomal protein L9, Elongation factor 4





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 213.12Å 271.72Å 436.83Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.52 – 2.60 49.52 – 2.59 | Depositor EDS |
| % Data completeness (in resolution range) | 99.4 (49.52-2.60) 98.7 (49.52-2.59) | Depositor EDS |
| R_{merge} | 0.26 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.00 (at 2.58Å) | Xtrriage |
| Refinement program | PHENIX 1.10.1-2155 | Depositor |
| R, R_{free} | 0.192 , 0.261 0.192 , 0.261 | Depositor DCC |
| R_{free} test set | 38580 reflections (5.04%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 47.7 | Xtrriage |
| Anisotropy | 0.255 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 47.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 155465 | wwPDB-VP |
| Average B, all atoms (Å ²) | 51.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, 5MC, SF4, 5MU, MG, MIA, PSU, 4SU, 7MG, ZN

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.69 | 11/69327 (0.0%) | 1.23 | 339/108217 (0.3%) |
| 2 | B | 0.51 | 0/2878 | 1.00 | 1/4490 (0.0%) |
| 3 | C | 0.36 | 0/1044 | 0.66 | 1/1413 (0.1%) |
| 4 | D | 0.50 | 0/2186 | 0.73 | 1/2944 (0.0%) |
| 5 | E | 0.45 | 0/1592 | 0.69 | 0/2149 |
| 6 | F | 0.46 | 0/1619 | 0.62 | 0/2193 |
| 7 | G | 0.38 | 0/1450 | 0.64 | 1/1959 (0.1%) |
| 8 | H | 0.42 | 0/1356 | 0.63 | 0/1834 |
| 9 | J | 0.32 | 0/640 | 0.55 | 0/889 |
| 10 | K | 0.43 | 0/1044 | 0.65 | 1/1416 (0.1%) |
| 11 | N | 0.41 | 0/1144 | 0.63 | 0/1543 |
| 12 | O | 0.49 | 0/943 | 0.68 | 1/1269 (0.1%) |
| 13 | P | 0.47 | 0/1152 | 0.74 | 1/1533 (0.1%) |
| 14 | Q | 0.46 | 0/1143 | 0.58 | 0/1527 |
| 15 | R | 0.38 | 0/982 | 0.66 | 0/1312 |
| 16 | S | 0.40 | 0/887 | 0.63 | 0/1180 |
| 17 | T | 0.43 | 0/1105 | 0.65 | 0/1477 |
| 18 | U | 0.46 | 0/977 | 0.69 | 2/1301 (0.2%) |
| 19 | V | 0.48 | 0/782 | 0.68 | 1/1049 (0.1%) |
| 20 | W | 0.46 | 0/897 | 0.63 | 0/1205 |
| 21 | X | 0.43 | 0/764 | 0.65 | 1/1025 (0.1%) |
| 22 | Y | 0.43 | 0/819 | 0.66 | 1/1095 (0.1%) |
| 23 | Z | 0.38 | 0/801 | 0.59 | 0/1079 |
| 24 | 0 | 0.43 | 0/599 | 0.64 | 0/798 |
| 25 | 1 | 0.52 | 0/762 | 0.74 | 1/1014 (0.1%) |
| 26 | 2 | 0.38 | 0/590 | 0.58 | 0/781 |
| 27 | 3 | 0.38 | 0/474 | 0.69 | 1/635 (0.2%) |
| 28 | 4 | 0.40 | 0/570 | 0.64 | 0/768 |
| 29 | 5 | 0.44 | 0/473 | 0.71 | 0/639 |
| 30 | 6 | 0.46 | 0/460 | 0.64 | 0/613 |
| 31 | 7 | 0.46 | 0/438 | 0.71 | 0/575 |
| 32 | 8 | 0.47 | 0/519 | 0.67 | 0/684 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | g | 0.49 | 0/310 | 0.73 | 0/407 |
| 34 | a | 0.62 | 2/36053 (0.0%) | 1.14 | 114/56270 (0.2%) |
| 35 | b | 0.37 | 0/1885 | 0.61 | 0/2547 |
| 36 | c | 0.41 | 1/1574 (0.1%) | 0.58 | 0/2127 |
| 37 | d | 0.38 | 0/1685 | 0.58 | 0/2262 |
| 38 | e | 0.42 | 0/1145 | 0.65 | 0/1543 |
| 39 | f | 0.39 | 0/819 | 0.57 | 0/1111 |
| 40 | g | 0.37 | 0/1246 | 0.54 | 0/1674 |
| 41 | h | 0.39 | 0/1108 | 0.64 | 1/1494 (0.1%) |
| 42 | i | 0.39 | 0/1002 | 0.61 | 0/1346 |
| 43 | j | 0.38 | 0/711 | 0.55 | 0/968 |
| 44 | k | 0.38 | 0/844 | 0.60 | 0/1145 |
| 45 | l | 0.48 | 0/946 | 0.76 | 2/1274 (0.2%) |
| 46 | m | 0.38 | 0/934 | 0.70 | 0/1256 |
| 47 | n | 0.46 | 0/501 | 0.65 | 0/664 |
| 48 | o | 0.39 | 0/739 | 0.61 | 0/985 |
| 49 | p | 0.37 | 0/697 | 0.65 | 0/939 |
| 50 | q | 0.44 | 0/836 | 0.68 | 1/1117 (0.1%) |
| 51 | r | 0.38 | 0/560 | 0.62 | 0/746 |
| 52 | s | 0.35 | 0/665 | 0.68 | 0/897 |
| 53 | t | 0.39 | 0/726 | 0.64 | 0/961 |
| 54 | u | 0.44 | 0/203 | 0.64 | 0/266 |
| 55 | v | 0.71 | 0/310 | 1.31 | 3/480 (0.6%) |
| 56 | w | 0.67 | 3/1602 (0.2%) | 1.69 | 31/2493 (1.2%) |
| 57 | x | 0.76 | 4/1747 (0.2%) | 1.48 | 32/2723 (1.2%) |
| 58 | y | 0.62 | 0/1628 | 1.49 | 31/2534 (1.2%) |
| 59 | z | 0.40 | 0/5296 | 0.65 | 4/7179 (0.1%) |
| All | All | 0.60 | 21/166189 (0.0%) | 1.08 | 572/248014 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 10 | K | 0 | 1 |
| 19 | V | 0 | 1 |
| 26 | 2 | 0 | 1 |
| 28 | 4 | 0 | 1 |
| 37 | d | 0 | 1 |
| 39 | f | 0 | 1 |
| 42 | i | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 52 | s | 0 | 2 |
| 53 | t | 0 | 1 |
| 59 | z | 0 | 6 |
| All | All | 0 | 17 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 56 | w | 71 | G | C6-N1 | -10.59 | 1.32 | 1.39 |
| 56 | w | 71 | G | N1-C2 | -10.38 | 1.29 | 1.37 |
| 57 | x | 14 | A | N7-C5 | -8.86 | 1.33 | 1.39 |
| 1 | A | 353 | A | N9-C4 | -7.12 | 1.33 | 1.37 |
| 1 | A | 1091 | A | C5-C6 | -7.12 | 1.34 | 1.41 |
| 57 | x | 14 | A | C8-N7 | -7.08 | 1.26 | 1.31 |
| 1 | A | 2298 | A | N9-C4 | -6.99 | 1.33 | 1.37 |
| 36 | c | 173 | VAL | C-N | -6.97 | 1.21 | 1.34 |
| 34 | a | 953 | A | N9-C4 | -6.84 | 1.33 | 1.37 |
| 1 | A | 1187 | A | N9-C4 | -6.75 | 1.33 | 1.37 |
| 1 | A | 1066 | A | N9-C4 | -6.07 | 1.34 | 1.37 |
| 1 | A | 552 | A | N9-C4 | -6.03 | 1.34 | 1.37 |
| 1 | A | 1744 | A | N9-C4 | -5.48 | 1.34 | 1.37 |
| 1 | A | 989 | A | N9-C4 | -5.46 | 1.34 | 1.37 |
| 34 | a | 1108 | U | P-O5' | 5.41 | 1.65 | 1.59 |
| 57 | x | 14 | A | N9-C4 | 5.38 | 1.41 | 1.37 |
| 1 | A | 353 | A | N3-C4 | -5.36 | 1.31 | 1.34 |
| 1 | A | 1955 | C | N3-C4 | -5.31 | 1.30 | 1.33 |
| 57 | x | 14 | A | C6-N6 | 5.24 | 1.38 | 1.33 |
| 56 | w | 2 | C | N3-C4 | -5.08 | 1.30 | 1.33 |
| 1 | A | 1853 | G | N3-C4 | -5.02 | 1.31 | 1.35 |

All (572) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 56 | w | 71 | G | N3-C2-N2 | 23.02 | 136.02 | 119.90 |
| 56 | w | 71 | G | C5-C6-O6 | 22.98 | 142.39 | 128.60 |
| 56 | w | 2 | C | N1-C2-O2 | 21.56 | 131.84 | 118.90 |
| 56 | w | 71 | G | N1-C2-N2 | -21.15 | 97.16 | 116.20 |
| 1 | A | 1091 | A | N9-C4-C5 | -17.30 | 98.88 | 105.80 |
| 56 | w | 71 | G | N1-C6-O6 | -15.20 | 110.78 | 119.90 |
| 1 | A | 1091 | A | C8-N9-C4 | 15.05 | 111.82 | 105.80 |
| 1 | A | 39 | C | C2-N3-C4 | 14.70 | 127.25 | 119.90 |
| 57 | x | 14 | A | C4-C5-C6 | 14.37 | 124.19 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 56 | w | 2 | C | C2-N3-C4 | 14.36 | 127.08 | 119.90 |
| 57 | x | 14 | A | C5-N7-C8 | 14.31 | 111.06 | 103.90 |
| 34 | a | 361 | U | C5-C6-N1 | -12.83 | 116.28 | 122.70 |
| 58 | y | 46 | G | C4-N9-C1' | 12.63 | 142.92 | 126.50 |
| 1 | A | 1775 | G | C4-C5-N7 | 12.58 | 115.83 | 110.80 |
| 56 | w | 2 | C | N3-C2-O2 | -12.28 | 113.31 | 121.90 |
| 1 | A | 1066 | A | C2-N3-C4 | -12.23 | 104.49 | 110.60 |
| 58 | y | 22 | G | C5-C6-O6 | -12.12 | 121.33 | 128.60 |
| 56 | w | 2 | C | C5-C6-N1 | 11.97 | 126.99 | 121.00 |
| 58 | y | 46 | G | C8-N9-C1' | -11.80 | 111.66 | 127.00 |
| 1 | A | 39 | C | N3-C4-C5 | 11.73 | 126.59 | 121.90 |
| 57 | x | 14 | A | C5-C6-N1 | -11.62 | 111.89 | 117.70 |
| 56 | w | 71 | G | C6-N1-C2 | 11.53 | 132.02 | 125.10 |
| 1 | A | 536 | G | O4'-C1'-N9 | 11.30 | 117.24 | 108.20 |
| 1 | A | 2298 | A | C2-N3-C4 | -11.26 | 104.97 | 110.60 |
| 1 | A | 2221 | C | C5-C6-N1 | 10.94 | 126.47 | 121.00 |
| 56 | w | 71 | G | C2-N3-C4 | -10.74 | 106.53 | 111.90 |
| 1 | A | 1091 | A | C4-C5-N7 | 10.48 | 115.94 | 110.70 |
| 1 | A | 1125 | C | N3-C2-O2 | -10.35 | 114.66 | 121.90 |
| 58 | y | 22 | G | N1-C6-O6 | 9.94 | 125.87 | 119.90 |
| 1 | A | 117 | U | O5'-P-OP1 | -9.94 | 96.76 | 105.70 |
| 34 | a | 1037 | C | O4'-C1'-N1 | 9.93 | 116.14 | 108.20 |
| 56 | w | 2 | C | C6-N1-C2 | -9.78 | 116.39 | 120.30 |
| 1 | A | 2018 | G | O5'-P-OP2 | -9.74 | 96.93 | 105.70 |
| 58 | y | 46 | G | N1-C2-N2 | -9.72 | 107.45 | 116.20 |
| 1 | A | 1187 | A | C2-N3-C4 | -9.70 | 105.75 | 110.60 |
| 57 | x | 76 | A | N1-C2-N3 | 9.64 | 134.12 | 129.30 |
| 1 | A | 1066 | A | N1-C2-N3 | 9.61 | 134.11 | 129.30 |
| 1 | A | 985 | A | O5'-P-OP1 | -9.61 | 97.06 | 105.70 |
| 56 | w | 71 | G | C5-C6-N1 | -9.40 | 106.80 | 111.50 |
| 1 | A | 2221 | C | C6-N1-C2 | -9.30 | 116.58 | 120.30 |
| 57 | x | 22 | G | C5-N7-C8 | -9.27 | 99.66 | 104.30 |
| 1 | A | 1957 | A | O4'-C1'-N9 | 9.24 | 115.59 | 108.20 |
| 57 | x | 17 | C | N1-C2-O2 | 9.12 | 124.38 | 118.90 |
| 1 | A | 1125 | C | N1-C2-O2 | 9.12 | 124.37 | 118.90 |
| 34 | a | 1313 | G | O4'-C1'-N9 | 9.10 | 115.48 | 108.20 |
| 58 | y | 22 | G | C6-C5-N7 | -8.98 | 125.01 | 130.40 |
| 1 | A | 1091 | A | N1-C6-N6 | 8.95 | 123.97 | 118.60 |
| 58 | y | 46 | G | O4'-C1'-N9 | 8.94 | 115.36 | 108.20 |
| 1 | A | 799 | C | O5'-P-OP1 | -8.92 | 97.67 | 105.70 |
| 1 | A | 1742 | G | O5'-P-OP2 | -8.89 | 97.70 | 105.70 |
| 58 | y | 46 | G | N3-C4-N9 | 8.88 | 131.33 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 34 | a | 1109 | U | C2-N1-C1' | 8.84 | 128.31 | 117.70 |
| 34 | a | 511 | G | O5'-P-OP2 | -8.76 | 97.81 | 105.70 |
| 1 | A | 1248 | A | O4'-C1'-N9 | 8.74 | 115.19 | 108.20 |
| 1 | A | 353 | A | N1-C2-N3 | 8.71 | 133.65 | 129.30 |
| 1 | A | 989 | A | C5-N7-C8 | -8.66 | 99.57 | 103.90 |
| 34 | a | 1109 | U | C5-C6-N1 | 8.66 | 127.03 | 122.70 |
| 34 | a | 1261 | A | N7-C8-N9 | 8.64 | 118.12 | 113.80 |
| 1 | A | 1877 | A | O4'-C1'-N9 | 8.62 | 115.10 | 108.20 |
| 1 | A | 1125 | C | C6-N1-C2 | -8.61 | 116.86 | 120.30 |
| 34 | a | 1480 | A | C5-N7-C8 | -8.60 | 99.60 | 103.90 |
| 58 | y | 45 | U | N3-C2-O2 | -8.59 | 116.19 | 122.20 |
| 1 | A | 2297 | A | N7-C8-N9 | 8.57 | 118.09 | 113.80 |
| 1 | A | 1775 | G | N9-C4-C5 | -8.56 | 101.97 | 105.40 |
| 1 | A | 2330 | G | N3-C4-C5 | 8.53 | 132.86 | 128.60 |
| 1 | A | 2221 | C | C2-N1-C1' | 8.52 | 128.17 | 118.80 |
| 1 | A | 2297 | A | C5-N7-C8 | -8.47 | 99.67 | 103.90 |
| 56 | w | 2 | C | C2-N1-C1' | 8.47 | 128.11 | 118.80 |
| 1 | A | 1775 | G | C5-N7-C8 | -8.38 | 100.11 | 104.30 |
| 34 | a | 1007 | C | C2-N1-C1' | 8.37 | 128.01 | 118.80 |
| 57 | x | 17 | C | C2-N1-C1' | 8.36 | 127.99 | 118.80 |
| 1 | A | 353 | A | C2-N3-C4 | -8.34 | 106.43 | 110.60 |
| 1 | A | 1589 | C | C2-N1-C1' | 8.32 | 127.95 | 118.80 |
| 34 | a | 961 | A | O5'-P-OP1 | -8.28 | 98.25 | 105.70 |
| 1 | A | 253 | A | C5-N7-C8 | -8.25 | 99.78 | 103.90 |
| 1 | A | 2457 | G | N1-C6-O6 | -8.24 | 114.96 | 119.90 |
| 1 | A | 2330 | G | N3-C4-N9 | -8.16 | 121.10 | 126.00 |
| 1 | A | 1589 | C | N1-C2-O2 | 8.14 | 123.78 | 118.90 |
| 34 | a | 262 | G | N3-C4-N9 | -8.11 | 121.13 | 126.00 |
| 34 | a | 953 | A | C5-N7-C8 | -8.11 | 99.85 | 103.90 |
| 57 | x | 46 | G | C6-N1-C2 | -8.09 | 120.24 | 125.10 |
| 1 | A | 1187 | A | N3-C4-N9 | -8.08 | 120.94 | 127.40 |
| 56 | w | 76 | A | N7-C8-N9 | 8.00 | 117.80 | 113.80 |
| 1 | A | 1091 | A | C6-N1-C2 | 8.00 | 123.40 | 118.60 |
| 34 | a | 570 | C | C6-N1-C2 | 7.99 | 123.50 | 120.30 |
| 1 | A | 2013 | G | P-O3'-C3' | 7.99 | 129.29 | 119.70 |
| 1 | A | 989 | A | N1-C6-N6 | 7.95 | 123.37 | 118.60 |
| 1 | A | 865 | A | O5'-P-OP1 | -7.85 | 98.63 | 105.70 |
| 58 | y | 46 | G | N3-C4-C5 | -7.81 | 124.69 | 128.60 |
| 1 | A | 2189 | G | C6-C5-N7 | -7.80 | 125.72 | 130.40 |
| 58 | y | 22 | G | C4-C5-N7 | 7.79 | 113.92 | 110.80 |
| 1 | A | 1187 | A | N3-C4-C5 | 7.76 | 132.23 | 126.80 |
| 1 | A | 2565 | U | O5'-P-OP1 | -7.74 | 98.73 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1091 | A | O4'-C1'-N9 | -7.72 | 102.02 | 108.20 |
| 58 | y | 22 | G | N3-C4-N9 | 7.72 | 130.63 | 126.00 |
| 34 | a | 262 | G | N3-C4-C5 | 7.69 | 132.45 | 128.60 |
| 34 | a | 1263 | U | N1-C2-O2 | 7.66 | 128.16 | 122.80 |
| 58 | y | 45 | U | N1-C2-O2 | 7.60 | 128.12 | 122.80 |
| 57 | x | 14 | A | C4-C5-N7 | -7.58 | 106.91 | 110.70 |
| 1 | A | 1091 | A | N1-C2-N3 | -7.57 | 125.52 | 129.30 |
| 1 | A | 2297 | A | C8-N9-C4 | -7.53 | 102.79 | 105.80 |
| 1 | A | 1066 | A | C5-N7-C8 | -7.53 | 100.14 | 103.90 |
| 58 | y | 46 | G | N1-C2-N3 | 7.50 | 128.40 | 123.90 |
| 57 | x | 76 | A | C2-N3-C4 | -7.50 | 106.85 | 110.60 |
| 57 | x | 76 | A | C5-N7-C8 | -7.45 | 100.17 | 103.90 |
| 7 | G | 82 | LEU | CA-CB-CG | 7.43 | 132.38 | 115.30 |
| 57 | x | 76 | A | C6-C5-N7 | -7.42 | 127.11 | 132.30 |
| 34 | a | 1480 | A | N7-C8-N9 | 7.40 | 117.50 | 113.80 |
| 57 | x | 17 | C | N3-C2-O2 | -7.37 | 116.74 | 121.90 |
| 1 | A | 1662 | C | O5'-P-OP1 | -7.37 | 99.07 | 105.70 |
| 55 | v | 13 | A | C5-N7-C8 | -7.35 | 100.22 | 103.90 |
| 1 | A | 1066 | A | N7-C8-N9 | 7.34 | 117.47 | 113.80 |
| 57 | x | 76 | A | O4'-C1'-N9 | 7.34 | 114.07 | 108.20 |
| 1 | A | 2249 | G | N3-C4-N9 | 7.33 | 130.40 | 126.00 |
| 1 | A | 994 | G | O5'-P-OP1 | -7.33 | 99.11 | 105.70 |
| 1 | A | 2298 | A | N3-C4-C5 | 7.33 | 131.93 | 126.80 |
| 34 | a | 1007 | C | N1-C2-O2 | 7.24 | 123.24 | 118.90 |
| 58 | y | 46 | G | C6-C5-N7 | -7.24 | 126.06 | 130.40 |
| 56 | w | 2 | C | C4-C5-C6 | -7.22 | 113.79 | 117.40 |
| 1 | A | 990 | G | N1-C6-O6 | -7.16 | 115.61 | 119.90 |
| 1 | A | 893 | U | C5-C6-N1 | -7.14 | 119.13 | 122.70 |
| 1 | A | 1248 | A | N1-C6-N6 | 7.14 | 122.88 | 118.60 |
| 56 | w | 72 | C | N1-C2-O2 | 7.13 | 123.18 | 118.90 |
| 1 | A | 1699 | G | N3-C4-C5 | -7.12 | 125.04 | 128.60 |
| 34 | a | 1261 | A | C5-N7-C8 | -7.11 | 100.35 | 103.90 |
| 1 | A | 1764 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 57 | x | 22 | G | N7-C8-N9 | 7.10 | 116.65 | 113.10 |
| 34 | a | 1261 | A | C8-N9-C4 | -7.08 | 102.97 | 105.80 |
| 1 | A | 2221 | C | N1-C2-O2 | 7.08 | 123.15 | 118.90 |
| 1 | A | 940 | U | C2-N1-C1' | 7.02 | 126.13 | 117.70 |
| 1 | A | 1812 | C | C6-N1-C2 | -7.00 | 117.50 | 120.30 |
| 1 | A | 977 | A | C5-N7-C8 | -7.00 | 100.40 | 103.90 |
| 1 | A | 989 | A | C4-C5-N7 | 7.00 | 114.20 | 110.70 |
| 34 | a | 939 | U | O5'-P-OP2 | -6.99 | 99.41 | 105.70 |
| 2 | B | 41 | U | C5-C6-N1 | -6.98 | 119.21 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1761 | G | C5-C6-O6 | -6.96 | 124.42 | 128.60 |
| 1 | A | 1693 | G | O4'-C1'-N9 | -6.95 | 102.64 | 108.20 |
| 34 | a | 317 | A | O5'-P-OP2 | -6.94 | 99.46 | 105.70 |
| 34 | a | 1389 | U | O5'-P-OP2 | -6.93 | 99.46 | 105.70 |
| 1 | A | 552 | A | C2-N3-C4 | -6.84 | 107.18 | 110.60 |
| 1 | A | 838 | G | O4'-C1'-N9 | -6.84 | 102.73 | 108.20 |
| 1 | A | 2457 | G | C5-C6-O6 | 6.83 | 132.70 | 128.60 |
| 1 | A | 2882 | A | O4'-C1'-N9 | 6.82 | 113.66 | 108.20 |
| 34 | a | 1006 | C | C2-N1-C1' | 6.74 | 126.22 | 118.80 |
| 1 | A | 792 | A | O4'-C1'-N9 | 6.73 | 113.59 | 108.20 |
| 56 | w | 60 | U | N3-C2-O2 | -6.73 | 117.49 | 122.20 |
| 34 | a | 1209 | A | C5-N7-C8 | -6.70 | 100.55 | 103.90 |
| 34 | a | 1019 | G | C4-N9-C1' | 6.70 | 135.21 | 126.50 |
| 58 | y | 22 | G | N9-C4-C5 | -6.67 | 102.73 | 105.40 |
| 56 | w | 2 | C | C5-C4-N4 | 6.66 | 124.86 | 120.20 |
| 1 | A | 2657 | C | O5'-P-OP2 | -6.64 | 99.72 | 105.70 |
| 34 | a | 732 | C | P-O3'-C3' | 6.64 | 127.66 | 119.70 |
| 1 | A | 186 | C | N1-C2-O2 | -6.63 | 114.92 | 118.90 |
| 1 | A | 353 | A | N3-C4-N9 | -6.62 | 122.10 | 127.40 |
| 34 | a | 1263 | U | C2-N1-C1' | 6.62 | 125.64 | 117.70 |
| 57 | x | 17 | C | O5'-P-OP1 | -6.62 | 99.74 | 105.70 |
| 1 | A | 1424 | A | O4'-C1'-N9 | -6.62 | 102.91 | 108.20 |
| 57 | x | 14 | A | C8-N9-C1' | -6.62 | 115.78 | 127.70 |
| 1 | A | 253 | A | C4-C5-N7 | 6.61 | 114.00 | 110.70 |
| 58 | y | 44 | G | C5-C6-O6 | -6.60 | 124.64 | 128.60 |
| 1 | A | 2189 | G | C4-N9-C1' | 6.60 | 135.08 | 126.50 |
| 1 | A | 1976 | U | C2-N1-C1' | -6.59 | 109.79 | 117.70 |
| 34 | a | 850 | A | O4'-C1'-N9 | 6.58 | 113.47 | 108.20 |
| 1 | A | 1853 | G | N3-C2-N2 | -6.58 | 115.30 | 119.90 |
| 1 | A | 1744 | A | C2-N3-C4 | -6.55 | 107.33 | 110.60 |
| 1 | A | 1699 | G | C8-N9-C4 | -6.54 | 103.78 | 106.40 |
| 1 | A | 1154 | C | C5-C6-N1 | 6.54 | 124.27 | 121.00 |
| 1 | A | 2189 | G | N3-C4-N9 | 6.54 | 129.92 | 126.00 |
| 1 | A | 2075 | A | C8-N9-C4 | 6.54 | 108.41 | 105.80 |
| 1 | A | 656 | A | C8-N9-C4 | 6.52 | 108.41 | 105.80 |
| 1 | A | 2592 | G | O4'-C1'-N9 | 6.52 | 113.42 | 108.20 |
| 1 | A | 552 | A | C5-N7-C8 | -6.51 | 100.64 | 103.90 |
| 1 | A | 1430 | G | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 1 | A | 1775 | G | C5-C6-O6 | -6.50 | 124.70 | 128.60 |
| 1 | A | 893 | U | C2-N1-C1' | -6.49 | 109.91 | 117.70 |
| 34 | a | 361 | U | C4-C5-C6 | 6.49 | 123.59 | 119.70 |
| 1 | A | 732 | G | N9-C4-C5 | -6.49 | 102.80 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1006 | G | N1-C6-O6 | -6.49 | 116.01 | 119.90 |
| 34 | a | 954 | G | N1-C6-O6 | 6.47 | 123.78 | 119.90 |
| 57 | x | 14 | A | C4-N9-C1' | 6.47 | 137.95 | 126.30 |
| 1 | A | 2577 | A | O4'-C1'-N9 | 6.46 | 113.37 | 108.20 |
| 1 | A | 2458 | G | C4-N9-C1' | -6.45 | 118.11 | 126.50 |
| 34 | a | 262 | G | C5-N7-C8 | -6.44 | 101.08 | 104.30 |
| 1 | A | 138 | A | N7-C8-N9 | 6.44 | 117.02 | 113.80 |
| 57 | x | 17 | C | O5'-P-OP2 | 6.42 | 118.41 | 110.70 |
| 1 | A | 977 | A | O4'-C1'-N9 | 6.42 | 113.34 | 108.20 |
| 1 | A | 11 | U | C2-N1-C1' | 6.38 | 125.36 | 117.70 |
| 56 | w | 76 | A | C8-N9-C4 | -6.38 | 103.25 | 105.80 |
| 57 | x | 76 | A | C4-C5-N7 | 6.37 | 113.89 | 110.70 |
| 57 | x | 76 | A | N7-C8-N9 | 6.37 | 116.99 | 113.80 |
| 1 | A | 2803 | C | N1-C2-O2 | -6.35 | 115.09 | 118.90 |
| 34 | a | 1268 | A | C5-N7-C8 | -6.34 | 100.73 | 103.90 |
| 34 | a | 1209 | A | N7-C8-N9 | 6.34 | 116.97 | 113.80 |
| 34 | a | 1340 | U | C5-C6-N1 | -6.34 | 119.53 | 122.70 |
| 1 | A | 669 | C | C5-C6-N1 | 6.33 | 124.17 | 121.00 |
| 1 | A | 1764 | U | C2-N1-C1' | -6.33 | 110.11 | 117.70 |
| 56 | w | 71 | G | C4-N9-C1' | 6.33 | 134.72 | 126.50 |
| 34 | a | 1109 | U | C6-N1-C2 | -6.32 | 117.21 | 121.00 |
| 34 | a | 1141 | C | C5-C6-N1 | -6.32 | 117.84 | 121.00 |
| 1 | A | 940 | U | N3-C2-O2 | -6.32 | 117.78 | 122.20 |
| 34 | a | 1109 | U | P-O3'-C3' | 6.31 | 127.27 | 119.70 |
| 34 | a | 1239 | U | N1-C2-O2 | 6.30 | 127.21 | 122.80 |
| 1 | A | 1604 | A | N1-C2-N3 | 6.30 | 132.45 | 129.30 |
| 59 | z | 373 | ALA | C-N-CD | -6.29 | 106.76 | 120.60 |
| 1 | A | 989 | A | C2-N3-C4 | -6.29 | 107.45 | 110.60 |
| 1 | A | 39 | C | N3-C4-N4 | -6.29 | 113.60 | 118.00 |
| 21 | X | 57 | LEU | CA-CB-CG | 6.29 | 129.76 | 115.30 |
| 34 | a | 1268 | A | N7-C8-N9 | 6.25 | 116.93 | 113.80 |
| 56 | w | 2 | C | N1-C2-N3 | -6.25 | 114.82 | 119.20 |
| 10 | K | 112 | MET | C-N-CD | 6.24 | 141.51 | 128.40 |
| 1 | A | 940 | U | N1-C2-O2 | 6.23 | 127.16 | 122.80 |
| 1 | A | 253 | A | N7-C8-N9 | 6.23 | 116.92 | 113.80 |
| 1 | A | 1604 | A | C2-N3-C4 | -6.23 | 107.48 | 110.60 |
| 56 | w | 71 | G | C8-N9-C1' | -6.22 | 118.92 | 127.00 |
| 1 | A | 1066 | A | C8-N9-C4 | -6.18 | 103.33 | 105.80 |
| 55 | v | 13 | A | N7-C8-N9 | 6.18 | 116.89 | 113.80 |
| 1 | A | 2623 | C | O5'-P-OP2 | -6.18 | 100.14 | 105.70 |
| 34 | a | 1480 | A | C4-C5-N7 | 6.17 | 113.78 | 110.70 |
| 1 | A | 214 | G | O4'-C1'-N9 | 6.17 | 113.14 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 2468 | U | N3-C2-O2 | -6.17 | 117.88 | 122.20 |
| 1 | A | 187 | A | OP1-P-OP2 | 6.16 | 128.85 | 119.60 |
| 34 | a | 1497 | A | C5-C6-N1 | -6.16 | 114.62 | 117.70 |
| 1 | A | 1764 | U | C6-N1-C1' | 6.15 | 129.81 | 121.20 |
| 1 | A | 2189 | G | C8-N9-C1' | -6.14 | 119.02 | 127.00 |
| 56 | w | 63 | G | N7-C8-N9 | 6.14 | 116.17 | 113.10 |
| 1 | A | 837 | C | N1-C2-O2 | -6.14 | 115.22 | 118.90 |
| 34 | a | 1263 | U | N3-C2-O2 | -6.13 | 117.91 | 122.20 |
| 57 | x | 22 | G | C4-C5-N7 | 6.13 | 113.25 | 110.80 |
| 1 | A | 553 | A | O4'-C1'-N9 | 6.12 | 113.10 | 108.20 |
| 1 | A | 577 | U | O4'-C1'-N1 | 6.11 | 113.09 | 108.20 |
| 34 | a | 1069 | U | C2-N1-C1' | 6.11 | 125.03 | 117.70 |
| 13 | P | 44 | GLY | C-N-CA | 6.10 | 136.96 | 121.70 |
| 34 | a | 1060 | G | O5'-P-OP2 | -6.10 | 100.21 | 105.70 |
| 1 | A | 1248 | A | C2-N3-C4 | -6.09 | 107.55 | 110.60 |
| 1 | A | 1773 | C | O4'-C1'-N1 | 6.08 | 113.07 | 108.20 |
| 58 | y | 46 | G | N3-C2-N2 | 6.07 | 124.15 | 119.90 |
| 1 | A | 1292 | A | N1-C6-N6 | 6.07 | 122.24 | 118.60 |
| 1 | A | 2302 | U | C5-C4-O4 | 6.06 | 129.54 | 125.90 |
| 18 | U | 74 | LEU | CA-CB-CG | 6.06 | 129.24 | 115.30 |
| 1 | A | 839 | A | N9-C4-C5 | -6.06 | 103.38 | 105.80 |
| 34 | a | 1019 | G | C8-N9-C1' | -6.06 | 119.12 | 127.00 |
| 1 | A | 2532 | C | N1-C2-O2 | -6.05 | 115.27 | 118.90 |
| 34 | a | 1203 | G | N1-C6-O6 | -6.04 | 116.27 | 119.90 |
| 1 | A | 1077 | A | N1-C6-N6 | 6.04 | 122.23 | 118.60 |
| 34 | a | 1480 | A | C8-N9-C4 | -6.04 | 103.38 | 105.80 |
| 18 | U | 92 | ARG | NE-CZ-NH2 | -6.03 | 117.28 | 120.30 |
| 1 | A | 1066 | A | N3-C4-N9 | -6.03 | 122.58 | 127.40 |
| 1 | A | 2090 | G | N1-C6-O6 | 6.01 | 123.50 | 119.90 |
| 58 | y | 45 | U | C2-N1-C1' | 6.01 | 124.91 | 117.70 |
| 1 | A | 1006 | G | C5-C6-O6 | 6.00 | 132.20 | 128.60 |
| 1 | A | 990 | G | C5-C6-O6 | 6.00 | 132.20 | 128.60 |
| 1 | A | 1744 | A | N3-C4-N9 | -6.00 | 122.60 | 127.40 |
| 1 | A | 1589 | C | C5-C6-N1 | 5.99 | 124.00 | 121.00 |
| 34 | a | 856 | G | N1-C6-O6 | -5.99 | 116.31 | 119.90 |
| 34 | a | 1502 | C | N1-C2-O2 | -5.98 | 115.31 | 118.90 |
| 56 | w | 48 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 57 | x | 14 | A | N7-C8-N9 | -5.97 | 110.81 | 113.80 |
| 1 | A | 1218 | A | OP1-P-O3' | 5.95 | 118.29 | 105.20 |
| 34 | a | 361 | U | C2-N3-C4 | -5.95 | 123.43 | 127.00 |
| 34 | a | 884 | G | C5-C6-O6 | -5.95 | 125.03 | 128.60 |
| 59 | z | 445 | GLN | N-CA-C | -5.94 | 94.95 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1699 | G | P-O3'-C3' | 5.94 | 126.83 | 119.70 |
| 1 | A | 2802 | A | C2-N3-C4 | 5.93 | 113.57 | 110.60 |
| 58 | y | 29 | G | N3-C4-N9 | 5.93 | 129.56 | 126.00 |
| 1 | A | 541 | C | C6-N1-C2 | 5.93 | 122.67 | 120.30 |
| 1 | A | 398 | G | O4'-C1'-N9 | 5.91 | 112.93 | 108.20 |
| 1 | A | 1589 | C | N3-C2-O2 | -5.91 | 117.76 | 121.90 |
| 1 | A | 1018 | G | O5'-P-OP2 | -5.91 | 100.38 | 105.70 |
| 1 | A | 1097 | C | C6-N1-C2 | -5.91 | 117.94 | 120.30 |
| 1 | A | 552 | A | C8-N9-C4 | -5.90 | 103.44 | 105.80 |
| 1 | A | 1370 | G | N1-C6-O6 | -5.89 | 116.36 | 119.90 |
| 1 | A | 798 | A | P-O3'-C3' | 5.89 | 126.77 | 119.70 |
| 1 | A | 2341 | G | N1-C6-O6 | -5.89 | 116.36 | 119.90 |
| 34 | a | 1046 | C | O5'-P-OP1 | -5.89 | 100.40 | 105.70 |
| 1 | A | 725 | C | C5-C6-N1 | -5.88 | 118.06 | 121.00 |
| 34 | a | 1006 | C | N1-C2-O2 | 5.88 | 122.43 | 118.90 |
| 1 | A | 552 | A | N7-C8-N9 | 5.85 | 116.73 | 113.80 |
| 34 | a | 514 | G | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 57 | x | 17 | C | C6-N1-C1' | -5.85 | 113.78 | 120.80 |
| 58 | y | 10 | G | N1-C6-O6 | 5.85 | 123.41 | 119.90 |
| 1 | A | 1589 | C | C6-N1-C2 | -5.84 | 117.96 | 120.30 |
| 1 | A | 2331 | A | N1-C6-N6 | 5.84 | 122.11 | 118.60 |
| 1 | A | 1965 | U | O5'-P-OP2 | -5.84 | 100.44 | 105.70 |
| 1 | A | 1796 | U | O5'-P-OP1 | -5.84 | 100.45 | 105.70 |
| 1 | A | 551 | C | C6-N1-C2 | 5.83 | 122.63 | 120.30 |
| 1 | A | 2189 | G | C4-C5-N7 | 5.83 | 113.13 | 110.80 |
| 34 | a | 1007 | C | C6-N1-C1' | -5.83 | 113.81 | 120.80 |
| 1 | A | 11 | U | N1-C2-O2 | 5.82 | 126.87 | 122.80 |
| 1 | A | 1026 | A | C8-N9-C4 | 5.82 | 108.13 | 105.80 |
| 1 | A | 2517 | U | C5-C4-O4 | -5.80 | 122.42 | 125.90 |
| 1 | A | 2297 | A | N9-C1'-C2' | 5.80 | 121.54 | 114.00 |
| 1 | A | 1091 | A | N3-C4-C5 | 5.79 | 130.86 | 126.80 |
| 1 | A | 136 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 1 | A | 789 | G | O5'-P-OP2 | -5.79 | 100.49 | 105.70 |
| 57 | x | 14 | A | N1-C6-N6 | 5.79 | 122.08 | 118.60 |
| 1 | A | 2081 | A | C8-N9-C4 | 5.79 | 108.12 | 105.80 |
| 1 | A | 794 | G | N7-C8-N9 | -5.79 | 110.21 | 113.10 |
| 1 | A | 2458 | G | C6-C5-N7 | 5.79 | 133.87 | 130.40 |
| 34 | a | 489 | G | N3-C4-C5 | -5.79 | 125.70 | 128.60 |
| 58 | y | 45 | U | C6-N1-C2 | -5.78 | 117.53 | 121.00 |
| 1 | A | 893 | U | N3-C4-O4 | -5.78 | 115.36 | 119.40 |
| 1 | A | 1343 | C | C6-N1-C2 | -5.78 | 117.99 | 120.30 |
| 1 | A | 2402 | G | O4'-C1'-N9 | 5.77 | 112.81 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2189 | G | C5-C6-O6 | -5.75 | 125.15 | 128.60 |
| 1 | A | 2221 | C | C2-N3-C4 | 5.75 | 122.78 | 119.90 |
| 1 | A | 253 | A | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 1 | A | 851 | G | C8-N9-C4 | 5.75 | 108.70 | 106.40 |
| 1 | A | 1868 | C | C6-N1-C2 | -5.74 | 118.00 | 120.30 |
| 1 | A | 136 | G | C4-C5-N7 | 5.74 | 113.09 | 110.80 |
| 1 | A | 138 | A | C5-N7-C8 | -5.74 | 101.03 | 103.90 |
| 57 | x | 46 | G | N3-C2-N2 | -5.73 | 115.89 | 119.90 |
| 1 | A | 138 | A | N1-C2-N3 | 5.72 | 132.16 | 129.30 |
| 34 | a | 750 | A | C8-N9-C4 | 5.72 | 108.09 | 105.80 |
| 34 | a | 884 | G | N1-C6-O6 | 5.72 | 123.33 | 119.90 |
| 1 | A | 1248 | A | N9-C4-C5 | -5.72 | 103.51 | 105.80 |
| 1 | A | 1985 | G | N1-C6-O6 | -5.72 | 116.47 | 119.90 |
| 58 | y | 33 | U | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 1 | A | 794 | G | C4-N9-C1' | -5.71 | 119.08 | 126.50 |
| 1 | A | 2458 | G | C8-N9-C1' | 5.70 | 134.41 | 127.00 |
| 1 | A | 839 | A | N1-C6-N6 | 5.70 | 122.02 | 118.60 |
| 34 | a | 1112 | C | C6-N1-C2 | -5.69 | 118.02 | 120.30 |
| 34 | a | 1037 | C | C1'-O4'-C4' | -5.69 | 105.35 | 109.90 |
| 58 | y | 44 | G | N1-C6-O6 | 5.69 | 123.31 | 119.90 |
| 34 | a | 732 | C | C2-N1-C1' | 5.69 | 125.06 | 118.80 |
| 34 | a | 1019 | G | N3-C4-N9 | 5.69 | 129.41 | 126.00 |
| 34 | a | 1317 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 1 | A | 89 | A | N7-C8-N9 | 5.68 | 116.64 | 113.80 |
| 1 | A | 1589 | C | C6-N1-C1' | -5.68 | 113.99 | 120.80 |
| 1 | A | 1951 | G | C4-N9-C1' | -5.67 | 119.12 | 126.50 |
| 34 | a | 717 | A | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 1 | A | 1744 | A | C5-N7-C8 | -5.67 | 101.07 | 103.90 |
| 1 | A | 1853 | G | N9-C4-C5 | 5.67 | 107.67 | 105.40 |
| 34 | a | 25 | U | C5-C4-O4 | -5.66 | 122.50 | 125.90 |
| 58 | y | 46 | G | C4-C5-C6 | 5.65 | 122.19 | 118.80 |
| 34 | a | 489 | G | C4-N9-C1' | 5.65 | 133.84 | 126.50 |
| 1 | A | 2801 | C | O4'-C1'-N1 | 5.64 | 112.72 | 108.20 |
| 1 | A | 2189 | G | N1-C6-O6 | 5.64 | 123.29 | 119.90 |
| 58 | y | 1 | G | C8-N9-C4 | -5.64 | 104.14 | 106.40 |
| 3 | C | 62 | VAL | CB-CA-C | 5.64 | 122.12 | 111.40 |
| 34 | a | 1380 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 1 | A | 1248 | A | C4-C5-N7 | 5.63 | 113.52 | 110.70 |
| 1 | A | 136 | G | N7-C8-N9 | 5.63 | 115.91 | 113.10 |
| 1 | A | 1298 | A | C2-N3-C4 | 5.63 | 113.41 | 110.60 |
| 57 | x | 25 | C | C2-N3-C4 | -5.63 | 117.09 | 119.90 |
| 1 | A | 2013 | G | OP1-P-O3' | -5.62 | 92.83 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 640 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 1 | A | 986 | G | OP2-P-O3' | 5.62 | 117.56 | 105.20 |
| 1 | A | 1256 | G | N9-C4-C5 | -5.62 | 103.15 | 105.40 |
| 1 | A | 805 | G | O5'-P-OP2 | -5.62 | 100.65 | 105.70 |
| 1 | A | 1005 | C | N1-C2-O2 | -5.62 | 115.53 | 118.90 |
| 1 | A | 1820 | C | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 34 | a | 1037 | C | C5'-C4'-O4' | 5.61 | 115.83 | 109.10 |
| 34 | a | 556 | A | N9-C4-C5 | 5.60 | 108.04 | 105.80 |
| 1 | A | 977 | A | C4-C5-N7 | 5.60 | 113.50 | 110.70 |
| 1 | A | 2001 | G | N3-C4-N9 | 5.60 | 129.36 | 126.00 |
| 4 | D | 274 | ARG | C-N-CA | 5.60 | 135.69 | 121.70 |
| 1 | A | 198 | C | N1-C2-O2 | -5.59 | 115.55 | 118.90 |
| 1 | A | 732 | G | N3-C4-N9 | 5.59 | 129.35 | 126.00 |
| 1 | A | 990 | G | C6-C5-N7 | 5.58 | 133.75 | 130.40 |
| 1 | A | 2840 | G | C8-N9-C4 | 5.58 | 108.63 | 106.40 |
| 1 | A | 989 | A | C6-C5-N7 | -5.58 | 128.40 | 132.30 |
| 1 | A | 2517 | U | N3-C4-O4 | 5.58 | 123.30 | 119.40 |
| 1 | A | 2400 | G | N3-C2-N2 | -5.56 | 116.00 | 119.90 |
| 1 | A | 800 | C | O5'-P-OP2 | -5.56 | 100.70 | 105.70 |
| 1 | A | 801 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 1 | A | 989 | A | O5'-P-OP1 | 5.55 | 117.36 | 110.70 |
| 1 | A | 2609 | A | O5'-P-OP2 | -5.55 | 100.71 | 105.70 |
| 12 | O | 8 | LEU | CA-CB-CG | 5.55 | 128.06 | 115.30 |
| 56 | w | 76 | A | C5-N7-C8 | -5.55 | 101.13 | 103.90 |
| 34 | a | 1048 | U | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 1 | A | 1773 | C | C5-C4-N4 | 5.54 | 124.08 | 120.20 |
| 34 | a | 1007 | C | N3-C2-O2 | -5.54 | 118.02 | 121.90 |
| 1 | A | 1091 | A | N7-C8-N9 | -5.54 | 111.03 | 113.80 |
| 34 | a | 1019 | G | C6-C5-N7 | -5.53 | 127.08 | 130.40 |
| 45 | l | 52 | LEU | CA-CB-CG | 5.53 | 128.01 | 115.30 |
| 1 | A | 839 | A | C5-C6-N6 | -5.52 | 119.28 | 123.70 |
| 1 | A | 1357 | U | N3-C2-O2 | -5.52 | 118.33 | 122.20 |
| 1 | A | 2458 | G | N3-C4-N9 | -5.52 | 122.69 | 126.00 |
| 1 | A | 138 | A | C8-N9-C4 | -5.52 | 103.59 | 105.80 |
| 59 | z | 292 | PRO | CA-C-N | 5.52 | 127.23 | 116.20 |
| 1 | A | 989 | A | N9-C1'-C2' | 5.51 | 121.17 | 114.00 |
| 34 | a | 1007 | C | C6-N1-C2 | -5.51 | 118.09 | 120.30 |
| 1 | A | 817 | G | C5-C6-O6 | -5.51 | 125.29 | 128.60 |
| 1 | A | 1359 | C | C6-N1-C2 | -5.51 | 118.09 | 120.30 |
| 1 | A | 2413 | C | N1-C2-O2 | 5.51 | 122.21 | 118.90 |
| 34 | a | 1141 | C | C4-C5-C6 | 5.51 | 120.15 | 117.40 |
| 56 | w | 12 | U | C5-C4-O4 | -5.50 | 122.60 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 57 | x | 14 | A | N1-C2-N3 | 5.50 | 132.05 | 129.30 |
| 34 | a | 550 | G | N1-C6-O6 | -5.50 | 116.60 | 119.90 |
| 1 | A | 2633 | C | N1-C2-O2 | -5.50 | 115.60 | 118.90 |
| 1 | A | 2622 | U | N1-C2-O2 | -5.49 | 118.96 | 122.80 |
| 1 | A | 2120 | U | N3-C2-O2 | -5.49 | 118.36 | 122.20 |
| 22 | Y | 67 | LEU | CA-CB-CG | 5.48 | 127.91 | 115.30 |
| 1 | A | 36 | C | N3-C2-O2 | -5.48 | 118.06 | 121.90 |
| 34 | a | 551 | G | C5-C6-O6 | -5.48 | 125.31 | 128.60 |
| 1 | A | 1746 | A | O5'-P-OP1 | -5.48 | 100.77 | 105.70 |
| 1 | A | 2583 | A | N1-C6-N6 | 5.48 | 121.89 | 118.60 |
| 1 | A | 1125 | C | C2-N1-C1' | 5.48 | 124.82 | 118.80 |
| 1 | A | 709 | G | N1-C6-O6 | -5.47 | 116.62 | 119.90 |
| 1 | A | 1662 | C | N1-C2-O2 | -5.47 | 115.62 | 118.90 |
| 58 | y | 46 | G | C6-N1-C2 | -5.47 | 121.82 | 125.10 |
| 1 | A | 1758 | C | C5-C6-N1 | 5.46 | 123.73 | 121.00 |
| 1 | A | 2554 | G | N1-C6-O6 | -5.46 | 116.62 | 119.90 |
| 1 | A | 598 | U | C5-C4-O4 | -5.45 | 122.63 | 125.90 |
| 1 | A | 1017 | A | C5-C6-N6 | 5.44 | 128.05 | 123.70 |
| 1 | A | 2398 | U | N3-C4-O4 | 5.44 | 123.21 | 119.40 |
| 34 | a | 361 | U | C6-N1-C2 | 5.44 | 124.27 | 121.00 |
| 34 | a | 116 | G | O5'-P-OP1 | -5.44 | 100.80 | 105.70 |
| 1 | A | 2431 | C | N3-C4-C5 | 5.44 | 124.08 | 121.90 |
| 34 | a | 1109 | U | N3-C4-O4 | 5.44 | 123.21 | 119.40 |
| 1 | A | 1746 | A | O5'-P-OP2 | 5.43 | 117.22 | 110.70 |
| 1 | A | 1106 | U | N3-C2-O2 | -5.42 | 118.40 | 122.20 |
| 41 | h | 112 | LEU | CA-CB-CG | 5.42 | 127.75 | 115.30 |
| 1 | A | 1066 | A | N3-C4-C5 | 5.41 | 130.59 | 126.80 |
| 1 | A | 701 | A | N1-C6-N6 | 5.41 | 121.85 | 118.60 |
| 25 | 1 | 80 | LEU | CA-CB-CG | -5.41 | 102.86 | 115.30 |
| 1 | A | 1366 | A | N1-C6-N6 | 5.41 | 121.85 | 118.60 |
| 1 | A | 2370 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 34 | a | 1445 | G | O5'-P-OP2 | -5.41 | 100.83 | 105.70 |
| 1 | A | 89 | A | C8-N9-C4 | -5.41 | 103.64 | 105.80 |
| 1 | A | 1292 | A | N9-C4-C5 | -5.41 | 103.64 | 105.80 |
| 1 | A | 2617 | C | C2-N1-C1' | -5.41 | 112.85 | 118.80 |
| 1 | A | 136 | G | C5-N7-C8 | -5.40 | 101.60 | 104.30 |
| 27 | 3 | 4 | LEU | CA-CB-CG | 5.39 | 127.70 | 115.30 |
| 56 | w | 63 | G | C6-C5-N7 | -5.39 | 127.16 | 130.40 |
| 1 | A | 1154 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 1 | A | 1818 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 1 | A | 989 | A | C5-C6-N6 | -5.38 | 119.40 | 123.70 |
| 1 | A | 1646 | G | N1-C6-O6 | -5.37 | 116.67 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1417 | U | N1-C2-O2 | 5.36 | 126.56 | 122.80 |
| 50 | q | 6 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |
| 1 | A | 2120 | U | N1-C2-O2 | 5.35 | 126.55 | 122.80 |
| 1 | A | 2591 | U | C2-N1-C1' | 5.35 | 124.12 | 117.70 |
| 34 | a | 797 | U | OP2-P-O3' | 5.35 | 116.97 | 105.20 |
| 34 | a | 891 | A | O5'-P-OP2 | -5.35 | 100.89 | 105.70 |
| 34 | a | 1267 | A | N1-C6-N6 | 5.35 | 121.81 | 118.60 |
| 1 | A | 2505 | G | C5-C6-O6 | 5.34 | 131.81 | 128.60 |
| 57 | x | 17 | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 1 | A | 657 | A | C8-N9-C4 | 5.34 | 107.94 | 105.80 |
| 34 | a | 28 | G | OP2-P-O3' | 5.33 | 116.94 | 105.20 |
| 1 | A | 989 | A | N7-C8-N9 | 5.33 | 116.47 | 113.80 |
| 34 | a | 417 | U | C2-N1-C1' | 5.33 | 124.10 | 117.70 |
| 34 | a | 1203 | G | C6-C5-N7 | 5.33 | 133.60 | 130.40 |
| 1 | A | 2456 | G | N3-C2-N2 | 5.33 | 123.63 | 119.90 |
| 57 | x | 76 | A | N1-C6-N6 | 5.33 | 121.80 | 118.60 |
| 1 | A | 1091 | A | C6-C5-N7 | -5.33 | 128.57 | 132.30 |
| 1 | A | 2801 | C | C2-N1-C1' | -5.33 | 112.94 | 118.80 |
| 1 | A | 2298 | A | N3-C4-N9 | -5.33 | 123.14 | 127.40 |
| 34 | a | 715 | G | O5'-P-OP2 | -5.33 | 100.91 | 105.70 |
| 1 | A | 1818 | C | N3-C2-O2 | -5.32 | 118.17 | 121.90 |
| 1 | A | 2589 | G | N3-C2-N2 | -5.32 | 116.17 | 119.90 |
| 1 | A | 1612 | A | N1-C2-N3 | -5.32 | 126.64 | 129.30 |
| 1 | A | 2018 | G | O5'-P-OP1 | 5.31 | 117.08 | 110.70 |
| 1 | A | 2428 | C | C6-N1-C2 | -5.31 | 118.18 | 120.30 |
| 1 | A | 2505 | G | N1-C6-O6 | -5.30 | 116.72 | 119.90 |
| 1 | A | 1256 | G | C8-N9-C4 | 5.30 | 108.52 | 106.40 |
| 1 | A | 2331 | A | N9-C4-C5 | -5.29 | 103.68 | 105.80 |
| 1 | A | 2070 | G | O5'-P-OP2 | -5.29 | 100.94 | 105.70 |
| 56 | w | 75 | C | N3-C2-O2 | -5.29 | 118.20 | 121.90 |
| 1 | A | 2535 | G | OP2-P-O3' | 5.28 | 116.83 | 105.20 |
| 34 | a | 872 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 1 | A | 2418 | G | C4-N9-C1' | 5.28 | 133.36 | 126.50 |
| 34 | a | 1301 | A | C8-N9-C4 | -5.28 | 103.69 | 105.80 |
| 1 | A | 542 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 34 | a | 891 | A | P-O3'-C3' | 5.28 | 126.03 | 119.70 |
| 1 | A | 88 | U | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 34 | a | 1503 | G | N1-C6-O6 | -5.27 | 116.74 | 119.90 |
| 1 | A | 1955 | C | N3-C4-N4 | -5.27 | 114.31 | 118.00 |
| 1 | A | 794 | G | C8-N9-C4 | 5.26 | 108.51 | 106.40 |
| 1 | A | 2831 | G | C5-C6-O6 | -5.26 | 125.44 | 128.60 |
| 34 | a | 877 | C | N1-C2-O2 | -5.26 | 115.74 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1768 | G | O5'-P-OP1 | -5.25 | 100.97 | 105.70 |
| 1 | A | 353 | A | N9-C4-C5 | 5.25 | 107.90 | 105.80 |
| 1 | A | 242 | G | O5'-P-OP2 | -5.25 | 100.98 | 105.70 |
| 1 | A | 1856 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 1 | A | 2891 | A | N1-C6-N6 | -5.25 | 115.45 | 118.60 |
| 1 | A | 2624 | U | C5-C6-N1 | -5.24 | 120.08 | 122.70 |
| 34 | a | 547 | A | N9-C4-C5 | -5.24 | 103.70 | 105.80 |
| 56 | w | 2 | C | N3-C4-N4 | -5.23 | 114.34 | 118.00 |
| 57 | x | 16 | C | OP1-P-O3' | 5.23 | 116.71 | 105.20 |
| 1 | A | 2189 | G | N9-C4-C5 | -5.22 | 103.31 | 105.40 |
| 1 | A | 1425 | G | O5'-P-OP2 | -5.22 | 101.00 | 105.70 |
| 1 | A | 2100 | U | N1-C2-O2 | -5.22 | 119.15 | 122.80 |
| 34 | a | 1441 | C | C6-N1-C2 | 5.22 | 122.39 | 120.30 |
| 56 | w | 72 | C | N3-C2-O2 | -5.22 | 118.25 | 121.90 |
| 1 | A | 1196 | G | C8-N9-C4 | 5.21 | 108.49 | 106.40 |
| 59 | z | 373 | ALA | C-N-CA | 5.21 | 143.87 | 122.00 |
| 1 | A | 441 | A | C2-N3-C4 | 5.20 | 113.20 | 110.60 |
| 1 | A | 598 | U | OP1-P-OP2 | 5.20 | 127.41 | 119.60 |
| 1 | A | 1865 | G | OP2-P-O3' | 5.20 | 116.64 | 105.20 |
| 34 | a | 953 | A | N7-C8-N9 | 5.20 | 116.40 | 113.80 |
| 34 | a | 1389 | U | C5-C6-N1 | -5.20 | 120.10 | 122.70 |
| 58 | y | 1 | G | N3-C4-C5 | -5.20 | 126.00 | 128.60 |
| 34 | a | 356 | A | N1-C6-N6 | -5.20 | 115.48 | 118.60 |
| 1 | A | 504 | A | N1-C6-N6 | -5.19 | 115.48 | 118.60 |
| 1 | A | 1853 | G | N3-C4-N9 | -5.19 | 122.88 | 126.00 |
| 1 | A | 11 | U | N3-C2-O2 | -5.19 | 118.56 | 122.20 |
| 1 | A | 2114 | G | C8-N9-C4 | 5.19 | 108.48 | 106.40 |
| 34 | a | 23 | G | N1-C6-O6 | 5.19 | 123.02 | 119.90 |
| 34 | a | 1420 | C | OP2-P-O3' | 5.19 | 116.62 | 105.20 |
| 34 | a | 1496 | A | C5-C6-N1 | -5.19 | 115.10 | 117.70 |
| 1 | A | 2297 | A | C5-C6-N1 | -5.19 | 115.11 | 117.70 |
| 1 | A | 538 | A | OP1-P-OP2 | 5.18 | 127.38 | 119.60 |
| 1 | A | 1774 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 34 | a | 1008 | C | C2-N1-C1' | 5.18 | 124.50 | 118.80 |
| 34 | a | 1482 | G | C6-N1-C2 | 5.18 | 128.21 | 125.10 |
| 1 | A | 942 | C | C2-N1-C1' | 5.17 | 124.49 | 118.80 |
| 1 | A | 1017 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 1 | A | 1814 | A | C8-N9-C4 | 5.16 | 107.86 | 105.80 |
| 34 | a | 514 | G | OP2-P-O3' | 5.16 | 116.55 | 105.20 |
| 1 | A | 837 | C | C2-N1-C1' | -5.16 | 113.13 | 118.80 |
| 58 | y | 25 | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 1 | A | 597 | A | O5'-P-OP1 | -5.15 | 101.06 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 2495 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 1 | A | 1761 | G | C4-N9-C1' | -5.14 | 119.82 | 126.50 |
| 34 | a | 25 | U | N3-C4-O4 | 5.14 | 123.00 | 119.40 |
| 1 | A | 1773 | C | C6-N1-C1' | 5.13 | 126.96 | 120.80 |
| 34 | a | 1398 | G | O5'-P-OP2 | -5.13 | 101.08 | 105.70 |
| 1 | A | 1808 | U | C2-N3-C4 | -5.13 | 123.92 | 127.00 |
| 1 | A | 552 | A | N3-C4-N9 | -5.12 | 123.30 | 127.40 |
| 1 | A | 854 | G | C8-N9-C4 | 5.12 | 108.45 | 106.40 |
| 1 | A | 553 | A | C5-N7-C8 | -5.12 | 101.34 | 103.90 |
| 58 | y | 19 | G | C4-N9-C1' | -5.12 | 119.84 | 126.50 |
| 1 | A | 2675 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 1 | A | 1185 | U | N1-C2-O2 | -5.11 | 119.22 | 122.80 |
| 34 | a | 671 | A | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 1 | A | 2092 | A | C8-N9-C4 | -5.11 | 103.76 | 105.80 |
| 1 | A | 554 | G | C5-N7-C8 | -5.11 | 101.75 | 104.30 |
| 1 | A | 1248 | A | C6-C5-N7 | -5.10 | 128.73 | 132.30 |
| 1 | A | 604 | G | C5-C6-O6 | 5.10 | 131.66 | 128.60 |
| 1 | A | 1821 | A | O5'-P-OP1 | -5.10 | 101.11 | 105.70 |
| 1 | A | 2528 | C | N3-C4-C5 | 5.10 | 123.94 | 121.90 |
| 1 | A | 554 | G | C4-C5-N7 | 5.10 | 112.84 | 110.80 |
| 1 | A | 2621 | C | C2-N3-C4 | -5.09 | 117.35 | 119.90 |
| 34 | a | 324 | C | O5'-P-OP1 | -5.09 | 101.12 | 105.70 |
| 1 | A | 2614 | G | N9-C4-C5 | 5.09 | 107.44 | 105.40 |
| 34 | a | 323 | A | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 34 | a | 293 | G | C8-N9-C4 | 5.09 | 108.44 | 106.40 |
| 34 | a | 1502 | C | C6-N1-C2 | 5.09 | 122.33 | 120.30 |
| 19 | V | 18 | LEU | CA-CB-CG | 5.08 | 126.99 | 115.30 |
| 1 | A | 604 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 55 | v | 13 | A | C4-C5-N7 | 5.08 | 113.24 | 110.70 |
| 1 | A | 732 | G | N3-C2-N2 | 5.08 | 123.45 | 119.90 |
| 1 | A | 1005 | C | O5'-P-OP2 | -5.08 | 101.13 | 105.70 |
| 56 | w | 75 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 1 | A | 182 | G | N9-C4-C5 | -5.07 | 103.37 | 105.40 |
| 34 | a | 847 | G | C5-C6-O6 | -5.07 | 125.56 | 128.60 |
| 1 | A | 989 | A | C8-N9-C4 | -5.07 | 103.77 | 105.80 |
| 1 | A | 1915 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 1 | A | 2249 | G | N3-C4-C5 | -5.07 | 126.07 | 128.60 |
| 34 | a | 953 | A | C4-C5-N7 | 5.07 | 113.23 | 110.70 |
| 1 | A | 1955 | C | C5-C4-N4 | 5.07 | 123.75 | 120.20 |
| 1 | A | 843 | C | N1-C2-O2 | -5.06 | 115.86 | 118.90 |
| 1 | A | 932 | C | O5'-P-OP2 | -5.06 | 101.15 | 105.70 |
| 34 | a | 844 | C | N1-C2-O2 | -5.06 | 115.87 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 2319 | G | C4-C5-N7 | 5.05 | 112.82 | 110.80 |
| 1 | A | 2120 | U | C2-N1-C1' | 5.05 | 123.76 | 117.70 |
| 45 | l | 84 | LEU | CA-CB-CG | 5.04 | 126.89 | 115.30 |
| 1 | A | 951 | G | C8-N9-C1' | 5.04 | 133.55 | 127.00 |
| 1 | A | 1699 | G | C4-N9-C1' | 5.04 | 133.05 | 126.50 |
| 1 | A | 2103 | A | O5'-P-OP2 | -5.04 | 101.17 | 105.70 |
| 1 | A | 1643 | C | C2-N1-C1' | 5.03 | 124.33 | 118.80 |
| 1 | A | 2219 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 1 | A | 592 | G | N1-C6-O6 | -5.03 | 116.89 | 119.90 |
| 1 | A | 1292 | A | C5-C6-N6 | -5.03 | 119.68 | 123.70 |
| 1 | A | 1853 | G | N1-C2-N2 | 5.03 | 120.72 | 116.20 |
| 1 | A | 2163 | C | C5-C6-N1 | 5.03 | 123.51 | 121.00 |
| 1 | A | 2591 | U | C5-C4-O4 | -5.02 | 122.89 | 125.90 |
| 34 | a | 1006 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 57 | x | 25 | C | N1-C2-O2 | -5.02 | 115.89 | 118.90 |
| 58 | y | 14 | A | N1-C6-N6 | 5.01 | 121.61 | 118.60 |
| 1 | A | 1761 | G | C4-C5-N7 | 5.01 | 112.80 | 110.80 |

There are no chirality outliers.

All (17) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 26 | 2 | 44 | LEU | Peptide |
| 28 | 4 | 65 | ASP | Peptide |
| 10 | K | 70 | LYS | Peptide |
| 19 | V | 43 | GLU | Peptide |
| 37 | d | 179 | GLU | Peptide |
| 39 | f | 97 | PHE | Peptide |
| 42 | i | 117 | HIS | Peptide |
| 42 | i | 45 | ALA | Peptide |
| 52 | s | 29 | ARG | Peptide |
| 52 | s | 8 | GLY | Peptide |
| 53 | t | 9 | ASN | Peptide |
| 59 | z | 185 | ILE | Peptide |
| 59 | z | 246 | THR | Peptide |
| 59 | z | 372 | THR | Peptide |
| 59 | z | 396 | LEU | Peptide |
| 59 | z | 419 | GLU | Peptide |
| 59 | z | 480 | GLU | Peptide |

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3 | C | 130/228 (57%) | 94 (72%) | 25 (19%) | 11 (8%) | 1 | 1 |
| 4 | D | 273/276 (99%) | 255 (93%) | 15 (6%) | 3 (1%) | 14 | 30 |
| 5 | E | 202/206 (98%) | 188 (93%) | 11 (5%) | 3 (2%) | 10 | 21 |
| 6 | F | 201/210 (96%) | 184 (92%) | 12 (6%) | 5 (2%) | 5 | 9 |
| 7 | G | 179/182 (98%) | 162 (90%) | 10 (6%) | 7 (4%) | 3 | 4 |
| 8 | H | 172/180 (96%) | 148 (86%) | 17 (10%) | 7 (4%) | 3 | 3 |
| 9 | J | 128/173 (74%) | 76 (59%) | 22 (17%) | 30 (23%) | 0 | 0 |
| 10 | K | 137/147 (93%) | 85 (62%) | 31 (23%) | 21 (15%) | 0 | 0 |
| 11 | N | 138/140 (99%) | 129 (94%) | 5 (4%) | 4 (3%) | 4 | 7 |
| 12 | O | 120/122 (98%) | 112 (93%) | 7 (6%) | 1 (1%) | 19 | 39 |
| 13 | P | 147/150 (98%) | 129 (88%) | 16 (11%) | 2 (1%) | 11 | 22 |
| 14 | Q | 139/141 (99%) | 131 (94%) | 7 (5%) | 1 (1%) | 22 | 43 |
| 15 | R | 116/118 (98%) | 111 (96%) | 5 (4%) | 0 | 100 | 100 |
| 16 | S | 108/112 (96%) | 96 (89%) | 10 (9%) | 2 (2%) | 8 | 15 |
| 17 | T | 129/146 (88%) | 123 (95%) | 5 (4%) | 1 (1%) | 19 | 39 |
| 18 | U | 114/118 (97%) | 113 (99%) | 1 (1%) | 0 | 100 | 100 |
| 19 | V | 99/101 (98%) | 94 (95%) | 3 (3%) | 2 (2%) | 7 | 14 |
| 20 | W | 110/113 (97%) | 105 (96%) | 5 (4%) | 0 | 100 | 100 |
| 21 | X | 93/96 (97%) | 89 (96%) | 3 (3%) | 1 (1%) | 14 | 30 |
| 22 | Y | 105/110 (96%) | 89 (85%) | 12 (11%) | 4 (4%) | 3 | 4 |
| 23 | Z | 92/206 (45%) | 84 (91%) | 8 (9%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 24 | 0 | 72/85 (85%) | 67 (93%) | 3 (4%) | 2 (3%) | 5 | 7 |
| 25 | 1 | 95/98 (97%) | 86 (90%) | 6 (6%) | 3 (3%) | 4 | 6 |
| 26 | 2 | 68/72 (94%) | 65 (96%) | 2 (3%) | 1 (2%) | 10 | 21 |
| 27 | 3 | 57/60 (95%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 28 | 4 | 67/71 (94%) | 45 (67%) | 15 (22%) | 7 (10%) | 0 | 0 |
| 29 | 5 | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 30 | 6 | 51/54 (94%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |
| 31 | 7 | 47/49 (96%) | 44 (94%) | 1 (2%) | 2 (4%) | 2 | 3 |
| 32 | 8 | 62/65 (95%) | 61 (98%) | 1 (2%) | 0 | 100 | 100 |
| 33 | 9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 35 | b | 229/256 (90%) | 192 (84%) | 23 (10%) | 14 (6%) | 1 | 1 |
| 36 | c | 204/239 (85%) | 177 (87%) | 20 (10%) | 7 (3%) | 3 | 5 |
| 37 | d | 206/209 (99%) | 187 (91%) | 16 (8%) | 3 (2%) | 10 | 21 |
| 38 | e | 146/162 (90%) | 130 (89%) | 13 (9%) | 3 (2%) | 7 | 13 |
| 39 | f | 98/101 (97%) | 84 (86%) | 11 (11%) | 3 (3%) | 4 | 6 |
| 40 | g | 153/156 (98%) | 135 (88%) | 13 (8%) | 5 (3%) | 4 | 6 |
| 41 | h | 135/138 (98%) | 130 (96%) | 5 (4%) | 0 | 100 | 100 |
| 42 | i | 125/128 (98%) | 113 (90%) | 5 (4%) | 7 (6%) | 2 | 2 |
| 43 | j | 94/105 (90%) | 79 (84%) | 6 (6%) | 9 (10%) | 0 | 0 |
| 44 | k | 112/129 (87%) | 107 (96%) | 4 (4%) | 1 (1%) | 17 | 35 |
| 45 | l | 120/132 (91%) | 112 (93%) | 7 (6%) | 1 (1%) | 19 | 39 |
| 46 | m | 117/126 (93%) | 102 (87%) | 9 (8%) | 6 (5%) | 2 | 2 |
| 47 | n | 58/61 (95%) | 57 (98%) | 0 | 1 (2%) | 9 | 18 |
| 48 | o | 86/89 (97%) | 78 (91%) | 5 (6%) | 3 (4%) | 3 | 5 |
| 49 | p | 80/88 (91%) | 72 (90%) | 7 (9%) | 1 (1%) | 12 | 24 |
| 50 | q | 97/105 (92%) | 86 (89%) | 8 (8%) | 3 (3%) | 4 | 6 |
| 51 | r | 66/88 (75%) | 60 (91%) | 6 (9%) | 0 | 100 | 100 |
| 52 | s | 81/93 (87%) | 72 (89%) | 4 (5%) | 5 (6%) | 1 | 1 |
| 53 | t | 94/106 (89%) | 84 (89%) | 4 (4%) | 6 (6%) | 1 | 1 |
| 54 | u | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 59 | z | 669/679 (98%) | 568 (85%) | 62 (9%) | 39 (6%) | 1 | 1 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|----------|-------------------|
| All | All | 6534/7143 (92%) | 5800 (89%) | 497 (8%) | 237 (4%) | 3 4 |

All (237) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 65 | PRO |
| 3 | C | 172 | HIS |
| 3 | C | 224 | ILE |
| 4 | D | 275 | LYS |
| 6 | F | 130 | ALA |
| 6 | F | 165 | ARG |
| 7 | G | 47 | LYS |
| 7 | G | 50 | ALA |
| 7 | G | 81 | LYS |
| 8 | H | 126 | PRO |
| 9 | J | 71 | LEU |
| 9 | J | 74 | LEU |
| 9 | J | 77 | PRO |
| 9 | J | 80 | VAL |
| 9 | J | 104 | ILE |
| 9 | J | 105 | PRO |
| 9 | J | 107 | VAL |
| 9 | J | 128 | LEU |
| 10 | K | 13 | PRO |
| 10 | K | 38 | VAL |
| 10 | K | 39 | LYS |
| 10 | K | 78 | ILE |
| 10 | K | 89 | HIS |
| 10 | K | 93 | ARG |
| 10 | K | 96 | VAL |
| 13 | P | 45 | LEU |
| 17 | T | 127 | ALA |
| 19 | V | 100 | ARG |
| 21 | X | 94 | GLY |
| 24 | 0 | 33 | ALA |
| 28 | 4 | 49 | PHE |
| 28 | 4 | 55 | ARG |
| 35 | b | 8 | LYS |
| 35 | b | 37 | ASN |
| 35 | b | 131 | PRO |
| 36 | c | 47 | LEU |
| 36 | c | 61 | ALA |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 39 | f | 62 | TRP |
| 43 | j | 29 | ARG |
| 43 | j | 55 | LYS |
| 43 | j | 79 | ARG |
| 46 | m | 85 | GLY |
| 47 | n | 3 | ARG |
| 48 | o | 88 | ARG |
| 49 | p | 67 | THR |
| 50 | q | 14 | LYS |
| 52 | s | 14 | HIS |
| 52 | s | 30 | LEU |
| 53 | t | 95 | ALA |
| 53 | t | 99 | LEU |
| 53 | t | 100 | ILE |
| 59 | z | 98 | ALA |
| 59 | z | 235 | LYS |
| 59 | z | 373 | ALA |
| 59 | z | 390 | VAL |
| 59 | z | 444 | ALA |
| 59 | z | 459 | ILE |
| 3 | C | 66 | HIS |
| 3 | C | 179 | SER |
| 3 | C | 183 | GLU |
| 4 | D | 125 | ILE |
| 5 | E | 118 | LYS |
| 6 | F | 22 | ALA |
| 7 | G | 52 | ILE |
| 7 | G | 126 | ASP |
| 7 | G | 147 | ASP |
| 8 | H | 47 | GLU |
| 8 | H | 92 | ILE |
| 9 | J | 75 | GLN |
| 9 | J | 91 | LYS |
| 9 | J | 93 | LEU |
| 9 | J | 123 | GLU |
| 9 | J | 125 | LEU |
| 9 | J | 132 | ASP |
| 10 | K | 29 | GLN |
| 10 | K | 77 | LEU |
| 10 | K | 91 | PRO |
| 12 | O | 5 | GLN |
| 14 | Q | 60 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 16 | S | 59 | LYS |
| 19 | V | 42 | GLY |
| 22 | Y | 2 | ARG |
| 22 | Y | 6 | HIS |
| 24 | 0 | 34 | GLY |
| 26 | 2 | 46 | GLN |
| 28 | 4 | 46 | GLN |
| 28 | 4 | 60 | GLN |
| 31 | 7 | 45 | ALA |
| 31 | 7 | 46 | VAL |
| 35 | b | 17 | PHE |
| 35 | b | 122 | PHE |
| 35 | b | 135 | GLN |
| 35 | b | 236 | TYR |
| 36 | c | 46 | GLU |
| 37 | d | 5 | ILE |
| 37 | d | 36 | ARG |
| 38 | e | 85 | GLY |
| 39 | f | 38 | GLU |
| 40 | g | 83 | ALA |
| 42 | i | 88 | TYR |
| 42 | i | 118 | LYS |
| 43 | j | 34 | VAL |
| 44 | k | 105 | VAL |
| 46 | m | 7 | VAL |
| 46 | m | 49 | THR |
| 50 | q | 68 | ARG |
| 52 | s | 26 | GLY |
| 59 | z | -35 | GLY |
| 59 | z | -34 | LEU |
| 59 | z | 64 | VAL |
| 59 | z | 97 | LEU |
| 59 | z | 268 | ILE |
| 59 | z | 272 | HIS |
| 59 | z | 384 | SER |
| 59 | z | 389 | GLU |
| 59 | z | 400 | THR |
| 59 | z | 417 | PRO |
| 59 | z | 542 | GLY |
| 59 | z | 564 | GLY |
| 3 | C | 178 | ALA |
| 4 | D | 3 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 8 | H | 122 | THR |
| 9 | J | 22 | GLY |
| 9 | J | 33 | PRO |
| 9 | J | 56 | ASN |
| 9 | J | 69 | PRO |
| 9 | J | 84 | GLU |
| 9 | J | 101 | PRO |
| 10 | K | 11 | GLN |
| 10 | K | 14 | ALA |
| 10 | K | 31 | GLY |
| 10 | K | 50 | ASP |
| 10 | K | 54 | PRO |
| 10 | K | 113 | PRO |
| 11 | N | 7 | LYS |
| 22 | Y | 5 | MET |
| 25 | 1 | 3 | LYS |
| 28 | 4 | 56 | VAL |
| 28 | 4 | 62 | ARG |
| 35 | b | 16 | HIS |
| 35 | b | 21 | ARG |
| 36 | c | 81 | GLY |
| 36 | c | 108 | ASN |
| 36 | c | 206 | GLU |
| 37 | d | 166 | LYS |
| 39 | f | 61 | LEU |
| 40 | g | 7 | ALA |
| 40 | g | 84 | ASN |
| 42 | i | 119 | ALA |
| 43 | j | 30 | SER |
| 45 | l | 19 | ARG |
| 59 | z | 288 | PRO |
| 59 | z | 292 | PRO |
| 59 | z | 326 | ASN |
| 59 | z | 382 | LEU |
| 59 | z | 418 | GLU |
| 59 | z | 461 | TYR |
| 3 | C | 159 | GLY |
| 3 | C | 210 | ARG |
| 5 | E | 52 | LEU |
| 6 | F | 23 | ASP |
| 8 | H | 3 | ARG |
| 9 | J | 72 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 10 | K | 16 | LYS |
| 10 | K | 81 | ALA |
| 10 | K | 114 | ASP |
| 11 | N | 88 | GLU |
| 16 | S | 84 | GLN |
| 22 | Y | 54 | LYS |
| 25 | 1 | 79 | GLY |
| 35 | b | 13 | ALA |
| 35 | b | 15 | VAL |
| 35 | b | 121 | LEU |
| 35 | b | 232 | PRO |
| 40 | g | 55 | GLY |
| 40 | g | 80 | VAL |
| 42 | i | 24 | GLY |
| 42 | i | 105 | ASP |
| 43 | j | 32 | ALA |
| 46 | m | 40 | ASN |
| 48 | o | 24 | SER |
| 52 | s | 29 | ARG |
| 59 | z | 43 | GLU |
| 59 | z | 294 | PHE |
| 59 | z | 445 | GLN |
| 59 | z | 460 | LEU |
| 59 | z | 503 | ALA |
| 3 | C | 220 | PRO |
| 5 | E | 72 | VAL |
| 6 | F | 7 | TYR |
| 9 | J | 5 | ARG |
| 9 | J | 31 | GLY |
| 9 | J | 120 | LYS |
| 10 | K | 4 | VAL |
| 10 | K | 88 | ALA |
| 11 | N | 2 | LYS |
| 11 | N | 19 | GLU |
| 25 | 1 | 83 | GLU |
| 35 | b | 52 | GLU |
| 36 | c | 66 | VAL |
| 38 | e | 8 | GLU |
| 38 | e | 69 | VAL |
| 42 | i | 12 | GLU |
| 46 | m | 86 | CYS |
| 50 | q | 49 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | s | 25 | LYS |
| 59 | z | 194 | ALA |
| 59 | z | 310 | SER |
| 59 | z | 325 | LEU |
| 59 | z | 421 | VAL |
| 59 | z | 472 | ARG |
| 59 | z | 553 | ALA |
| 3 | C | 180 | PHE |
| 7 | G | 145 | THR |
| 8 | H | 99 | VAL |
| 9 | J | 20 | ALA |
| 9 | J | 114 | GLY |
| 43 | j | 77 | PRO |
| 43 | j | 78 | ASN |
| 53 | t | 10 | LEU |
| 53 | t | 97 | ALA |
| 59 | z | 81 | ILE |
| 59 | z | 267 | ALA |
| 43 | j | 75 | ILE |
| 46 | m | 6 | GLY |
| 48 | o | 87 | ILE |
| 59 | z | 274 | VAL |
| 53 | t | 47 | GLY |
| 8 | H | 100 | GLY |
| 9 | J | 53 | VAL |
| 9 | J | 86 | PRO |
| 9 | J | 85 | ASP |
| 28 | 4 | 19 | GLY |
| 42 | i | 74 | ILE |
| 59 | z | 186 | PRO |
| 9 | J | 73 | GLY |
| 13 | P | 72 | PRO |

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | C | 103/180 (57%) | 79 (77%) | 24 (23%) | 1 | 1 |
| 4 | D | 215/218 (99%) | 186 (86%) | 29 (14%) | 4 | 6 |
| 5 | E | 164/166 (99%) | 138 (84%) | 26 (16%) | 2 | 4 |
| 6 | F | 160/166 (96%) | 135 (84%) | 25 (16%) | 2 | 4 |
| 7 | G | 143/156 (92%) | 116 (81%) | 27 (19%) | 1 | 2 |
| 8 | H | 144/148 (97%) | 128 (89%) | 16 (11%) | 6 | 11 |
| 10 | K | 104/111 (94%) | 71 (68%) | 33 (32%) | 0 | 0 |
| 11 | N | 118/119 (99%) | 96 (81%) | 22 (19%) | 1 | 2 |
| 12 | O | 100/100 (100%) | 91 (91%) | 9 (9%) | 9 | 18 |
| 13 | P | 115/116 (99%) | 103 (90%) | 12 (10%) | 7 | 13 |
| 14 | Q | 111/111 (100%) | 94 (85%) | 17 (15%) | 2 | 4 |
| 15 | R | 101/101 (100%) | 84 (83%) | 17 (17%) | 2 | 3 |
| 16 | S | 87/88 (99%) | 77 (88%) | 10 (12%) | 5 | 10 |
| 17 | T | 115/127 (91%) | 100 (87%) | 15 (13%) | 4 | 7 |
| 18 | U | 93/94 (99%) | 80 (86%) | 13 (14%) | 3 | 6 |
| 19 | V | 80/82 (98%) | 67 (84%) | 13 (16%) | 2 | 3 |
| 20 | W | 90/92 (98%) | 79 (88%) | 11 (12%) | 5 | 9 |
| 21 | X | 77/78 (99%) | 69 (90%) | 8 (10%) | 7 | 13 |
| 22 | Y | 85/91 (93%) | 75 (88%) | 10 (12%) | 5 | 9 |
| 23 | Z | 84/179 (47%) | 73 (87%) | 11 (13%) | 4 | 7 |
| 24 | 0 | 59/67 (88%) | 55 (93%) | 4 (7%) | 16 | 32 |
| 25 | 1 | 80/83 (96%) | 69 (86%) | 11 (14%) | 3 | 6 |
| 26 | 2 | 65/67 (97%) | 54 (83%) | 11 (17%) | 2 | 3 |
| 27 | 3 | 51/52 (98%) | 44 (86%) | 7 (14%) | 3 | 6 |
| 28 | 4 | 60/63 (95%) | 45 (75%) | 15 (25%) | 0 | 1 |
| 29 | 5 | 51/52 (98%) | 45 (88%) | 6 (12%) | 5 | 9 |
| 30 | 6 | 51/52 (98%) | 47 (92%) | 4 (8%) | 12 | 25 |
| 31 | 7 | 42/42 (100%) | 34 (81%) | 8 (19%) | 1 | 2 |
| 32 | 8 | 53/55 (96%) | 48 (91%) | 5 (9%) | 8 | 17 |
| 33 | 9 | 34/34 (100%) | 29 (85%) | 5 (15%) | 3 | 5 |
| 35 | b | 193/220 (88%) | 150 (78%) | 43 (22%) | 1 | 1 |
| 36 | c | 142/188 (76%) | 130 (92%) | 12 (8%) | 10 | 21 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 37 | d | 169/181 (93%) | 143 (85%) | 26 (15%) | 2 | 4 |
| 38 | e | 113/123 (92%) | 95 (84%) | 18 (16%) | 2 | 4 |
| 39 | f | 83/90 (92%) | 69 (83%) | 14 (17%) | 2 | 3 |
| 40 | g | 118/127 (93%) | 99 (84%) | 19 (16%) | 2 | 4 |
| 41 | h | 114/119 (96%) | 99 (87%) | 15 (13%) | 4 | 7 |
| 42 | i | 90/99 (91%) | 76 (84%) | 14 (16%) | 2 | 4 |
| 43 | j | 65/92 (71%) | 53 (82%) | 12 (18%) | 1 | 2 |
| 44 | k | 82/99 (83%) | 74 (90%) | 8 (10%) | 8 | 15 |
| 45 | l | 97/109 (89%) | 85 (88%) | 12 (12%) | 4 | 8 |
| 46 | m | 89/101 (88%) | 76 (85%) | 13 (15%) | 3 | 5 |
| 47 | n | 49/50 (98%) | 41 (84%) | 8 (16%) | 2 | 3 |
| 48 | o | 78/80 (98%) | 71 (91%) | 7 (9%) | 9 | 18 |
| 49 | p | 69/74 (93%) | 59 (86%) | 10 (14%) | 3 | 5 |
| 50 | q | 94/97 (97%) | 81 (86%) | 13 (14%) | 3 | 6 |
| 51 | r | 59/77 (77%) | 50 (85%) | 9 (15%) | 2 | 4 |
| 52 | s | 68/80 (85%) | 58 (85%) | 10 (15%) | 3 | 5 |
| 53 | t | 69/82 (84%) | 61 (88%) | 8 (12%) | 5 | 10 |
| 54 | u | 18/22 (82%) | 16 (89%) | 2 (11%) | 6 | 11 |
| 59 | z | 542/560 (97%) | 436 (80%) | 106 (20%) | 1 | 2 |
| All | All | 5236/5760 (91%) | 4433 (85%) | 803 (15%) | 2 | 4 |

All (803) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 3 | HIS |
| 3 | C | 5 | LYS |
| 3 | C | 8 | ARG |
| 3 | C | 11 | LEU |
| 3 | C | 23 | ASP |
| 3 | C | 39 | GLU |
| 3 | C | 42 | GLU |
| 3 | C | 46 | LYS |
| 3 | C | 49 | ILE |
| 3 | C | 55 | ASP |
| 3 | C | 61 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | C | 68 | LEU |
| 3 | C | 162 | GLU |
| 3 | C | 163 | PHE |
| 3 | C | 164 | ARG |
| 3 | C | 168 | THR |
| 3 | C | 184 | LYS |
| 3 | C | 185 | LEU |
| 3 | C | 209 | LEU |
| 3 | C | 210 | ARG |
| 3 | C | 211 | SER |
| 3 | C | 216 | THR |
| 3 | C | 222 | VAL |
| 3 | C | 224 | ILE |
| 4 | D | 5 | LYS |
| 4 | D | 18 | VAL |
| 4 | D | 27 | THR |
| 4 | D | 37 | LEU |
| 4 | D | 38 | LYS |
| 4 | D | 61 | LEU |
| 4 | D | 71 | ASP |
| 4 | D | 88 | ARG |
| 4 | D | 94 | LEU |
| 4 | D | 103 | ARG |
| 4 | D | 111 | LEU |
| 4 | D | 112 | GLN |
| 4 | D | 116 | GLN |
| 4 | D | 122 | ASP |
| 4 | D | 140 | THR |
| 4 | D | 141 | VAL |
| 4 | D | 142 | VAL |
| 4 | D | 150 | LYS |
| 4 | D | 183 | ARG |
| 4 | D | 200 | ASP |
| 4 | D | 202 | LYS |
| 4 | D | 211 | ARG |
| 4 | D | 221 | VAL |
| 4 | D | 229 | VAL |
| 4 | D | 242 | ARG |
| 4 | D | 257 | LEU |
| 4 | D | 259 | THR |
| 4 | D | 260 | ARG |
| 4 | D | 274 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | E | 7 | VAL |
| 5 | E | 9 | VAL |
| 5 | E | 21 | VAL |
| 5 | E | 24 | THR |
| 5 | E | 33 | VAL |
| 5 | E | 34 | VAL |
| 5 | E | 41 | LYS |
| 5 | E | 47 | VAL |
| 5 | E | 49 | LEU |
| 5 | E | 52 | LEU |
| 5 | E | 78 | LEU |
| 5 | E | 82 | ARG |
| 5 | E | 85 | ASN |
| 5 | E | 89 | ASP |
| 5 | E | 94 | GLU |
| 5 | E | 116 | VAL |
| 5 | E | 119 | ARG |
| 5 | E | 140 | SER |
| 5 | E | 144 | ARG |
| 5 | E | 149 | ARG |
| 5 | E | 152 | LYS |
| 5 | E | 154 | LYS |
| 5 | E | 163 | GLU |
| 5 | E | 175 | VAL |
| 5 | E | 181 | LEU |
| 5 | E | 196 | VAL |
| 6 | F | 20 | LEU |
| 6 | F | 24 | LEU |
| 6 | F | 28 | ILE |
| 6 | F | 33 | LEU |
| 6 | F | 38 | ARG |
| 6 | F | 53 | THR |
| 6 | F | 74 | ARG |
| 6 | F | 88 | VAL |
| 6 | F | 106 | ARG |
| 6 | F | 120 | GLU |
| 6 | F | 124 | LEU |
| 6 | F | 125 | LEU |
| 6 | F | 135 | LYS |
| 6 | F | 162 | LEU |
| 6 | F | 164 | ARG |
| 6 | F | 165 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | F | 168 | ARG |
| 6 | F | 170 | LEU |
| 6 | F | 175 | THR |
| 6 | F | 176 | LEU |
| 6 | F | 191 | ARG |
| 6 | F | 192 | LEU |
| 6 | F | 195 | ASP |
| 6 | F | 201 | VAL |
| 6 | F | 206 | ILE |
| 7 | G | 3 | LEU |
| 7 | G | 5 | VAL |
| 7 | G | 7 | LEU |
| 7 | G | 26 | GLN |
| 7 | G | 33 | ARG |
| 7 | G | 34 | LEU |
| 7 | G | 43 | LEU |
| 7 | G | 49 | ASP |
| 7 | G | 51 | ARG |
| 7 | G | 75 | LYS |
| 7 | G | 78 | SER |
| 7 | G | 80 | PHE |
| 7 | G | 82 | LEU |
| 7 | G | 86 | MET |
| 7 | G | 91 | ARG |
| 7 | G | 115 | ARG |
| 7 | G | 133 | LEU |
| 7 | G | 139 | LEU |
| 7 | G | 140 | ILE |
| 7 | G | 145 | THR |
| 7 | G | 146 | TYR |
| 7 | G | 148 | MET |
| 7 | G | 149 | VAL |
| 7 | G | 159 | VAL |
| 7 | G | 164 | GLU |
| 7 | G | 175 | LEU |
| 7 | G | 181 | ARG |
| 8 | H | 3 | ARG |
| 8 | H | 23 | ARG |
| 8 | H | 32 | GLU |
| 8 | H | 43 | VAL |
| 8 | H | 57 | ASP |
| 8 | H | 69 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 8 | H | 71 | LEU |
| 8 | H | 80 | SER |
| 8 | H | 92 | ILE |
| 8 | H | 99 | VAL |
| 8 | H | 101 | ARG |
| 8 | H | 104 | GLU |
| 8 | H | 105 | LEU |
| 8 | H | 114 | VAL |
| 8 | H | 116 | GLU |
| 8 | H | 160 | LYS |
| 10 | K | 2 | LYS |
| 10 | K | 4 | VAL |
| 10 | K | 5 | VAL |
| 10 | K | 7 | VAL |
| 10 | K | 11 | GLN |
| 10 | K | 18 | THR |
| 10 | K | 30 | HIS |
| 10 | K | 47 | ASN |
| 10 | K | 48 | MET |
| 10 | K | 50 | ASP |
| 10 | K | 53 | VAL |
| 10 | K | 58 | THR |
| 10 | K | 64 | SER |
| 10 | K | 65 | PHE |
| 10 | K | 66 | THR |
| 10 | K | 69 | THR |
| 10 | K | 75 | SER |
| 10 | K | 80 | LYS |
| 10 | K | 86 | LYS |
| 10 | K | 93 | ARG |
| 10 | K | 94 | GLU |
| 10 | K | 95 | LYS |
| 10 | K | 102 | GLU |
| 10 | K | 103 | GLN |
| 10 | K | 105 | LEU |
| 10 | K | 107 | ILE |
| 10 | K | 112 | MET |
| 10 | K | 115 | LEU |
| 10 | K | 117 | THR |
| 10 | K | 118 | THR |
| 10 | K | 132 | ARG |
| 10 | K | 134 | MET |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 10 | K | 138 | VAL |
| 11 | N | 1 | MET |
| 11 | N | 5 | VAL |
| 11 | N | 9 | VAL |
| 11 | N | 10 | GLU |
| 11 | N | 12 | ARG |
| 11 | N | 14 | VAL |
| 11 | N | 28 | THR |
| 11 | N | 33 | LEU |
| 11 | N | 34 | LEU |
| 11 | N | 48 | MET |
| 11 | N | 55 | VAL |
| 11 | N | 62 | VAL |
| 11 | N | 67 | LEU |
| 11 | N | 87 | LEU |
| 11 | N | 90 | MET |
| 11 | N | 97 | ARG |
| 11 | N | 99 | LEU |
| 11 | N | 120 | LEU |
| 11 | N | 131 | GLN |
| 11 | N | 133 | GLN |
| 11 | N | 139 | GLU |
| 11 | N | 140 | VAL |
| 12 | O | 8 | LEU |
| 12 | O | 10 | VAL |
| 12 | O | 23 | ARG |
| 12 | O | 24 | VAL |
| 12 | O | 63 | VAL |
| 12 | O | 69 | ILE |
| 12 | O | 94 | ARG |
| 12 | O | 98 | VAL |
| 12 | O | 116 | SER |
| 13 | P | 1 | MET |
| 13 | P | 45 | LEU |
| 13 | P | 55 | ARG |
| 13 | P | 65 | ARG |
| 13 | P | 98 | GLU |
| 13 | P | 102 | ARG |
| 13 | P | 115 | LEU |
| 13 | P | 117 | GLU |
| 13 | P | 125 | VAL |
| 13 | P | 131 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 13 | P | 137 | LYS |
| 13 | P | 148 | LEU |
| 14 | Q | 3 | MET |
| 14 | Q | 5 | ARG |
| 14 | Q | 16 | ARG |
| 14 | Q | 45 | GLN |
| 14 | Q | 56 | ARG |
| 14 | Q | 57 | HIS |
| 14 | Q | 60 | ARG |
| 14 | Q | 63 | LYS |
| 14 | Q | 75 | THR |
| 14 | Q | 81 | VAL |
| 14 | Q | 82 | ARG |
| 14 | Q | 85 | LYS |
| 14 | Q | 109 | VAL |
| 14 | Q | 110 | THR |
| 14 | Q | 111 | GLU |
| 14 | Q | 130 | LYS |
| 14 | Q | 135 | ASP |
| 15 | R | 6 | SER |
| 15 | R | 18 | LEU |
| 15 | R | 28 | LEU |
| 15 | R | 29 | LEU |
| 15 | R | 33 | ARG |
| 15 | R | 36 | THR |
| 15 | R | 40 | LYS |
| 15 | R | 44 | LEU |
| 15 | R | 54 | LEU |
| 15 | R | 60 | LEU |
| 15 | R | 65 | LEU |
| 15 | R | 79 | LEU |
| 15 | R | 89 | ASP |
| 15 | R | 91 | GLN |
| 15 | R | 100 | LEU |
| 15 | R | 111 | LEU |
| 15 | R | 114 | VAL |
| 16 | S | 3 | ARG |
| 16 | S | 15 | ARG |
| 16 | S | 20 | ARG |
| 16 | S | 36 | TYR |
| 16 | S | 43 | GLU |
| 16 | S | 48 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 16 | S | 49 | VAL |
| 16 | S | 69 | VAL |
| 16 | S | 73 | LEU |
| 16 | S | 78 | LEU |
| 17 | T | 6 | LEU |
| 17 | T | 13 | ARG |
| 17 | T | 16 | ARG |
| 17 | T | 23 | ARG |
| 17 | T | 39 | ARG |
| 17 | T | 41 | ARG |
| 17 | T | 49 | VAL |
| 17 | T | 50 | ILE |
| 17 | T | 59 | THR |
| 17 | T | 64 | ARG |
| 17 | T | 74 | ARG |
| 17 | T | 96 | ARG |
| 17 | T | 108 | ARG |
| 17 | T | 118 | ARG |
| 17 | T | 125 | ARG |
| 18 | U | 18 | LEU |
| 18 | U | 31 | SER |
| 18 | U | 34 | LYS |
| 18 | U | 36 | ARG |
| 18 | U | 52 | ARG |
| 18 | U | 59 | ARG |
| 18 | U | 74 | LEU |
| 18 | U | 83 | LEU |
| 18 | U | 85 | LYS |
| 18 | U | 92 | ARG |
| 18 | U | 95 | LEU |
| 18 | U | 104 | GLN |
| 18 | U | 108 | GLU |
| 19 | V | 25 | LEU |
| 19 | V | 43 | GLU |
| 19 | V | 46 | VAL |
| 19 | V | 51 | VAL |
| 19 | V | 57 | VAL |
| 19 | V | 58 | VAL |
| 19 | V | 62 | LEU |
| 19 | V | 66 | ARG |
| 19 | V | 71 | LEU |
| 19 | V | 72 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 19 | V | 79 | VAL |
| 19 | V | 80 | GLN |
| 19 | V | 95 | LEU |
| 20 | W | 6 | ILE |
| 20 | W | 11 | ARG |
| 20 | W | 19 | LEU |
| 20 | W | 23 | LEU |
| 20 | W | 37 | ARG |
| 20 | W | 51 | LEU |
| 20 | W | 63 | ASP |
| 20 | W | 92 | ARG |
| 20 | W | 100 | THR |
| 20 | W | 107 | LEU |
| 20 | W | 111 | HIS |
| 21 | X | 23 | GLU |
| 21 | X | 35 | THR |
| 21 | X | 51 | VAL |
| 21 | X | 57 | LEU |
| 21 | X | 65 | ARG |
| 21 | X | 72 | LYS |
| 21 | X | 80 | ILE |
| 21 | X | 95 | LEU |
| 22 | Y | 7 | VAL |
| 22 | Y | 23 | ARG |
| 22 | Y | 43 | ASN |
| 22 | Y | 61 | ILE |
| 22 | Y | 67 | LEU |
| 22 | Y | 72 | VAL |
| 22 | Y | 85 | VAL |
| 22 | Y | 90 | LEU |
| 22 | Y | 99 | CYS |
| 22 | Y | 106 | LEU |
| 23 | Z | 5 | LEU |
| 23 | Z | 18 | LEU |
| 23 | Z | 31 | ARG |
| 23 | Z | 37 | VAL |
| 23 | Z | 41 | LEU |
| 23 | Z | 42 | VAL |
| 23 | Z | 50 | GLN |
| 23 | Z | 72 | ARG |
| 23 | Z | 78 | LYS |
| 23 | Z | 91 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | Z | 93 | ASP |
| 24 | 0 | 20 | ARG |
| 24 | 0 | 23 | VAL |
| 24 | 0 | 27 | GLU |
| 24 | 0 | 74 | ARG |
| 25 | 1 | 13 | ILE |
| 25 | 1 | 14 | VAL |
| 25 | 1 | 21 | ARG |
| 25 | 1 | 35 | THR |
| 25 | 1 | 40 | ARG |
| 25 | 1 | 51 | VAL |
| 25 | 1 | 52 | ARG |
| 25 | 1 | 69 | LYS |
| 25 | 1 | 71 | TYR |
| 25 | 1 | 80 | LEU |
| 25 | 1 | 95 | LEU |
| 26 | 2 | 1 | MET |
| 26 | 2 | 20 | GLU |
| 26 | 2 | 22 | GLU |
| 26 | 2 | 27 | GLU |
| 26 | 2 | 30 | ARG |
| 26 | 2 | 32 | LEU |
| 26 | 2 | 34 | GLU |
| 26 | 2 | 40 | SER |
| 26 | 2 | 53 | LEU |
| 26 | 2 | 68 | ARG |
| 26 | 2 | 70 | GLN |
| 27 | 3 | 3 | ARG |
| 27 | 3 | 4 | LEU |
| 27 | 3 | 8 | LEU |
| 27 | 3 | 18 | ASP |
| 27 | 3 | 23 | LEU |
| 27 | 3 | 40 | THR |
| 27 | 3 | 54 | VAL |
| 28 | 4 | 9 | LEU |
| 28 | 4 | 22 | ILE |
| 28 | 4 | 34 | GLU |
| 28 | 4 | 35 | VAL |
| 28 | 4 | 49 | PHE |
| 28 | 4 | 50 | VAL |
| 28 | 4 | 52 | THR |
| 28 | 4 | 58 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 28 | 4 | 59 | PHE |
| 28 | 4 | 60 | GLN |
| 28 | 4 | 61 | ARG |
| 28 | 4 | 62 | ARG |
| 28 | 4 | 63 | TYR |
| 28 | 4 | 67 | TYR |
| 28 | 4 | 68 | ARG |
| 29 | 5 | 9 | LYS |
| 29 | 5 | 16 | ARG |
| 29 | 5 | 29 | THR |
| 29 | 5 | 40 | LYS |
| 29 | 5 | 48 | GLU |
| 29 | 5 | 56 | LYS |
| 30 | 6 | 6 | ARG |
| 30 | 6 | 17 | LYS |
| 30 | 6 | 24 | GLU |
| 30 | 6 | 27 | LYS |
| 31 | 7 | 1 | MET |
| 31 | 7 | 14 | LYS |
| 31 | 7 | 23 | ARG |
| 31 | 7 | 32 | LYS |
| 31 | 7 | 43 | THR |
| 31 | 7 | 46 | VAL |
| 31 | 7 | 47 | ARG |
| 31 | 7 | 49 | ARG |
| 32 | 8 | 14 | VAL |
| 32 | 8 | 23 | VAL |
| 32 | 8 | 26 | LYS |
| 32 | 8 | 31 | HIS |
| 32 | 8 | 32 | LEU |
| 33 | 9 | 7 | VAL |
| 33 | 9 | 12 | ASP |
| 33 | 9 | 22 | ARG |
| 33 | 9 | 35 | ARG |
| 33 | 9 | 36 | GLN |
| 35 | b | 8 | LYS |
| 35 | b | 9 | GLU |
| 35 | b | 10 | LEU |
| 35 | b | 11 | LEU |
| 35 | b | 12 | GLU |
| 35 | b | 15 | VAL |
| 35 | b | 17 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 35 | b | 21 | ARG |
| 35 | b | 24 | TRP |
| 35 | b | 37 | ASN |
| 35 | b | 45 | GLN |
| 35 | b | 48 | MET |
| 35 | b | 56 | ARG |
| 35 | b | 76 | GLN |
| 35 | b | 79 | ASP |
| 35 | b | 80 | ILE |
| 35 | b | 93 | VAL |
| 35 | b | 97 | TRP |
| 35 | b | 118 | LEU |
| 35 | b | 119 | GLU |
| 35 | b | 122 | PHE |
| 35 | b | 124 | SER |
| 35 | b | 127 | ILE |
| 35 | b | 128 | GLU |
| 35 | b | 135 | GLN |
| 35 | b | 136 | VAL |
| 35 | b | 138 | LEU |
| 35 | b | 142 | LEU |
| 35 | b | 144 | ARG |
| 35 | b | 145 | LEU |
| 35 | b | 146 | GLN |
| 35 | b | 155 | LEU |
| 35 | b | 156 | LYS |
| 35 | b | 178 | ARG |
| 35 | b | 179 | LYS |
| 35 | b | 185 | ILE |
| 35 | b | 187 | LEU |
| 35 | b | 196 | LEU |
| 35 | b | 208 | ILE |
| 35 | b | 212 | GLN |
| 35 | b | 217 | ARG |
| 35 | b | 221 | LEU |
| 35 | b | 223 | ILE |
| 36 | c | 3 | ASN |
| 36 | c | 47 | LEU |
| 36 | c | 52 | LEU |
| 36 | c | 70 | VAL |
| 36 | c | 104 | GLN |
| 36 | c | 165 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | c | 178 | LEU |
| 36 | c | 190 | ARG |
| 36 | c | 191 | THR |
| 36 | c | 192 | THR |
| 36 | c | 195 | VAL |
| 36 | c | 196 | LEU |
| 37 | d | 5 | ILE |
| 37 | d | 9 | CYS |
| 37 | d | 15 | GLU |
| 37 | d | 18 | LYS |
| 37 | d | 21 | LEU |
| 37 | d | 28 | SER |
| 37 | d | 58 | LEU |
| 37 | d | 76 | ARG |
| 37 | d | 107 | ARG |
| 37 | d | 108 | LEU |
| 37 | d | 132 | ARG |
| 37 | d | 135 | LEU |
| 37 | d | 137 | SER |
| 37 | d | 141 | ARG |
| 37 | d | 150 | GLU |
| 37 | d | 156 | GLU |
| 37 | d | 158 | ILE |
| 37 | d | 162 | LEU |
| 37 | d | 163 | GLU |
| 37 | d | 168 | ARG |
| 37 | d | 170 | VAL |
| 37 | d | 173 | TRP |
| 37 | d | 174 | LEU |
| 37 | d | 188 | LEU |
| 37 | d | 194 | LEU |
| 37 | d | 201 | GLN |
| 38 | e | 20 | GLN |
| 38 | e | 31 | LEU |
| 38 | e | 34 | VAL |
| 38 | e | 37 | ARG |
| 38 | e | 38 | GLN |
| 38 | e | 41 | VAL |
| 38 | e | 47 | LYS |
| 38 | e | 57 | LYS |
| 38 | e | 69 | VAL |
| 38 | e | 71 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 38 | e | 80 | ILE |
| 38 | e | 91 | LEU |
| 38 | e | 112 | LEU |
| 38 | e | 116 | THR |
| 38 | e | 121 | LYS |
| 38 | e | 123 | LEU |
| 38 | e | 151 | LEU |
| 38 | e | 152 | ARG |
| 39 | f | 9 | VAL |
| 39 | f | 14 | LEU |
| 39 | f | 15 | ASP |
| 39 | f | 21 | LEU |
| 39 | f | 32 | ASN |
| 39 | f | 54 | LYS |
| 39 | f | 61 | LEU |
| 39 | f | 69 | GLU |
| 39 | f | 73 | ASN |
| 39 | f | 74 | ASP |
| 39 | f | 83 | ASP |
| 39 | f | 87 | ARG |
| 39 | f | 94 | GLN |
| 39 | f | 98 | LEU |
| 40 | g | 12 | LEU |
| 40 | g | 15 | ASP |
| 40 | g | 22 | LEU |
| 40 | g | 32 | ARG |
| 40 | g | 37 | ASN |
| 40 | g | 51 | GLN |
| 40 | g | 59 | LEU |
| 40 | g | 64 | GLN |
| 40 | g | 72 | ARG |
| 40 | g | 75 | VAL |
| 40 | g | 104 | LEU |
| 40 | g | 113 | GLU |
| 40 | g | 115 | ARG |
| 40 | g | 131 | LYS |
| 40 | g | 137 | LYS |
| 40 | g | 138 | LYS |
| 40 | g | 140 | ASP |
| 40 | g | 144 | MET |
| 40 | g | 155 | ARG |
| 41 | h | 2 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 41 | h | 23 | SER |
| 41 | h | 29 | SER |
| 41 | h | 50 | ARG |
| 41 | h | 52 | ASP |
| 41 | h | 63 | LEU |
| 41 | h | 78 | GLN |
| 41 | h | 84 | ARG |
| 41 | h | 85 | ARG |
| 41 | h | 91 | ARG |
| 41 | h | 99 | GLU |
| 41 | h | 112 | LEU |
| 41 | h | 116 | LYS |
| 41 | h | 122 | ARG |
| 41 | h | 133 | LEU |
| 42 | i | 27 | THR |
| 42 | i | 38 | GLN |
| 42 | i | 41 | VAL |
| 42 | i | 47 | LEU |
| 42 | i | 48 | GLU |
| 42 | i | 56 | LEU |
| 42 | i | 58 | HIS |
| 42 | i | 64 | THR |
| 42 | i | 65 | VAL |
| 42 | i | 75 | ASP |
| 42 | i | 83 | ARG |
| 42 | i | 108 | VAL |
| 42 | i | 121 | ARG |
| 42 | i | 124 | GLN |
| 43 | j | 15 | THR |
| 43 | j | 16 | LEU |
| 43 | j | 30 | SER |
| 43 | j | 35 | SER |
| 43 | j | 43 | ARG |
| 43 | j | 46 | ARG |
| 43 | j | 70 | ARG |
| 43 | j | 72 | VAL |
| 43 | j | 89 | ASP |
| 43 | j | 92 | THR |
| 43 | j | 96 | ILE |
| 43 | j | 100 | THR |
| 44 | k | 48 | ILE |
| 44 | k | 54 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 44 | k | 70 | LYS |
| 44 | k | 83 | ILE |
| 44 | k | 93 | GLN |
| 44 | k | 99 | GLN |
| 44 | k | 104 | GLN |
| 44 | k | 109 | VAL |
| 45 | l | 18 | VAL |
| 45 | l | 27 | LEU |
| 45 | l | 33 | ARG |
| 45 | l | 41 | ARG |
| 45 | l | 52 | LEU |
| 45 | l | 53 | ARG |
| 45 | l | 60 | LEU |
| 45 | l | 67 | THR |
| 45 | l | 83 | VAL |
| 45 | l | 84 | LEU |
| 45 | l | 86 | ARG |
| 45 | l | 89 | ARG |
| 46 | m | 9 | ILE |
| 46 | m | 11 | ARG |
| 46 | m | 15 | VAL |
| 46 | m | 34 | LEU |
| 46 | m | 40 | ASN |
| 46 | m | 49 | THR |
| 46 | m | 70 | LEU |
| 46 | m | 73 | GLU |
| 46 | m | 80 | ARG |
| 46 | m | 88 | ARG |
| 46 | m | 102 | ARG |
| 46 | m | 116 | THR |
| 46 | m | 120 | LYS |
| 47 | n | 3 | ARG |
| 47 | n | 6 | LEU |
| 47 | n | 7 | ILE |
| 47 | n | 8 | GLU |
| 47 | n | 18 | VAL |
| 47 | n | 33 | VAL |
| 47 | n | 41 | ARG |
| 47 | n | 50 | LYS |
| 48 | o | 24 | SER |
| 48 | o | 26 | GLU |
| 48 | o | 39 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 48 | o | 66 | LEU |
| 48 | o | 67 | LEU |
| 48 | o | 82 | ILE |
| 48 | o | 83 | GLU |
| 49 | p | 3 | LYS |
| 49 | p | 5 | ARG |
| 49 | p | 19 | ILE |
| 49 | p | 21 | VAL |
| 49 | p | 25 | ARG |
| 49 | p | 27 | LYS |
| 49 | p | 45 | THR |
| 49 | p | 60 | LEU |
| 49 | p | 62 | VAL |
| 49 | p | 79 | VAL |
| 50 | q | 4 | LYS |
| 50 | q | 6 | LEU |
| 50 | q | 9 | VAL |
| 50 | q | 11 | VAL |
| 50 | q | 13 | ASP |
| 50 | q | 52 | LYS |
| 50 | q | 63 | ARG |
| 50 | q | 68 | ARG |
| 50 | q | 70 | ARG |
| 50 | q | 72 | ARG |
| 50 | q | 74 | LEU |
| 50 | q | 78 | GLU |
| 50 | q | 96 | GLU |
| 51 | r | 21 | LYS |
| 51 | r | 31 | LEU |
| 51 | r | 32 | ARG |
| 51 | r | 35 | ARG |
| 51 | r | 42 | ARG |
| 51 | r | 49 | LYS |
| 51 | r | 58 | LEU |
| 51 | r | 84 | LYS |
| 51 | r | 87 | ARG |
| 52 | s | 5 | LEU |
| 52 | s | 14 | HIS |
| 52 | s | 15 | LEU |
| 52 | s | 28 | LYS |
| 52 | s | 37 | ARG |
| 52 | s | 45 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 52 | s | 48 | THR |
| 52 | s | 65 | ASN |
| 52 | s | 67 | VAL |
| 52 | s | 71 | LEU |
| 53 | t | 9 | ASN |
| 53 | t | 10 | LEU |
| 53 | t | 24 | LEU |
| 53 | t | 43 | LEU |
| 53 | t | 51 | GLU |
| 53 | t | 62 | LEU |
| 53 | t | 80 | ARG |
| 53 | t | 84 | LEU |
| 54 | u | 7 | ARG |
| 54 | u | 12 | LYS |
| 59 | z | -68 | MET |
| 59 | z | -60 | LEU |
| 59 | z | -54 | VAL |
| 59 | z | -34 | LEU |
| 59 | z | -25 | LEU |
| 59 | z | -24 | LYS |
| 59 | z | -22 | LEU |
| 59 | z | -12 | ARG |
| 59 | z | -11 | LEU |
| 59 | z | -7 | LYS |
| 59 | z | 2 | ILE |
| 59 | z | 5 | ASN |
| 59 | z | 10 | ARG |
| 59 | z | 15 | ILE |
| 59 | z | 28 | ARG |
| 59 | z | 32 | LEU |
| 59 | z | 40 | GLU |
| 59 | z | 43 | GLU |
| 59 | z | 46 | LEU |
| 59 | z | 50 | GLU |
| 59 | z | 54 | GLU |
| 59 | z | 67 | THR |
| 59 | z | 75 | GLU |
| 59 | z | 80 | LEU |
| 59 | z | 88 | ASP |
| 59 | z | 101 | GLU |
| 59 | z | 105 | LEU |
| 59 | z | 113 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 59 | z | 126 | GLU |
| 59 | z | 131 | ILE |
| 59 | z | 140 | LEU |
| 59 | z | 142 | ASN |
| 59 | z | 150 | LEU |
| 59 | z | 175 | GLU |
| 59 | z | 181 | ILE |
| 59 | z | 184 | ARG |
| 59 | z | 204 | VAL |
| 59 | z | 208 | TYR |
| 59 | z | 209 | GLN |
| 59 | z | 212 | ILE |
| 59 | z | 216 | ARG |
| 59 | z | 229 | ARG |
| 59 | z | 241 | LYS |
| 59 | z | 245 | PHE |
| 59 | z | 248 | GLN |
| 59 | z | 250 | LEU |
| 59 | z | 251 | VAL |
| 59 | z | 268 | ILE |
| 59 | z | 269 | ARG |
| 59 | z | 274 | VAL |
| 59 | z | 280 | ILE |
| 59 | z | 282 | LEU |
| 59 | z | 298 | LYS |
| 59 | z | 309 | ASP |
| 59 | z | 312 | ASP |
| 59 | z | 316 | LEU |
| 59 | z | 317 | ARG |
| 59 | z | 322 | LYS |
| 59 | z | 325 | LEU |
| 59 | z | 326 | ASN |
| 59 | z | 336 | SER |
| 59 | z | 338 | THR |
| 59 | z | 345 | ARG |
| 59 | z | 355 | GLU |
| 59 | z | 360 | ARG |
| 59 | z | 362 | GLU |
| 59 | z | 369 | LEU |
| 59 | z | 370 | ILE |
| 59 | z | 382 | LEU |
| 59 | z | 384 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 59 | z | 387 | GLU |
| 59 | z | 401 | ARG |
| 59 | z | 402 | ILE |
| 59 | z | 405 | ILE |
| 59 | z | 413 | THR |
| 59 | z | 418 | GLU |
| 59 | z | 419 | GLU |
| 59 | z | 424 | LEU |
| 59 | z | 434 | ARG |
| 59 | z | 438 | MET |
| 59 | z | 441 | LEU |
| 59 | z | 445 | GLN |
| 59 | z | 447 | ARG |
| 59 | z | 450 | LEU |
| 59 | z | 461 | TYR |
| 59 | z | 467 | LEU |
| 59 | z | 468 | LYS |
| 59 | z | 471 | SER |
| 59 | z | 476 | SER |
| 59 | z | 480 | GLU |
| 59 | z | 481 | GLN |
| 59 | z | 490 | VAL |
| 59 | z | 495 | LEU |
| 59 | z | 512 | LYS |
| 59 | z | 516 | MET |
| 59 | z | 518 | ARG |
| 59 | z | 521 | VAL |
| 59 | z | 541 | ILE |
| 59 | z | 545 | ILE |
| 59 | z | 546 | ILE |
| 59 | z | 548 | ARG |
| 59 | z | 550 | THR |
| 59 | z | 572 | LYS |
| 59 | z | 576 | LYS |
| 59 | z | 592 | VAL |
| 59 | z | 595 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | D | 115 | GLN |
| 4 | D | 166 | GLN |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | D | 253 | GLN |
| 5 | E | 85 | ASN |
| 6 | F | 8 | GLN |
| 6 | F | 69 | HIS |
| 6 | F | 169 | ASN |
| 7 | G | 26 | GLN |
| 7 | G | 40 | ASN |
| 7 | G | 108 | ASN |
| 8 | H | 139 | GLN |
| 11 | N | 8 | GLN |
| 14 | Q | 12 | GLN |
| 17 | T | 43 | GLN |
| 17 | T | 123 | GLN |
| 18 | U | 72 | HIS |
| 21 | X | 31 | HIS |
| 21 | X | 82 | GLN |
| 23 | Z | 50 | GLN |
| 23 | Z | 54 | HIS |
| 23 | Z | 65 | GLN |
| 24 | 0 | 17 | GLN |
| 24 | 0 | 35 | ASN |
| 25 | 1 | 19 | GLN |
| 25 | 1 | 56 | GLN |
| 26 | 2 | 70 | GLN |
| 28 | 4 | 20 | ASN |
| 28 | 4 | 60 | GLN |
| 33 | 9 | 36 | GLN |
| 35 | b | 16 | HIS |
| 35 | b | 45 | GLN |
| 35 | b | 94 | ASN |
| 35 | b | 113 | HIS |
| 35 | b | 212 | GLN |
| 36 | c | 6 | HIS |
| 36 | c | 37 | GLN |
| 36 | c | 104 | GLN |
| 36 | c | 108 | ASN |
| 36 | c | 118 | GLN |
| 36 | c | 162 | GLN |
| 36 | c | 176 | HIS |
| 36 | c | 181 | ASN |
| 37 | d | 77 | ASN |
| 37 | d | 123 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | d | 125 | HIS |
| 37 | d | 201 | GLN |
| 38 | e | 73 | ASN |
| 38 | e | 141 | GLN |
| 39 | f | 73 | ASN |
| 39 | f | 100 | ASN |
| 40 | g | 28 | ASN |
| 40 | g | 68 | ASN |
| 40 | g | 148 | ASN |
| 42 | i | 89 | ASN |
| 42 | i | 124 | GLN |
| 43 | j | 56 | HIS |
| 44 | k | 38 | ASN |
| 44 | k | 93 | GLN |
| 45 | l | 99 | HIS |
| 46 | m | 40 | ASN |
| 48 | o | 28 | GLN |
| 50 | q | 16 | GLN |
| 52 | s | 14 | HIS |
| 52 | s | 57 | HIS |
| 52 | s | 65 | ASN |
| 52 | s | 83 | HIS |
| 53 | t | 16 | HIS |
| 53 | t | 75 | ASN |
| 59 | z | 127 | HIS |
| 59 | z | 183 | GLN |
| 59 | z | 248 | GLN |
| 59 | z | 275 | GLN |
| 59 | z | 326 | ASN |
| 59 | z | 426 | GLN |
| 59 | z | 429 | GLN |
| 59 | z | 538 | GLN |
| 59 | z | 577 | GLN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 2868/2915 (98%) | 464 (16%) | 42 (1%) |
| 2 | B | 119/121 (98%) | 14 (11%) | 0 |
| 34 | a | 1496/1521 (98%) | 243 (16%) | 0 |
| 55 | v | 12/24 (50%) | 1 (8%) | 0 |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 56 | w | 71/76 (93%) | 26 (36%) | 0 |
| 57 | x | 76/77 (98%) | 13 (17%) | 0 |
| 58 | y | 71/76 (93%) | 28 (39%) | 0 |
| All | All | 4713/4810 (97%) | 789 (16%) | 42 (0%) |

All (789) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 7 | A |
| 1 | A | 10 | G |
| 1 | A | 14 | G |
| 1 | A | 34 | G |
| 1 | A | 44 | C |
| 1 | A | 58 | G |
| 1 | A | 69 | A |
| 1 | A | 72 | A |
| 1 | A | 73 | G |
| 1 | A | 82 | A |
| 1 | A | 86 | G |
| 1 | A | 88 | U |
| 1 | A | 89 | A |
| 1 | A | 93 | G |
| 1 | A | 115 | A |
| 1 | A | 116 | A |
| 1 | A | 117 | U |
| 1 | A | 136 | G |
| 1 | A | 138 | A |
| 1 | A | 161 | G |
| 1 | A | 162 | C |
| 1 | A | 169 | A |
| 1 | A | 184 | A |
| 1 | A | 187 | A |
| 1 | A | 188 | U |
| 1 | A | 193 | G |
| 1 | A | 202 | G |
| 1 | A | 203 | G |
| 1 | A | 204 | A |
| 1 | A | 209 | A |
| 1 | A | 210 | A |
| 1 | A | 217 | A |
| 1 | A | 221 | A |
| 1 | A | 236 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 253 | A |
| 1 | A | 268 | G |
| 1 | A | 270 | U |
| 1 | A | 271 | U |
| 1 | A | 272 | G |
| 1 | A | 277 | G |
| 1 | A | 286 | G |
| 1 | A | 287 | U |
| 1 | A | 288 | G |
| 1 | A | 295 | U |
| 1 | A | 298 | G |
| 1 | A | 302 | C |
| 1 | A | 306 | A |
| 1 | A | 334 | A |
| 1 | A | 350 | G |
| 1 | A | 352 | G |
| 1 | A | 353 | A |
| 1 | A | 356 | G |
| 1 | A | 375 | G |
| 1 | A | 376 | G |
| 1 | A | 386 | G |
| 1 | A | 412 | G |
| 1 | A | 422 | G |
| 1 | A | 431 | U |
| 1 | A | 437 | G |
| 1 | A | 438 | A |
| 1 | A | 469 | C |
| 1 | A | 473 | U |
| 1 | A | 479 | A |
| 1 | A | 480 | C |
| 1 | A | 481 | C |
| 1 | A | 482 | A |
| 1 | A | 504 | A |
| 1 | A | 506 | G |
| 1 | A | 528 | U |
| 1 | A | 529 | A |
| 1 | A | 530 | G |
| 1 | A | 532 | G |
| 1 | A | 533 | C |
| 1 | A | 555 | C |
| 1 | A | 556 | A |
| 1 | A | 557 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 568 | G |
| 1 | A | 569 | C |
| 1 | A | 585 | G |
| 1 | A | 595 | G |
| 1 | A | 597 | A |
| 1 | A | 608 | A |
| 1 | A | 615 | G |
| 1 | A | 625 | A |
| 1 | A | 626 | G |
| 1 | A | 629 | U |
| 1 | A | 638 | G |
| 1 | A | 640 | G |
| 1 | A | 651 | A |
| 1 | A | 661 | A |
| 1 | A | 665 | C |
| 1 | A | 669 | C |
| 1 | A | 670 | A |
| 1 | A | 678 | A |
| 1 | A | 679 | G |
| 1 | A | 680 | C |
| 1 | A | 681 | G |
| 1 | A | 696 | C |
| 1 | A | 697 | G |
| 1 | A | 698 | C |
| 1 | A | 702 | G |
| 1 | A | 732 | G |
| 1 | A | 763 | G |
| 1 | A | 776 | C |
| 1 | A | 798 | A |
| 1 | A | 799 | C |
| 1 | A | 811 | G |
| 1 | A | 821 | G |
| 1 | A | 822 | G |
| 1 | A | 828 | A |
| 1 | A | 830 | A |
| 1 | A | 831 | G |
| 1 | A | 838 | G |
| 1 | A | 851 | G |
| 1 | A | 858 | C |
| 1 | A | 865 | A |
| 1 | A | 873 | U |
| 1 | A | 874 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 876 | G |
| 1 | A | 905 | G |
| 1 | A | 912 | A |
| 1 | A | 915 | G |
| 1 | A | 921 | G |
| 1 | A | 924 | A |
| 1 | A | 926 | G |
| 1 | A | 931 | C |
| 1 | A | 932 | C |
| 1 | A | 933 | A |
| 1 | A | 934 | C |
| 1 | A | 935 | C |
| 1 | A | 936 | A |
| 1 | A | 937 | G |
| 1 | A | 938 | C |
| 1 | A | 940 | U |
| 1 | A | 941 | A |
| 1 | A | 942 | C |
| 1 | A | 943 | C |
| 1 | A | 944 | A |
| 1 | A | 945 | A |
| 1 | A | 946 | A |
| 1 | A | 955 | A |
| 1 | A | 962 | A |
| 1 | A | 976 | G |
| 1 | A | 985 | A |
| 1 | A | 989 | A |
| 1 | A | 990 | G |
| 1 | A | 1005 | C |
| 1 | A | 1018 | G |
| 1 | A | 1019 | C |
| 1 | A | 1028 | A |
| 1 | A | 1041 | A |
| 1 | A | 1050 | C |
| 1 | A | 1057 | U |
| 1 | A | 1058 | C |
| 1 | A | 1060 | G |
| 1 | A | 1067 | G |
| 1 | A | 1078 | U |
| 1 | A | 1084 | G |
| 1 | A | 1090 | A |
| 1 | A | 1091 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 1092 | G |
| 1 | A | 1093 | A |
| 1 | A | 1096 | G |
| 1 | A | 1097 | C |
| 1 | A | 1098 | C |
| 1 | A | 1099 | A |
| 1 | A | 1103 | G |
| 1 | A | 1106 | U |
| 1 | A | 1107 | G |
| 1 | A | 1111 | U |
| 1 | A | 1114 | A |
| 1 | A | 1115 | A |
| 1 | A | 1117 | C |
| 1 | A | 1118 | A |
| 1 | A | 1120 | C |
| 1 | A | 1121 | C |
| 1 | A | 1125 | C |
| 1 | A | 1127 | U |
| 1 | A | 1128 | U |
| 1 | A | 1131 | A |
| 1 | A | 1132 | G |
| 1 | A | 1133 | A |
| 1 | A | 1135 | U |
| 1 | A | 1136 | G |
| 1 | A | 1142 | U |
| 1 | A | 1145 | C |
| 1 | A | 1154 | C |
| 1 | A | 1156 | A |
| 1 | A | 1157 | G |
| 1 | A | 1173 | A |
| 1 | A | 1174 | A |
| 1 | A | 1175 | U |
| 1 | A | 1179 | C |
| 1 | A | 1180 | G |
| 1 | A | 1185 | U |
| 1 | A | 1186 | U |
| 1 | A | 1187 | A |
| 1 | A | 1194 | G |
| 1 | A | 1216 | G |
| 1 | A | 1217 | G |
| 1 | A | 1218 | A |
| 1 | A | 1219 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 1220 | G |
| 1 | A | 1221 | A |
| 1 | A | 1222 | C |
| 1 | A | 1254 | A |
| 1 | A | 1255 | U |
| 1 | A | 1264 | A |
| 1 | A | 1265 | C |
| 1 | A | 1281 | G |
| 1 | A | 1284 | G |
| 1 | A | 1289 | G |
| 1 | A | 1293 | G |
| 1 | A | 1295 | G |
| 1 | A | 1298 | A |
| 1 | A | 1301 | G |
| 1 | A | 1302 | C |
| 1 | A | 1316 | G |
| 1 | A | 1317 | A |
| 1 | A | 1318 | U |
| 1 | A | 1345 | U |
| 1 | A | 1346 | A |
| 1 | A | 1350 | C |
| 1 | A | 1404 | A |
| 1 | A | 1410 | A |
| 1 | A | 1417 | U |
| 1 | A | 1425 | G |
| 1 | A | 1430 | G |
| 1 | A | 1461 | G |
| 1 | A | 1462 | C |
| 1 | A | 1465 | U |
| 1 | A | 1466 | G |
| 1 | A | 1473 | C |
| 1 | A | 1482 | C |
| 1 | A | 1490 | A |
| 1 | A | 1501 | G |
| 1 | A | 1506 | A |
| 1 | A | 1507 | G |
| 1 | A | 1513 | C |
| 1 | A | 1517 | A |
| 1 | A | 1528 | G |
| 1 | A | 1529 | G |
| 1 | A | 1539 | A |
| 1 | A | 1553 | A |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 1554 | C |
| 1 | A | 1555 | A |
| 1 | A | 1557 | G |
| 1 | A | 1578 | C |
| 1 | A | 1588 | A |
| 1 | A | 1589 | C |
| 1 | A | 1600 | A |
| 1 | A | 1604 | A |
| 1 | A | 1606 | G |
| 1 | A | 1612 | A |
| 1 | A | 1615 | A |
| 1 | A | 1624 | U |
| 1 | A | 1626 | A |
| 1 | A | 1627 | G |
| 1 | A | 1630 | C |
| 1 | A | 1631 | A |
| 1 | A | 1653 | A |
| 1 | A | 1654 | A |
| 1 | A | 1655 | A |
| 1 | A | 1662 | C |
| 1 | A | 1694 | C |
| 1 | A | 1700 | A |
| 1 | A | 1720 | G |
| 1 | A | 1742 | G |
| 1 | A | 1746 | A |
| 1 | A | 1761 | G |
| 1 | A | 1765 | G |
| 1 | A | 1766 | A |
| 1 | A | 1767 | U |
| 1 | A | 1768 | G |
| 1 | A | 1769 | A |
| 1 | A | 1770 | G |
| 1 | A | 1773 | C |
| 1 | A | 1774 | C |
| 1 | A | 1775 | G |
| 1 | A | 1776 | G |
| 1 | A | 1777 | G |
| 1 | A | 1778 | G |
| 1 | A | 1788 | G |
| 1 | A | 1793 | G |
| 1 | A | 1794 | G |
| 1 | A | 1799 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 1803 | A |
| 1 | A | 1821 | A |
| 1 | A | 1830 | C |
| 1 | A | 1831 | G |
| 1 | A | 1846 | G |
| 1 | A | 1869 | G |
| 1 | A | 1877 | A |
| 1 | A | 1897 | A |
| 1 | A | 1898 | A |
| 1 | A | 1899 | G |
| 1 | A | 1921 | A |
| 1 | A | 1927 | G |
| 1 | A | 1950 | G |
| 1 | A | 1951 | G |
| 1 | A | 1958 | A |
| 1 | A | 1959 | A |
| 1 | A | 1962 | C |
| 1 | A | 1976 | U |
| 1 | A | 1981 | A |
| 1 | A | 1984 | U |
| 1 | A | 1988 | C |
| 1 | A | 1991 | A |
| 1 | A | 1992 | A |
| 1 | A | 1993 | A |
| 1 | A | 2013 | G |
| 1 | A | 2014 | U |
| 1 | A | 2018 | G |
| 1 | A | 2041 | A |
| 1 | A | 2044 | G |
| 1 | A | 2052 | A |
| 1 | A | 2053 | G |
| 1 | A | 2054 | A |
| 1 | A | 2064 | C |
| 1 | A | 2076 | C |
| 1 | A | 2077 | G |
| 1 | A | 2081 | A |
| 1 | A | 2082 | G |
| 1 | A | 2083 | A |
| 1 | A | 2090 | G |
| 1 | A | 2120 | U |
| 1 | A | 2123 | U |
| 1 | A | 2124 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 2125 | G |
| 1 | A | 2126 | C |
| 1 | A | 2127 | G |
| 1 | A | 2128 | C |
| 1 | A | 2130 | U |
| 1 | A | 2134 | U |
| 1 | A | 2137 | G |
| 1 | A | 2140 | A |
| 1 | A | 2141 | G |
| 1 | A | 2142 | G |
| 1 | A | 2147 | A |
| 1 | A | 2149 | C |
| 1 | A | 2152 | G |
| 1 | A | 2153 | U |
| 1 | A | 2155 | A |
| 1 | A | 2156 | A |
| 1 | A | 2157 | C |
| 1 | A | 2159 | C |
| 1 | A | 2160 | C |
| 1 | A | 2161 | C |
| 1 | A | 2164 | C |
| 1 | A | 2165 | U |
| 1 | A | 2167 | C |
| 1 | A | 2168 | G |
| 1 | A | 2177 | G |
| 1 | A | 2178 | G |
| 1 | A | 2179 | A |
| 1 | A | 2180 | G |
| 1 | A | 2181 | G |
| 1 | A | 2182 | C |
| 1 | A | 2186 | G |
| 1 | A | 2187 | G |
| 1 | A | 2188 | U |
| 1 | A | 2189 | G |
| 1 | A | 2190 | A |
| 1 | A | 2193 | U |
| 1 | A | 2199 | C |
| 1 | A | 2200 | C |
| 1 | A | 2203 | G |
| 1 | A | 2205 | G |
| 1 | A | 2206 | C |
| 1 | A | 2208 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 2211 | G |
| 1 | A | 2213 | G |
| 1 | A | 2214 | G |
| 1 | A | 2219 | A |
| 1 | A | 2220 | A |
| 1 | A | 2221 | C |
| 1 | A | 2226 | G |
| 1 | A | 2227 | G |
| 1 | A | 2228 | A |
| 1 | A | 2230 | G |
| 1 | A | 2236 | A |
| 1 | A | 2249 | G |
| 1 | A | 2250 | G |
| 1 | A | 2284 | A |
| 1 | A | 2286 | C |
| 1 | A | 2294 | C |
| 1 | A | 2298 | A |
| 1 | A | 2316 | A |
| 1 | A | 2318 | G |
| 1 | A | 2319 | G |
| 1 | A | 2330 | G |
| 1 | A | 2331 | A |
| 1 | A | 2332 | G |
| 1 | A | 2333 | A |
| 1 | A | 2336 | G |
| 1 | A | 2338 | A |
| 1 | A | 2345 | G |
| 1 | A | 2347 | A |
| 1 | A | 2354 | C |
| 1 | A | 2358 | C |
| 1 | A | 2365 | G |
| 1 | A | 2372 | A |
| 1 | A | 2394 | G |
| 1 | A | 2396 | C |
| 1 | A | 2399 | A |
| 1 | A | 2404 | A |
| 1 | A | 2417 | U |
| 1 | A | 2425 | G |
| 1 | A | 2432 | G |
| 1 | A | 2433 | A |
| 1 | A | 2435 | C |
| 1 | A | 2436 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 2440 | G |
| 1 | A | 2441 | A |
| 1 | A | 2446 | A |
| 1 | A | 2450 | A |
| 1 | A | 2452 | C |
| 1 | A | 2459 | A |
| 1 | A | 2487 | A |
| 1 | A | 2513 | G |
| 1 | A | 2516 | G |
| 1 | A | 2517 | U |
| 1 | A | 2529 | A |
| 1 | A | 2540 | G |
| 1 | A | 2565 | U |
| 1 | A | 2577 | A |
| 1 | A | 2578 | G |
| 1 | A | 2584 | C |
| 1 | A | 2589 | G |
| 1 | A | 2596 | U |
| 1 | A | 2613 | A |
| 1 | A | 2620 | U |
| 1 | A | 2622 | U |
| 1 | A | 2623 | C |
| 1 | A | 2632 | A |
| 1 | A | 2641 | G |
| 1 | A | 2643 | A |
| 1 | A | 2654 | G |
| 1 | A | 2665 | A |
| 1 | A | 2674 | G |
| 1 | A | 2675 | G |
| 1 | A | 2694 | C |
| 1 | A | 2700 | U |
| 1 | A | 2702 | C |
| 1 | A | 2724 | A |
| 1 | A | 2725 | A |
| 1 | A | 2726 | G |
| 1 | A | 2738 | U |
| 1 | A | 2745 | A |
| 1 | A | 2769 | A |
| 1 | A | 2777 | A |
| 1 | A | 2778 | G |
| 1 | A | 2790 | A |
| 1 | A | 2802 | A |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 2803 | C |
| 1 | A | 2812 | G |
| 1 | A | 2816 | G |
| 1 | A | 2829 | A |
| 1 | A | 2830 | A |
| 1 | A | 2844 | A |
| 1 | A | 2848 | G |
| 1 | A | 2881 | G |
| 1 | A | 2891 | A |
| 1 | A | 2902 | G |
| 2 | B | 2 | C |
| 2 | B | 7 | G |
| 2 | B | 31 | C |
| 2 | B | 35 | U |
| 2 | B | 45 | A |
| 2 | B | 56 | G |
| 2 | B | 65 | C |
| 2 | B | 66 | A |
| 2 | B | 67 | G |
| 2 | B | 72 | G |
| 2 | B | 73 | A |
| 2 | B | 85 | G |
| 2 | B | 110 | G |
| 2 | B | 120 | A |
| 34 | a | 7 | G |
| 34 | a | 8 | G |
| 34 | a | 10 | G |
| 34 | a | 23 | G |
| 34 | a | 32 | G |
| 34 | a | 33 | A |
| 34 | a | 40 | G |
| 34 | a | 49 | C |
| 34 | a | 52 | A |
| 34 | a | 62 | G |
| 34 | a | 72 | C |
| 34 | a | 73 | C |
| 34 | a | 74 | G |
| 34 | a | 76 | G |
| 34 | a | 78 | G |
| 34 | a | 87 | C |
| 34 | a | 88 | C |
| 34 | a | 89 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | a | 91 | G |
| 34 | a | 92 | G |
| 34 | a | 93 | U |
| 34 | a | 95 | A |
| 34 | a | 114 | A |
| 34 | a | 115 | C |
| 34 | a | 126 | C |
| 34 | a | 137 | G |
| 34 | a | 138 | A |
| 34 | a | 139 | G |
| 34 | a | 152 | G |
| 34 | a | 154 | G |
| 34 | a | 155 | A |
| 34 | a | 158 | C |
| 34 | a | 177 | U |
| 34 | a | 204 | A |
| 34 | a | 209 | U |
| 34 | a | 210 | U |
| 34 | a | 211 | U |
| 34 | a | 212 | G |
| 34 | a | 216 | G |
| 34 | a | 243 | G |
| 34 | a | 247 | G |
| 34 | a | 262 | G |
| 34 | a | 263 | C |
| 34 | a | 282 | G |
| 34 | a | 285 | G |
| 34 | a | 314 | G |
| 34 | a | 317 | A |
| 34 | a | 324 | C |
| 34 | a | 328 | G |
| 34 | a | 338 | C |
| 34 | a | 339 | U |
| 34 | a | 340 | A |
| 34 | a | 341 | C |
| 34 | a | 342 | G |
| 34 | a | 343 | G |
| 34 | a | 348 | C |
| 34 | a | 349 | A |
| 34 | a | 350 | G |
| 34 | a | 352 | A |
| 34 | a | 363 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | a | 368 | C |
| 34 | a | 380 | G |
| 34 | a | 394 | C |
| 34 | a | 402 | G |
| 34 | a | 407 | A |
| 34 | a | 408 | A |
| 34 | a | 409 | G |
| 34 | a | 410 | A |
| 34 | a | 420 | G |
| 34 | a | 425 | U |
| 34 | a | 426 | A |
| 34 | a | 433 | U |
| 34 | a | 441 | G |
| 34 | a | 447 | A |
| 34 | a | 451 | C |
| 34 | a | 455 | A |
| 34 | a | 456 | C |
| 34 | a | 457 | G |
| 34 | a | 470 | G |
| 34 | a | 481 | A |
| 34 | a | 482 | U |
| 34 | a | 489 | G |
| 34 | a | 493 | A |
| 34 | a | 494 | A |
| 34 | a | 495 | C |
| 34 | a | 502 | C |
| 34 | a | 508 | G |
| 34 | a | 511 | G |
| 34 | a | 514 | G |
| 34 | a | 515 | U |
| 34 | a | 516 | A |
| 34 | a | 531 | A |
| 34 | a | 543 | A |
| 34 | a | 545 | U |
| 34 | a | 556 | A |
| 34 | a | 557 | A |
| 34 | a | 558 | A |
| 34 | a | 560 | G |
| 34 | a | 561 | G |
| 34 | a | 591 | A |
| 34 | a | 614 | G |
| 34 | a | 615 | G |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | a | 616 | A |
| 34 | a | 621 | G |
| 34 | a | 634 | G |
| 34 | a | 637 | A |
| 34 | a | 649 | A |
| 34 | a | 650 | G |
| 34 | a | 671 | A |
| 34 | a | 672 | G |
| 34 | a | 679 | A |
| 34 | a | 707 | U |
| 34 | a | 715 | G |
| 34 | a | 718 | G |
| 34 | a | 733 | C |
| 34 | a | 739 | G |
| 34 | a | 761 | A |
| 34 | a | 777 | U |
| 34 | a | 778 | A |
| 34 | a | 799 | A |
| 34 | a | 801 | C |
| 34 | a | 803 | A |
| 34 | a | 812 | A |
| 34 | a | 823 | U |
| 34 | a | 824 | C |
| 34 | a | 825 | U |
| 34 | a | 826 | C |
| 34 | a | 837 | A |
| 34 | a | 852 | G |
| 34 | a | 880 | G |
| 34 | a | 892 | A |
| 34 | a | 904 | G |
| 34 | a | 905 | G |
| 34 | a | 912 | C |
| 34 | a | 913 | A |
| 34 | a | 920 | G |
| 34 | a | 938 | U |
| 34 | a | 939 | U |
| 34 | a | 944 | G |
| 34 | a | 946 | A |
| 34 | a | 947 | A |
| 34 | a | 949 | G |
| 34 | a | 953 | A |
| 34 | a | 954 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | a | 955 | A |
| 34 | a | 971 | G |
| 34 | a | 978 | U |
| 34 | a | 985 | C |
| 34 | a | 986 | C |
| 34 | a | 988 | G |
| 34 | a | 989 | G |
| 34 | a | 996 | G |
| 34 | a | 1002 | G |
| 34 | a | 1003 | G |
| 34 | a | 1004 | U |
| 34 | a | 1005 | G |
| 34 | a | 1006 | C |
| 34 | a | 1007 | C |
| 34 | a | 1008 | C |
| 34 | a | 1009 | C |
| 34 | a | 1010 | G |
| 34 | a | 1014 | G |
| 34 | a | 1016 | G |
| 34 | a | 1017 | G |
| 34 | a | 1019 | G |
| 34 | a | 1020 | C |
| 34 | a | 1027 | A |
| 34 | a | 1037 | C |
| 34 | a | 1049 | C |
| 34 | a | 1068 | U |
| 34 | a | 1071 | G |
| 34 | a | 1077 | G |
| 34 | a | 1078 | U |
| 34 | a | 1084 | A |
| 34 | a | 1107 | G |
| 34 | a | 1108 | U |
| 34 | a | 1109 | U |
| 34 | a | 1110 | G |
| 34 | a | 1112 | C |
| 34 | a | 1113 | A |
| 34 | a | 1114 | G |
| 34 | a | 1116 | G |
| 34 | a | 1120 | C |
| 34 | a | 1122 | G |
| 34 | a | 1123 | C |
| 34 | a | 1128 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | a | 1129 | A |
| 34 | a | 1135 | A |
| 34 | a | 1140 | A |
| 34 | a | 1141 | C |
| 34 | a | 1142 | U |
| 34 | a | 1143 | G |
| 34 | a | 1164 | G |
| 34 | a | 1178 | U |
| 34 | a | 1179 | G |
| 34 | a | 1195 | A |
| 34 | a | 1209 | A |
| 34 | a | 1218 | A |
| 34 | a | 1220 | A |
| 34 | a | 1222 | U |
| 34 | a | 1239 | U |
| 34 | a | 1240 | G |
| 34 | a | 1252 | C |
| 34 | a | 1260 | U |
| 34 | a | 1262 | A |
| 34 | a | 1267 | A |
| 34 | a | 1268 | A |
| 34 | a | 1269 | A |
| 34 | a | 1272 | G |
| 34 | a | 1281 | A |
| 34 | a | 1282 | G |
| 34 | a | 1283 | U |
| 34 | a | 1284 | U |
| 34 | a | 1287 | G |
| 34 | a | 1302 | C |
| 34 | a | 1304 | C |
| 34 | a | 1320 | G |
| 34 | a | 1328 | A |
| 34 | a | 1329 | G |
| 34 | a | 1347 | U |
| 34 | a | 1353 | G |
| 34 | a | 1360 | A |
| 34 | a | 1377 | A |
| 34 | a | 1380 | C |
| 34 | a | 1381 | A |
| 34 | a | 1402 | G |
| 34 | a | 1423 | C |
| 34 | a | 1425 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | a | 1431 | U |
| 34 | a | 1432 | A |
| 34 | a | 1433 | C |
| 34 | a | 1434 | G |
| 34 | a | 1447 | G |
| 34 | a | 1470 | A |
| 34 | a | 1471 | A |
| 34 | a | 1472 | G |
| 34 | a | 1481 | A |
| 34 | a | 1484 | U |
| 34 | a | 1495 | G |
| 34 | a | 1498 | G |
| 34 | a | 1507 | G |
| 34 | a | 1508 | G |
| 34 | a | 1509 | A |
| 55 | v | 24 | A |
| 56 | w | 6 | G |
| 56 | w | 8 | 4SU |
| 56 | w | 9 | A |
| 56 | w | 13 | C |
| 56 | w | 15 | G |
| 56 | w | 19 | G |
| 56 | w | 20 | U |
| 56 | w | 21 | A |
| 56 | w | 26 | A |
| 56 | w | 44 | G |
| 56 | w | 45 | U |
| 56 | w | 46 | 7MG |
| 56 | w | 47 | U |
| 56 | w | 48 | C |
| 56 | w | 49 | C |
| 56 | w | 55 | PSU |
| 56 | w | 56 | C |
| 56 | w | 58 | A |
| 56 | w | 59 | U |
| 56 | w | 60 | U |
| 56 | w | 61 | C |
| 56 | w | 63 | G |
| 56 | w | 64 | A |
| 56 | w | 71 | G |
| 56 | w | 74 | C |
| 56 | w | 76 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 57 | x | 2 | G |
| 57 | x | 9 | G |
| 57 | x | 14 | A |
| 57 | x | 16 | C |
| 57 | x | 17 | C |
| 57 | x | 17(A) | U |
| 57 | x | 18 | G |
| 57 | x | 19 | G |
| 57 | x | 31 | G |
| 57 | x | 47 | U |
| 57 | x | 48 | C |
| 57 | x | 61 | C |
| 57 | x | 76 | A |
| 58 | y | 2 | C |
| 58 | y | 5 | G |
| 58 | y | 7 | A |
| 58 | y | 8 | 4SU |
| 58 | y | 9 | A |
| 58 | y | 13 | C |
| 58 | y | 19 | G |
| 58 | y | 20 | U |
| 58 | y | 21 | A |
| 58 | y | 22 | G |
| 58 | y | 25 | C |
| 58 | y | 26 | A |
| 58 | y | 29 | G |
| 58 | y | 30 | G |
| 58 | y | 32 | PSU |
| 58 | y | 33 | U |
| 58 | y | 35 | A |
| 58 | y | 41 | C |
| 58 | y | 43 | C |
| 58 | y | 44 | G |
| 58 | y | 45 | U |
| 58 | y | 46 | G |
| 58 | y | 47 | U |
| 58 | y | 48 | C |
| 58 | y | 56 | C |
| 58 | y | 59 | U |
| 58 | y | 60 | U |
| 58 | y | 66 | U |

All (42) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 33 | C |
| 1 | A | 88 | U |
| 1 | A | 184 | A |
| 1 | A | 270 | U |
| 1 | A | 271 | U |
| 1 | A | 301 | A |
| 1 | A | 385 | U |
| 1 | A | 514 | G |
| 1 | A | 669 | C |
| 1 | A | 677 | A |
| 1 | A | 731 | A |
| 1 | A | 792 | A |
| 1 | A | 798 | A |
| 1 | A | 810 | A |
| 1 | A | 1008 | C |
| 1 | A | 1018 | G |
| 1 | A | 1037 | C |
| 1 | A | 1097 | C |
| 1 | A | 1120 | C |
| 1 | A | 1132 | G |
| 1 | A | 1153 | U |
| 1 | A | 1218 | A |
| 1 | A | 1220 | G |
| 1 | A | 1238 | A |
| 1 | A | 1254 | A |
| 1 | A | 1424 | A |
| 1 | A | 1465 | U |
| 1 | A | 1653 | A |
| 1 | A | 1699 | G |
| 1 | A | 2013 | G |
| 1 | A | 2123 | U |
| 1 | A | 2166 | C |
| 1 | A | 2202 | G |
| 1 | A | 2212 | G |
| 1 | A | 2329 | G |
| 1 | A | 2417 | U |
| 1 | A | 2432 | G |
| 1 | A | 2433 | A |
| 1 | A | 2450 | A |
| 1 | A | 2622 | U |
| 1 | A | 2768 | U |
| 1 | A | 2901 | G |

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

17 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 |
| 58 | PSU | y | 39 | 58 | 18,21,22 | 1.47 | 2 (11%) | 22,30,33 | 1.80 | 5 (22%) |
| 56 | MIA | w | 37 | 56 | 24,29,32 | 2.20 | 3 (12%) | 25,41,47 | 2.83 | 10 (40%) |
| 56 | 5MU | w | 54 | 56 | 19,22,23 | 1.40 | 4 (21%) | 28,32,35 | 1.80 | 7 (25%) |
| 57 | PSU | x | 55 | 57 | 18,21,22 | 1.42 | 3 (16%) | 22,30,33 | 1.84 | 5 (22%) |
| 58 | MIA | y | 37 | 58,34 | 18,24,32 | 1.26 | 2 (11%) | 18,35,47 | 1.25 | 2 (11%) |
| 57 | 5MU | x | 54 | 60,57 | 19,22,23 | 1.30 | 4 (21%) | 28,32,35 | 2.11 | 6 (21%) |
| 56 | PSU | w | 55 | 56 | 18,21,22 | 1.34 | 2 (11%) | 22,30,33 | 1.76 | 4 (18%) |
| 56 | 7MG | w | 46 | 56 | 22,26,27 | 1.40 | 5 (22%) | 29,39,42 | 2.40 | 7 (24%) |
| 58 | 4SU | y | 8 | 58 | 18,21,22 | 4.60 | 7 (38%) | 26,30,33 | 11.78 | 8 (30%) |
| 57 | 4SU | x | 8 | 57 | 18,21,22 | 2.11 | 6 (33%) | 26,30,33 | 2.02 | 5 (19%) |
| 56 | PSU | w | 32 | 56 | 18,21,22 | 1.43 | 2 (11%) | 22,30,33 | 1.87 | 5 (22%) |
| 58 | PSU | y | 32 | 58 | 18,21,22 | 1.40 | 3 (16%) | 22,30,33 | 1.80 | 3 (13%) |
| 58 | PSU | y | 55 | 58 | 18,21,22 | 1.39 | 2 (11%) | 22,30,33 | 1.89 | 4 (18%) |
| 57 | 5MC | x | 32 | 57 | 18,22,23 | 0.98 | 2 (11%) | 26,32,35 | 1.15 | 2 (7%) |
| 56 | 4SU | w | 8 | 56 | 18,21,22 | 1.81 | 5 (27%) | 26,30,33 | 1.95 | 5 (19%) |
| 56 | PSU | w | 39 | 56 | 18,21,22 | 1.29 | 2 (11%) | 22,30,33 | 1.90 | 5 (22%) |
| 58 | 5MU | y | 54 | 58 | 19,22,23 | 1.44 | 6 (31%) | 28,32,35 | 1.97 | 8 (28%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 58 | PSU | y | 39 | 58 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | MIA | w | 37 | 56 | - | 6/10/31/34 | 0/3/3/3 |
| 56 | 5MU | w | 54 | 56 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 57 | PSU | x | 55 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 58 | MIA | y | 37 | 58,34 | - | 2/3/25/34 | 0/3/3/3 |
| 57 | 5MU | x | 54 | 60,57 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | PSU | w | 55 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | 7MG | w | 46 | 56 | - | 3/7/37/38 | 0/3/3/3 |
| 58 | 4SU | y | 8 | 58 | - | 2/7/25/26 | 0/2/2/2 |
| 57 | 4SU | x | 8 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | PSU | w | 32 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 58 | PSU | y | 32 | 58 | - | 4/7/25/26 | 0/2/2/2 |
| 58 | PSU | y | 55 | 58 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | 5MC | x | 32 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | 4SU | w | 8 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | PSU | w | 39 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 58 | 5MU | y | 54 | 58 | - | 0/7/25/26 | 0/2/2/2 |

All (60) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 58 | y | 8 | 4SU | O2-C2 | -12.52 | 1.00 | 1.23 |
| 58 | y | 8 | 4SU | C4-N3 | 10.94 | 1.49 | 1.37 |
| 56 | w | 37 | MIA | C2-S10 | -7.24 | 1.69 | 1.75 |
| 56 | w | 37 | MIA | C13-C14 | 6.90 | 1.52 | 1.32 |
| 57 | x | 8 | 4SU | C4-N3 | -5.80 | 1.31 | 1.37 |
| 58 | y | 8 | 4SU | C6-C5 | 5.13 | 1.47 | 1.35 |
| 58 | y | 8 | 4SU | C2-N1 | 4.79 | 1.46 | 1.38 |
| 58 | y | 8 | 4SU | C5-C4 | 4.75 | 1.48 | 1.42 |
| 58 | y | 8 | 4SU | C4-S4 | -4.58 | 1.59 | 1.68 |
| 56 | w | 8 | 4SU | C4-S4 | -4.38 | 1.60 | 1.68 |
| 58 | y | 39 | PSU | C6-C5 | 4.02 | 1.40 | 1.35 |
| 57 | x | 8 | 4SU | C2-N3 | -4.01 | 1.30 | 1.38 |
| 56 | w | 32 | PSU | C6-C5 | 4.01 | 1.40 | 1.35 |
| 56 | w | 8 | 4SU | C4-N3 | -3.81 | 1.33 | 1.37 |
| 58 | y | 32 | PSU | C6-C5 | 3.52 | 1.39 | 1.35 |
| 56 | w | 55 | PSU | C6-C5 | 3.50 | 1.39 | 1.35 |
| 58 | y | 55 | PSU | C6-C5 | 3.49 | 1.39 | 1.35 |
| 56 | w | 39 | PSU | C6-C5 | 3.36 | 1.39 | 1.35 |
| 57 | x | 55 | PSU | C4-N3 | -3.31 | 1.32 | 1.38 |
| 56 | w | 46 | 7MG | C5-C4 | 3.20 | 1.48 | 1.38 |
| 56 | w | 46 | 7MG | C4-N9 | -3.13 | 1.34 | 1.37 |
| 58 | y | 37 | MIA | C2-N3 | 3.01 | 1.36 | 1.32 |
| 56 | w | 54 | 5MU | C6-C5 | 2.95 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 58 | y | 37 | MIA | C5-C4 | 2.91 | 1.48 | 1.40 |
| 57 | x | 54 | 5MU | C4-N3 | -2.82 | 1.33 | 1.38 |
| 58 | y | 39 | PSU | C4-N3 | -2.79 | 1.33 | 1.38 |
| 58 | y | 54 | 5MU | C2-N1 | 2.77 | 1.42 | 1.38 |
| 57 | x | 8 | 4SU | C5-C4 | -2.70 | 1.39 | 1.42 |
| 56 | w | 32 | PSU | C4-N3 | -2.69 | 1.33 | 1.38 |
| 57 | x | 8 | 4SU | C6-C5 | 2.68 | 1.41 | 1.35 |
| 57 | x | 32 | 5MC | C6-N1 | -2.67 | 1.33 | 1.38 |
| 58 | y | 32 | PSU | C4-N3 | -2.67 | 1.33 | 1.38 |
| 57 | x | 54 | 5MU | C6-C5 | 2.63 | 1.38 | 1.34 |
| 58 | y | 55 | PSU | C4-N3 | -2.63 | 1.34 | 1.38 |
| 57 | x | 8 | 4SU | C4-S4 | -2.61 | 1.63 | 1.68 |
| 56 | w | 8 | 4SU | C5-C4 | -2.57 | 1.39 | 1.42 |
| 56 | w | 54 | 5MU | C4-N3 | -2.56 | 1.34 | 1.38 |
| 57 | x | 8 | 4SU | O2-C2 | 2.52 | 1.27 | 1.23 |
| 56 | w | 55 | PSU | C4-N3 | -2.50 | 1.34 | 1.38 |
| 58 | y | 54 | 5MU | C6-C5 | 2.48 | 1.38 | 1.34 |
| 57 | x | 32 | 5MC | C6-C5 | 2.46 | 1.38 | 1.34 |
| 56 | w | 39 | PSU | C4-N3 | -2.45 | 1.34 | 1.38 |
| 56 | w | 46 | 7MG | C8-N9 | 2.44 | 1.47 | 1.46 |
| 58 | y | 54 | 5MU | C4-C5 | 2.43 | 1.48 | 1.44 |
| 57 | x | 55 | PSU | C2-N3 | -2.39 | 1.33 | 1.37 |
| 56 | w | 54 | 5MU | C4-C5 | 2.36 | 1.48 | 1.44 |
| 56 | w | 54 | 5MU | C2-N1 | 2.36 | 1.42 | 1.38 |
| 58 | y | 8 | 4SU | C6-N1 | 2.35 | 1.43 | 1.38 |
| 58 | y | 54 | 5MU | C4-N3 | -2.34 | 1.34 | 1.38 |
| 57 | x | 54 | 5MU | C6-N1 | -2.32 | 1.34 | 1.38 |
| 56 | w | 8 | 4SU | C2-N3 | -2.27 | 1.33 | 1.38 |
| 56 | w | 46 | 7MG | C6-N1 | -2.25 | 1.34 | 1.38 |
| 56 | w | 8 | 4SU | C2-N1 | 2.21 | 1.42 | 1.38 |
| 56 | w | 37 | MIA | C5-C4 | 2.17 | 1.46 | 1.40 |
| 57 | x | 55 | PSU | C6-C5 | 2.13 | 1.37 | 1.35 |
| 58 | y | 32 | PSU | C4-C5 | 2.10 | 1.50 | 1.44 |
| 56 | w | 46 | 7MG | C5-C6 | 2.09 | 1.48 | 1.43 |
| 58 | y | 54 | 5MU | C2-N3 | -2.08 | 1.34 | 1.38 |
| 58 | y | 54 | 5MU | C6-N1 | -2.05 | 1.34 | 1.38 |
| 57 | x | 54 | 5MU | C2-N3 | -2.04 | 1.34 | 1.38 |

All (91) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 58 | y | 8 | 4SU | O2-C2-N1 | -40.28 | 69.25 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 58 | y | 8 | 4SU | O2-C2-N3 | -39.78 | 47.40 | 121.50 |
| 58 | y | 8 | 4SU | C6-C5-C4 | -12.81 | 108.86 | 119.95 |
| 58 | y | 8 | 4SU | C5-C4-N3 | 11.26 | 125.13 | 114.69 |
| 56 | w | 46 | 7MG | N9-C4-N3 | 8.37 | 137.99 | 125.47 |
| 56 | w | 37 | MIA | C12-C13-C14 | -7.94 | 111.69 | 127.14 |
| 58 | y | 8 | 4SU | C5-C4-S4 | -6.78 | 115.74 | 124.47 |
| 56 | w | 37 | MIA | C11-S10-C2 | -6.68 | 97.28 | 102.27 |
| 57 | x | 8 | 4SU | C4-N3-C2 | 6.58 | 133.73 | 127.34 |
| 58 | y | 8 | 4SU | C4-N3-C2 | -6.32 | 121.20 | 127.34 |
| 56 | w | 32 | PSU | N1-C2-N3 | 6.11 | 122.06 | 115.13 |
| 57 | x | 55 | PSU | N1-C2-N3 | 5.97 | 121.90 | 115.13 |
| 58 | y | 39 | PSU | N1-C2-N3 | 5.85 | 121.75 | 115.13 |
| 58 | y | 32 | PSU | N1-C2-N3 | 5.77 | 121.67 | 115.13 |
| 58 | y | 55 | PSU | N1-C2-N3 | 5.76 | 121.65 | 115.13 |
| 56 | w | 39 | PSU | N1-C2-N3 | 5.71 | 121.59 | 115.13 |
| 56 | w | 8 | 4SU | C4-N3-C2 | -5.41 | 122.08 | 127.34 |
| 57 | x | 54 | 5MU | N3-C2-N1 | 5.39 | 122.04 | 114.89 |
| 56 | w | 8 | 4SU | C5-C4-N3 | 5.27 | 119.57 | 114.69 |
| 56 | w | 55 | PSU | N1-C2-N3 | 5.26 | 121.09 | 115.13 |
| 56 | w | 46 | 7MG | N9-C8-N7 | -5.11 | 96.08 | 103.38 |
| 57 | x | 54 | 5MU | C4-N3-C2 | -5.07 | 120.78 | 127.35 |
| 56 | w | 46 | 7MG | C5-C4-N3 | -5.04 | 118.53 | 128.13 |
| 56 | w | 37 | MIA | C16-C14-C13 | -4.84 | 108.65 | 122.65 |
| 58 | y | 54 | 5MU | C4-N3-C2 | -4.53 | 121.49 | 127.35 |
| 56 | w | 54 | 5MU | N3-C2-N1 | 4.36 | 120.67 | 114.89 |
| 56 | w | 39 | PSU | C4-N3-C2 | -4.28 | 120.17 | 126.34 |
| 57 | x | 54 | 5MU | O4-C4-C5 | -4.19 | 120.04 | 124.90 |
| 58 | y | 54 | 5MU | C5-C4-N3 | 4.18 | 118.88 | 115.31 |
| 58 | y | 54 | 5MU | N3-C2-N1 | 4.16 | 120.41 | 114.89 |
| 56 | w | 46 | 7MG | C2-N3-C4 | 4.15 | 119.70 | 112.30 |
| 58 | y | 55 | PSU | C4-N3-C2 | -4.14 | 120.38 | 126.34 |
| 56 | w | 54 | 5MU | C4-N3-C2 | -4.06 | 122.09 | 127.35 |
| 58 | y | 54 | 5MU | O4-C4-C5 | -3.96 | 120.31 | 124.90 |
| 57 | x | 55 | PSU | C4-N3-C2 | -3.94 | 120.66 | 126.34 |
| 56 | w | 55 | PSU | C4-N3-C2 | -3.89 | 120.73 | 126.34 |
| 57 | x | 54 | 5MU | O2-C2-N1 | -3.89 | 117.62 | 122.79 |
| 56 | w | 37 | MIA | C2-N3-C4 | 3.88 | 120.67 | 115.32 |
| 56 | w | 8 | 4SU | N3-C2-N1 | 3.76 | 119.88 | 114.89 |
| 57 | x | 54 | 5MU | C5-C4-N3 | 3.73 | 118.50 | 115.31 |
| 57 | x | 8 | 4SU | C6-C5-C4 | -3.73 | 116.72 | 119.95 |
| 56 | w | 32 | PSU | C4-N3-C2 | -3.70 | 121.01 | 126.34 |
| 56 | w | 37 | MIA | C15-C14-C13 | -3.68 | 112.01 | 122.65 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56 | w | 54 | 5MU | C5-C4-N3 | 3.67 | 118.44 | 115.31 |
| 58 | y | 37 | MIA | N3-C2-N1 | -3.62 | 123.02 | 128.68 |
| 57 | x | 8 | 4SU | S4-C4-N3 | -3.58 | 116.68 | 120.21 |
| 58 | y | 39 | PSU | C4-N3-C2 | -3.58 | 121.18 | 126.34 |
| 58 | y | 32 | PSU | C4-N3-C2 | -3.57 | 121.20 | 126.34 |
| 57 | x | 8 | 4SU | C5-C4-S4 | 3.56 | 129.05 | 124.47 |
| 57 | x | 54 | 5MU | C5-C6-N1 | -3.50 | 119.74 | 123.34 |
| 57 | x | 32 | 5MC | C5-C6-N1 | -3.47 | 119.77 | 123.34 |
| 57 | x | 8 | 4SU | O2-C2-N1 | 3.43 | 127.34 | 122.79 |
| 56 | w | 54 | 5MU | O4-C4-C5 | -3.40 | 120.96 | 124.90 |
| 58 | y | 54 | 5MU | C5-C6-N1 | -3.39 | 119.85 | 123.34 |
| 58 | y | 8 | 4SU | C5-C6-N1 | 3.37 | 127.45 | 121.81 |
| 56 | w | 37 | MIA | C5-C6-N1 | -3.10 | 118.24 | 120.81 |
| 58 | y | 55 | PSU | O2-C2-N1 | -2.96 | 119.53 | 122.79 |
| 56 | w | 8 | 4SU | C5-C4-S4 | -2.81 | 120.85 | 124.47 |
| 58 | y | 32 | PSU | O2-C2-N1 | -2.71 | 119.81 | 122.79 |
| 56 | w | 37 | MIA | C2-N1-C6 | 2.68 | 121.98 | 117.19 |
| 56 | w | 54 | 5MU | C5-C6-N1 | -2.65 | 120.61 | 123.34 |
| 56 | w | 39 | PSU | C5-C6-N1 | -2.60 | 118.22 | 122.11 |
| 56 | w | 37 | MIA | C12-N6-C6 | -2.57 | 118.74 | 122.55 |
| 56 | w | 39 | PSU | O2-C2-N1 | -2.53 | 120.00 | 122.79 |
| 56 | w | 32 | PSU | O2-C2-N1 | -2.50 | 120.04 | 122.79 |
| 57 | x | 32 | 5MC | C5-C4-N3 | -2.49 | 118.98 | 121.67 |
| 58 | y | 55 | PSU | C6-C5-C4 | -2.47 | 116.47 | 118.20 |
| 56 | w | 8 | 4SU | C1'-N1-C2 | 2.44 | 121.98 | 117.57 |
| 58 | y | 54 | 5MU | C5M-C5-C4 | 2.43 | 121.44 | 118.77 |
| 57 | x | 55 | PSU | C5-C6-N1 | -2.43 | 118.47 | 122.11 |
| 58 | y | 8 | 4SU | C1'-N1-C2 | 2.42 | 121.95 | 117.57 |
| 58 | y | 39 | PSU | C5-C6-N1 | -2.41 | 118.49 | 122.11 |
| 56 | w | 46 | 7MG | CM7-N7-C5 | 2.34 | 132.44 | 126.40 |
| 58 | y | 37 | MIA | C4-C5-N7 | -2.34 | 106.96 | 109.40 |
| 56 | w | 46 | 7MG | C5-C6-N1 | 2.30 | 115.05 | 110.99 |
| 56 | w | 37 | MIA | N3-C2-N1 | -2.27 | 122.81 | 126.98 |
| 58 | y | 39 | PSU | O2-C2-N3 | -2.25 | 117.58 | 121.82 |
| 57 | x | 55 | PSU | O2-C2-N3 | -2.23 | 117.61 | 121.82 |
| 58 | y | 39 | PSU | O4'-C1'-C2' | 2.22 | 108.27 | 105.14 |
| 56 | w | 46 | 7MG | C5-C4-N9 | -2.21 | 103.48 | 106.35 |
| 56 | w | 55 | PSU | O2-C2-N1 | -2.17 | 120.41 | 122.79 |
| 56 | w | 37 | MIA | C4-C5-N7 | -2.15 | 107.16 | 109.40 |
| 56 | w | 32 | PSU | C5-C6-N1 | -2.12 | 118.93 | 122.11 |
| 57 | x | 55 | PSU | O2-C2-N1 | -2.09 | 120.48 | 122.79 |
| 56 | w | 32 | PSU | O2-C2-N3 | -2.07 | 117.91 | 121.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56 | w | 54 | 5MU | C5M-C5-C4 | 2.07 | 121.04 | 118.77 |
| 56 | w | 54 | 5MU | C1'-N1-C2 | 2.07 | 121.31 | 117.57 |
| 58 | y | 54 | 5MU | C5M-C5-C6 | -2.06 | 120.09 | 122.85 |
| 58 | y | 54 | 5MU | C1'-N1-C2 | 2.04 | 121.26 | 117.57 |
| 56 | w | 55 | PSU | C5-C6-N1 | -2.03 | 119.06 | 122.11 |
| 56 | w | 39 | PSU | O4'-C1'-C2' | 2.02 | 107.99 | 105.14 |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 56 | w | 37 | MIA | C5-C6-N6-C12 |
| 56 | w | 37 | MIA | C12-C13-C14-C15 |
| 56 | w | 37 | MIA | C12-C13-C14-C16 |
| 58 | y | 32 | PSU | C2'-C1'-C5-C4 |
| 58 | y | 32 | PSU | C2'-C1'-C5-C6 |
| 56 | w | 46 | 7MG | O4'-C4'-C5'-O5' |
| 56 | w | 46 | 7MG | C3'-C4'-C5'-O5' |
| 58 | y | 8 | 4SU | C2'-C1'-N1-C2 |
| 58 | y | 8 | 4SU | C2'-C1'-N1-C6 |
| 56 | w | 37 | MIA | N1-C6-N6-C12 |
| 58 | y | 37 | MIA | C3'-C4'-C5'-O5' |
| 58 | y | 32 | PSU | C4'-C5'-O5'-P |
| 56 | w | 37 | MIA | N1-C2-S10-C11 |
| 58 | y | 32 | PSU | C3'-C4'-C5'-O5' |
| 56 | w | 37 | MIA | N3-C2-S10-C11 |
| 56 | w | 46 | 7MG | C4'-C5'-O5'-P |
| 58 | y | 37 | MIA | O4'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 927 ligands modelled in this entry, 925 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 62 | SF4 | d | 302 | 37 | 0,12,12 | - | - | - | | |
| 63 | GCP | z | 703 | 60 | 27,34,34 | 2.08 | 7 (25%) | 34,54,54 | 1.93 | 8 (23%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 62 | SF4 | d | 302 | 37 | - | - | 0/6/5/5 |
| 63 | GCP | z | 703 | 60 | - | 9/15/38/38 | 0/3/3/3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 63 | z | 703 | GCP | PB-O2B | -6.34 | 1.41 | 1.56 |
| 63 | z | 703 | GCP | PG-O3G | -4.32 | 1.45 | 1.54 |
| 63 | z | 703 | GCP | C2'-C1' | -2.97 | 1.49 | 1.53 |
| 63 | z | 703 | GCP | PB-O1B | 2.77 | 1.58 | 1.51 |
| 63 | z | 703 | GCP | C5-C6 | 2.73 | 1.46 | 1.41 |
| 63 | z | 703 | GCP | PG-O1G | 2.37 | 1.55 | 1.50 |
| 63 | z | 703 | GCP | PA-O2A | -2.21 | 1.44 | 1.55 |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 63 | z | 703 | GCP | C2-N3-C4 | 5.03 | 121.10 | 115.36 |
| 63 | z | 703 | GCP | C4-C5-C6 | -3.70 | 117.27 | 120.80 |
| 63 | z | 703 | GCP | C2-N1-C6 | 3.44 | 121.40 | 115.93 |
| 63 | z | 703 | GCP | C5-C6-N1 | -3.24 | 119.00 | 123.43 |
| 63 | z | 703 | GCP | N3-C2-N1 | -3.14 | 123.04 | 127.22 |
| 63 | z | 703 | GCP | O3'-C3'-C2' | -2.79 | 102.79 | 111.82 |
| 63 | z | 703 | GCP | O3G-PG-O2G | 2.45 | 115.24 | 108.08 |
| 63 | z | 703 | GCP | O2G-PG-O1G | -2.24 | 106.47 | 112.39 |

There are no chirality outliers.

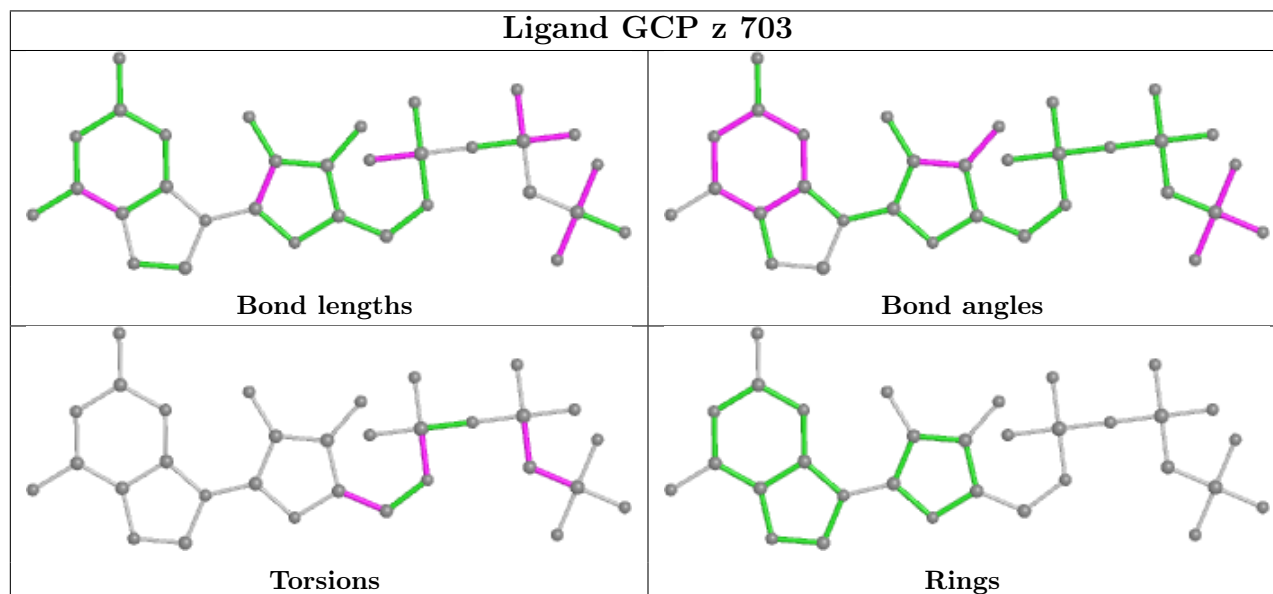
All (9) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 63 | z | 703 | GCP | PB-C3B-PG-O1G |
| 63 | z | 703 | GCP | PB-C3B-PG-O2G |
| 63 | z | 703 | GCP | PG-C3B-PB-O1B |
| 63 | z | 703 | GCP | C5'-O5'-PA-O3A |
| 63 | z | 703 | GCP | O4'-C4'-C5'-O5' |
| 63 | z | 703 | GCP | C3'-C4'-C5'-O5' |
| 63 | z | 703 | GCP | C5'-O5'-PA-O1A |
| 63 | z | 703 | GCP | C5'-O5'-PA-O2A |
| 63 | z | 703 | GCP | PB-C3B-PG-O3G |

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-----------|
| 1 | A | 2874/2915 (98%) | 0.19 | 151 (5%) 26 20 | 22, 39, 92, 112 | 465 (16%) |
| 2 | B | 120/121 (99%) | 0.15 | 0 100 100 | 36, 57, 73, 93 | 18 (15%) |
| 3 | C | 136/228 (59%) | 2.05 | 60 (44%) 0 0 | 72, 89, 95, 97 | 104 (76%) |
| 4 | D | 275/276 (99%) | -0.01 | 1 (0%) 92 91 | 18, 37, 49, 69 | 42 (15%) |
| 5 | E | 204/206 (99%) | 0.18 | 5 (2%) 57 51 | 20, 41, 63, 76 | 38 (18%) |
| 6 | F | 203/210 (96%) | 0.09 | 3 (1%) 73 70 | 22, 50, 75, 90 | 31 (15%) |
| 7 | G | 181/182 (99%) | 0.35 | 10 (5%) 25 19 | 42, 58, 78, 84 | 38 (20%) |
| 8 | H | 174/180 (96%) | 0.30 | 8 (4%) 32 26 | 39, 54, 70, 73 | 30 (17%) |
| 9 | J | 130/173 (75%) | 3.73 | 89 (68%) 0 0 | 84, 138, 186, 214 | 10 (7%) |
| 10 | K | 139/147 (94%) | 4.74 | 112 (80%) 0 0 | 93, 102, 107, 110 | 115 (82%) |
| 11 | N | 140/140 (100%) | 0.07 | 3 (2%) 63 58 | 26, 43, 65, 83 | 27 (19%) |
| 12 | O | 122/122 (100%) | -0.06 | 0 100 100 | 27, 39, 50, 65 | 7 (5%) |
| 13 | P | 149/150 (99%) | 0.20 | 3 (2%) 65 60 | 21, 48, 65, 83 | 38 (25%) |
| 14 | Q | 141/141 (100%) | -0.03 | 3 (2%) 63 58 | 27, 42, 59, 87 | 36 (25%) |
| 15 | R | 118/118 (100%) | 0.10 | 0 100 100 | 26, 43, 54, 69 | 16 (13%) |
| 16 | S | 110/112 (98%) | 0.29 | 1 (0%) 84 82 | 40, 52, 65, 75 | 24 (21%) |
| 17 | T | 131/146 (89%) | 0.23 | 3 (2%) 60 54 | 34, 45, 72, 92 | 22 (16%) |
| 18 | U | 116/118 (98%) | 0.13 | 0 100 100 | 26, 40, 49, 53 | 23 (19%) |
| 19 | V | 101/101 (100%) | 0.07 | 1 (0%) 82 80 | 28, 48, 59, 66 | 12 (11%) |
| 20 | W | 112/113 (99%) | 0.15 | 1 (0%) 84 82 | 28, 41, 63, 79 | 24 (21%) |
| 21 | X | 95/96 (98%) | 0.24 | 3 (3%) 47 40 | 39, 50, 72, 84 | 14 (14%) |
| 22 | Y | 107/110 (97%) | 0.44 | 8 (7%) 14 10 | 44, 54, 81, 87 | 24 (22%) |
| 23 | Z | 94/206 (45%) | 0.48 | 5 (5%) 26 20 | 42, 59, 74, 97 | 15 (15%) |
| 24 | 0 | 74/85 (87%) | -0.01 | 0 100 100 | 26, 39, 52, 65 | 16 (21%) |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-----------|
| 25 | 1 | 97/98 (98%) | 0.29 | 5 (5%) 27 21 | 24, 39, 70, 81 | 21 (21%) |
| 26 | 2 | 70/72 (97%) | 0.51 | 2 (2%) 51 45 | 44, 57, 67, 79 | 13 (18%) |
| 27 | 3 | 59/60 (98%) | 0.53 | 5 (8%) 10 7 | 29, 43, 66, 78 | 12 (20%) |
| 28 | 4 | 69/71 (97%) | 1.18 | 16 (23%) 0 0 | 52, 73, 94, 99 | 26 (37%) |
| 29 | 5 | 59/60 (98%) | 0.04 | 0 100 100 | 22, 43, 62, 71 | 8 (13%) |
| 30 | 6 | 53/54 (98%) | 0.17 | 0 100 100 | 35, 41, 52, 58 | 11 (20%) |
| 31 | 7 | 49/49 (100%) | 0.05 | 2 (4%) 37 30 | 25, 30, 54, 70 | 9 (18%) |
| 32 | 8 | 64/65 (98%) | 0.00 | 0 100 100 | 26, 34, 40, 51 | 7 (10%) |
| 33 | 9 | 37/37 (100%) | 0.33 | 2 (5%) 25 20 | 32, 39, 51, 58 | 11 (29%) |
| 34 | a | 1498/1521 (98%) | 0.22 | 73 (4%) 29 23 | 28, 45, 92, 113 | 228 (15%) |
| 35 | b | 231/256 (90%) | 0.82 | 30 (12%) 3 2 | 51, 71, 92, 100 | 56 (24%) |
| 36 | c | 206/239 (86%) | 0.24 | 6 (2%) 51 45 | 40, 58, 73, 83 | 19 (9%) |
| 37 | d | 208/209 (99%) | 0.41 | 7 (3%) 45 38 | 47, 59, 79, 86 | 49 (23%) |
| 38 | e | 148/162 (91%) | 0.06 | 3 (2%) 65 60 | 33, 48, 60, 78 | 23 (15%) |
| 39 | f | 100/101 (99%) | 0.40 | 7 (7%) 16 12 | 48, 66, 76, 86 | 17 (17%) |
| 40 | g | 155/156 (99%) | 0.57 | 13 (8%) 11 7 | 41, 58, 89, 98 | 40 (25%) |
| 41 | h | 137/138 (99%) | 0.17 | 1 (0%) 87 86 | 39, 48, 57, 65 | 14 (10%) |
| 42 | i | 127/128 (99%) | 0.36 | 3 (2%) 59 53 | 35, 61, 77, 83 | 15 (11%) |
| 43 | j | 96/105 (91%) | 1.00 | 18 (18%) 1 0 | 34, 65, 87, 94 | 27 (28%) |
| 44 | k | 114/129 (88%) | 0.25 | 3 (2%) 56 50 | 32, 54, 67, 72 | 16 (14%) |
| 45 | l | 122/132 (92%) | -0.02 | 1 (0%) 86 84 | 28, 40, 55, 65 | 23 (18%) |
| 46 | m | 119/126 (94%) | 0.63 | 13 (10%) 5 3 | 32, 57, 77, 82 | 24 (20%) |
| 47 | n | 60/61 (98%) | 0.22 | 0 100 100 | 33, 44, 54, 63 | 4 (6%) |
| 48 | o | 88/89 (98%) | 0.41 | 2 (2%) 60 54 | 37, 50, 65, 74 | 21 (23%) |
| 49 | p | 82/88 (93%) | 0.59 | 5 (6%) 21 16 | 43, 55, 69, 76 | 14 (17%) |
| 50 | q | 99/105 (94%) | 0.10 | 0 100 100 | 41, 49, 61, 65 | 18 (18%) |
| 51 | r | 68/88 (77%) | 0.56 | 3 (4%) 34 27 | 48, 59, 78, 86 | 14 (20%) |
| 52 | s | 83/93 (89%) | 0.47 | 7 (8%) 11 7 | 39, 55, 75, 80 | 13 (15%) |
| 53 | t | 96/106 (90%) | 0.36 | 1 (1%) 82 80 | 40, 49, 59, 71 | 16 (16%) |
| 54 | u | 23/27 (85%) | 0.44 | 0 100 100 | 38, 45, 50, 51 | 4 (17%) |
| 55 | v | 13/24 (54%) | 0.58 | 1 (7%) 13 10 | 36, 48, 70, 81 | 4 (30%) |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|------------|
| 56 | w | 67/76 (88%) | 2.16 | 32 (47%) 0 0 | 47, 92, 104, 107 | 54 (80%) |
| 57 | x | 73/77 (94%) | 0.33 | 4 (5%) 25 19 | 27, 49, 72, 88 | 13 (17%) |
| 58 | y | 68/76 (89%) | 1.34 | 16 (23%) 0 0 | 29, 84, 103, 108 | 39 (57%) |
| 59 | z | 671/679 (98%) | 0.52 | 52 (7%) 13 10 | 32, 66, 85, 99 | 164 (24%) |
| All | All | 11355/11953 (94%) | 0.40 | 803 (7%) 16 11 | 18, 49, 93, 214 | 2236 (19%) |

All (803) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 10 | K | 92 | GLY | 15.0 |
| 1 | A | 934 | C | 14.8 |
| 10 | K | 122 | ALA | 14.7 |
| 10 | K | 135 | GLY | 13.9 |
| 10 | K | 139 | VAL | 12.3 |
| 10 | K | 116 | ASN | 12.0 |
| 10 | K | 9 | LYS | 11.7 |
| 40 | g | 82 | GLY | 11.1 |
| 9 | J | 49 | ALA | 10.8 |
| 9 | J | 116 | ILE | 10.7 |
| 10 | K | 52 | ILE | 10.6 |
| 10 | K | 45 | THR | 10.6 |
| 10 | K | 43 | ALA | 10.2 |
| 10 | K | 93 | ARG | 9.9 |
| 10 | K | 77 | LEU | 9.8 |
| 9 | J | 97 | ALA | 9.7 |
| 10 | K | 47 | ASN | 9.7 |
| 10 | K | 34 | ILE | 9.2 |
| 9 | J | 130 | THR | 9.0 |
| 10 | K | 46 | ALA | 9.0 |
| 10 | K | 4 | VAL | 9.0 |
| 3 | C | 198 | ALA | 8.8 |
| 9 | J | 129 | PRO | 8.7 |
| 10 | K | 140 | GLY | 8.6 |
| 9 | J | 43 | ALA | 8.6 |
| 3 | C | 200 | LYS | 8.6 |
| 10 | K | 17 | ALA | 8.6 |
| 10 | K | 7 | VAL | 8.5 |
| 9 | J | 55 | LYS | 8.4 |
| 9 | J | 39 | ALA | 8.4 |
| 10 | K | 59 | ILE | 8.2 |
| 9 | J | 53 | VAL | 8.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 935 | C | 8.1 |
| 10 | K | 18 | THR | 8.0 |
| 34 | a | 1012 | G | 8.0 |
| 10 | K | 10 | LEU | 8.0 |
| 10 | K | 104 | VAL | 8.0 |
| 34 | a | 984 | A | 7.9 |
| 1 | A | 938 | C | 7.8 |
| 9 | J | 118 | THR | 7.8 |
| 10 | K | 94 | GLU | 7.7 |
| 40 | g | 81 | GLY | 7.7 |
| 9 | J | 103 | GLY | 7.7 |
| 1 | A | 2806 | C | 7.6 |
| 9 | J | 123 | GLU | 7.6 |
| 40 | g | 80 | VAL | 7.6 |
| 9 | J | 121 | ASP | 7.6 |
| 34 | a | 1014 | G | 7.5 |
| 10 | K | 49 | GLY | 7.4 |
| 1 | A | 1220 | G | 7.4 |
| 46 | m | 120 | LYS | 7.4 |
| 10 | K | 138 | VAL | 7.4 |
| 58 | y | 44 | G | 7.4 |
| 9 | J | 94 | VAL | 7.4 |
| 9 | J | 117 | LEU | 7.3 |
| 9 | J | 88 | ALA | 7.3 |
| 34 | a | 1013 | A | 7.3 |
| 1 | A | 1219 | U | 7.3 |
| 34 | a | 1015 | G | 7.3 |
| 10 | K | 41 | PHE | 7.2 |
| 27 | 3 | 2 | PRO | 7.2 |
| 34 | a | 74 | G | 7.2 |
| 34 | a | 985 | C | 7.2 |
| 9 | J | 35 | LYS | 7.1 |
| 9 | J | 50 | ARG | 7.1 |
| 10 | K | 25 | PRO | 7.1 |
| 9 | J | 105 | PRO | 7.0 |
| 1 | A | 2812 | G | 7.0 |
| 10 | K | 2 | LYS | 7.0 |
| 9 | J | 133 | GLU | 6.9 |
| 3 | C | 205 | LYS | 6.9 |
| 1 | A | 933 | A | 6.9 |
| 1 | A | 2167 | C | 6.8 |
| 9 | J | 46 | GLN | 6.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 9 | J | 99 | SER | 6.8 |
| 9 | J | 100 | ASN | 6.8 |
| 1 | A | 932 | C | 6.8 |
| 10 | K | 98 | ARG | 6.7 |
| 9 | J | 93 | LEU | 6.7 |
| 10 | K | 3 | LYS | 6.7 |
| 10 | K | 5 | VAL | 6.6 |
| 10 | K | 95 | LYS | 6.6 |
| 3 | C | 209 | LEU | 6.6 |
| 10 | K | 117 | THR | 6.5 |
| 34 | a | 982 | G | 6.5 |
| 9 | J | 85 | ASP | 6.4 |
| 56 | w | 19 | G | 6.4 |
| 1 | A | 273 | U | 6.4 |
| 28 | 4 | 56 | VAL | 6.4 |
| 10 | K | 44 | ALA | 6.4 |
| 10 | K | 13 | PRO | 6.3 |
| 9 | J | 89 | ALA | 6.3 |
| 9 | J | 37 | THR | 6.2 |
| 10 | K | 6 | ALA | 6.2 |
| 1 | A | 1554 | C | 6.2 |
| 46 | m | 119 | GLY | 6.1 |
| 9 | J | 54 | ALA | 6.1 |
| 10 | K | 118 | THR | 6.1 |
| 10 | K | 100 | THR | 6.0 |
| 3 | C | 223 | ARG | 5.9 |
| 10 | K | 14 | ALA | 5.9 |
| 10 | K | 54 | PRO | 5.9 |
| 34 | a | 1005 | G | 5.9 |
| 9 | J | 101 | PRO | 5.9 |
| 34 | a | 1004 | U | 5.9 |
| 34 | a | 211 | U | 5.8 |
| 1 | A | 217 | A | 5.8 |
| 9 | J | 87 | VAL | 5.8 |
| 1 | A | 937 | G | 5.8 |
| 10 | K | 33 | ASN | 5.8 |
| 10 | K | 48 | MET | 5.8 |
| 9 | J | 48 | GLY | 5.8 |
| 9 | J | 17 | LEU | 5.7 |
| 10 | K | 62 | ASP | 5.7 |
| 1 | A | 2805 | G | 5.7 |
| 1 | A | 2185 | C | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 10 | K | 137 | GLU | 5.7 |
| 10 | K | 37 | PHE | 5.6 |
| 9 | J | 47 | ASN | 5.6 |
| 34 | a | 1019 | G | 5.6 |
| 9 | J | 10 | LEU | 5.5 |
| 23 | Z | 93 | ASP | 5.5 |
| 9 | J | 122 | VAL | 5.5 |
| 10 | K | 53 | VAL | 5.5 |
| 9 | J | 76 | GLY | 5.5 |
| 28 | 4 | 54 | GLY | 5.5 |
| 10 | K | 30 | HIS | 5.4 |
| 3 | C | 210 | ARG | 5.4 |
| 1 | A | 2168 | G | 5.4 |
| 1 | A | 2813 | C | 5.4 |
| 9 | J | 75 | GLN | 5.3 |
| 56 | w | 57 | G | 5.3 |
| 10 | K | 16 | LYS | 5.3 |
| 1 | A | 2165 | U | 5.3 |
| 3 | C | 158 | ALA | 5.3 |
| 10 | K | 28 | GLY | 5.3 |
| 1 | A | 1120 | C | 5.2 |
| 1 | A | 1762 | G | 5.2 |
| 10 | K | 63 | ARG | 5.2 |
| 1 | A | 2814 | C | 5.2 |
| 3 | C | 196 | LEU | 5.2 |
| 9 | J | 131 | MET | 5.2 |
| 1 | A | 682 | G | 5.1 |
| 10 | K | 15 | GLY | 5.1 |
| 3 | C | 14 | VAL | 5.1 |
| 9 | J | 98 | LYS | 5.0 |
| 1 | A | 2166 | C | 5.0 |
| 35 | b | 234 | PRO | 5.0 |
| 1 | A | 2804 | G | 5.0 |
| 11 | N | 8 | GLN | 5.0 |
| 59 | z | 525 | ALA | 5.0 |
| 9 | J | 91 | LYS | 5.0 |
| 34 | a | 986 | C | 5.0 |
| 1 | A | 1091 | A | 5.0 |
| 9 | J | 92 | THR | 5.0 |
| 9 | J | 77 | PRO | 5.0 |
| 3 | C | 19 | ILE | 5.0 |
| 10 | K | 8 | VAL | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 936 | A | 4.9 |
| 56 | w | 24 | G | 5.0 |
| 1 | A | 2163 | C | 4.9 |
| 10 | K | 96 | VAL | 4.9 |
| 1 | A | 2802 | A | 4.9 |
| 35 | b | 232 | PRO | 4.9 |
| 10 | K | 88 | ALA | 4.9 |
| 1 | A | 1567 | G | 4.9 |
| 9 | J | 7 | VAL | 4.8 |
| 1 | A | 696 | C | 4.8 |
| 1 | A | 297 | G | 4.8 |
| 1 | A | 678 | A | 4.8 |
| 28 | 4 | 57 | GLU | 4.8 |
| 1 | A | 1774 | C | 4.8 |
| 10 | K | 50 | ASP | 4.8 |
| 1 | A | 1123 | U | 4.8 |
| 1 | A | 569 | C | 4.8 |
| 9 | J | 72 | ASP | 4.7 |
| 10 | K | 125 | ARG | 4.7 |
| 10 | K | 58 | THR | 4.7 |
| 28 | 4 | 49 | PHE | 4.7 |
| 56 | w | 18 | G | 4.7 |
| 9 | J | 52 | PHE | 4.7 |
| 10 | K | 136 | VAL | 4.7 |
| 34 | a | 1022 | C | 4.7 |
| 9 | J | 23 | SER | 4.6 |
| 9 | J | 6 | ASN | 4.6 |
| 7 | G | 50 | ALA | 4.6 |
| 3 | C | 199 | HIS | 4.6 |
| 1 | A | 2137 | G | 4.6 |
| 10 | K | 60 | TYR | 4.6 |
| 23 | Z | 17 | ALA | 4.6 |
| 51 | r | 20 | ALA | 4.6 |
| 1 | A | 2164 | C | 4.6 |
| 10 | K | 36 | GLU | 4.6 |
| 9 | J | 14 | LYS | 4.5 |
| 9 | J | 8 | GLU | 4.5 |
| 1 | A | 1458 | G | 4.5 |
| 34 | a | 1002 | G | 4.5 |
| 1 | A | 2158 | C | 4.5 |
| 34 | a | 160 | C | 4.5 |
| 59 | z | 288 | PRO | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 58 | y | 20 | U | 4.5 |
| 1 | A | 695 | C | 4.5 |
| 34 | a | 1021 | C | 4.5 |
| 10 | K | 105 | LEU | 4.5 |
| 56 | w | 51 | U | 4.5 |
| 22 | Y | 53 | PRO | 4.4 |
| 1 | A | 929 | G | 4.4 |
| 1 | A | 1583 | G | 4.4 |
| 3 | C | 194 | ARG | 4.4 |
| 10 | K | 38 | VAL | 4.4 |
| 10 | K | 31 | GLY | 4.4 |
| 43 | j | 27 | ALA | 4.4 |
| 1 | A | 2213 | G | 4.4 |
| 34 | a | 1010 | G | 4.4 |
| 10 | K | 124 | ALA | 4.4 |
| 9 | J | 42 | GLN | 4.4 |
| 1 | A | 939 | C | 4.4 |
| 3 | C | 29 | VAL | 4.4 |
| 9 | J | 9 | LEU | 4.4 |
| 1 | A | 926 | G | 4.3 |
| 1 | A | 1775 | G | 4.3 |
| 34 | a | 980 | G | 4.3 |
| 58 | y | 12 | U | 4.3 |
| 35 | b | 233 | SER | 4.3 |
| 10 | K | 101 | TRP | 4.3 |
| 56 | w | 25 | C | 4.3 |
| 59 | z | 397 | PRO | 4.3 |
| 9 | J | 34 | ALA | 4.3 |
| 3 | C | 11 | LEU | 4.2 |
| 3 | C | 225 | ASN | 4.2 |
| 7 | G | 51 | ARG | 4.2 |
| 56 | w | 58 | A | 4.2 |
| 39 | f | 15 | ASP | 4.2 |
| 25 | 1 | 2 | SER | 4.2 |
| 9 | J | 36 | GLU | 4.2 |
| 9 | J | 22 | GLY | 4.2 |
| 34 | a | 1003 | G | 4.1 |
| 1 | A | 2188 | U | 4.1 |
| 35 | b | 126 | GLU | 4.1 |
| 9 | J | 132 | ASP | 4.1 |
| 10 | K | 107 | ILE | 4.1 |
| 9 | J | 11 | ALA | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 10 | K | 26 | ALA | 4.1 |
| 10 | K | 12 | LEU | 4.1 |
| 1 | A | 2136 | G | 4.1 |
| 10 | K | 73 | PRO | 4.1 |
| 10 | K | 102 | GLU | 4.1 |
| 43 | j | 88 | LEU | 4.1 |
| 34 | a | 1017 | G | 4.1 |
| 28 | 4 | 53 | GLU | 4.0 |
| 34 | a | 987 | C | 4.0 |
| 58 | y | 34 | G | 4.0 |
| 34 | a | 983 | A | 4.0 |
| 28 | 4 | 68 | ARG | 4.0 |
| 1 | A | 298 | G | 4.0 |
| 1 | A | 927 | G | 4.0 |
| 1 | A | 2903 | U | 4.0 |
| 34 | a | 152 | G | 4.0 |
| 34 | a | 826 | C | 4.0 |
| 3 | C | 38 | ASP | 3.9 |
| 7 | G | 48 | GLU | 3.9 |
| 9 | J | 38 | HIS | 3.9 |
| 10 | K | 35 | MET | 3.9 |
| 10 | K | 61 | ALA | 3.9 |
| 56 | w | 15 | G | 3.9 |
| 1 | A | 2811 | A | 3.9 |
| 34 | a | 75 | C | 3.9 |
| 56 | w | 71 | G | 3.9 |
| 34 | a | 209 | U | 3.9 |
| 10 | K | 42 | ASN | 3.9 |
| 1 | A | 940 | U | 3.9 |
| 10 | K | 66 | THR | 3.9 |
| 9 | J | 86 | PRO | 3.9 |
| 9 | J | 18 | GLU | 3.9 |
| 56 | w | 20 | U | 3.9 |
| 1 | A | 2178 | G | 3.8 |
| 28 | 4 | 55 | ARG | 3.8 |
| 42 | i | 94 | ALA | 3.8 |
| 10 | K | 82 | ALA | 3.8 |
| 3 | C | 68 | LEU | 3.8 |
| 9 | J | 44 | LEU | 3.8 |
| 22 | Y | 93 | GLY | 3.8 |
| 8 | H | 21 | PRO | 3.8 |
| 34 | a | 1020 | C | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | 1 | 82 | LEU | 3.8 |
| 1 | A | 2152 | G | 3.8 |
| 10 | K | 11 | GLN | 3.8 |
| 10 | K | 29 | GLN | 3.8 |
| 10 | K | 76 | TYR | 3.7 |
| 1 | A | 1763 | G | 3.7 |
| 34 | a | 825 | U | 3.7 |
| 56 | w | 56 | C | 3.7 |
| 9 | J | 56 | ASN | 3.7 |
| 1 | A | 1222 | C | 3.7 |
| 1 | A | 2157 | C | 3.7 |
| 34 | a | 981 | G | 3.7 |
| 34 | a | 1120 | C | 3.7 |
| 17 | T | 126 | ALA | 3.7 |
| 34 | a | 73 | C | 3.7 |
| 10 | K | 99 | ILE | 3.7 |
| 10 | K | 121 | GLU | 3.7 |
| 35 | b | 137 | ARG | 3.7 |
| 10 | K | 69 | THR | 3.7 |
| 56 | w | 14 | A | 3.7 |
| 10 | K | 57 | ILE | 3.7 |
| 43 | j | 75 | ILE | 3.7 |
| 56 | w | 3 | C | 3.7 |
| 1 | A | 1584 | G | 3.7 |
| 3 | C | 17 | ASN | 3.6 |
| 34 | a | 1000 | G | 3.6 |
| 56 | w | 52 | G | 3.6 |
| 10 | K | 20 | ALA | 3.6 |
| 1 | A | 1457 | A | 3.6 |
| 3 | C | 206 | GLY | 3.6 |
| 35 | b | 119 | GLU | 3.6 |
| 1 | A | 677 | A | 3.6 |
| 1 | A | 944 | A | 3.6 |
| 3 | C | 212 | VAL | 3.6 |
| 10 | K | 68 | VAL | 3.6 |
| 39 | f | 40 | VAL | 3.6 |
| 1 | A | 2905 | U | 3.6 |
| 58 | y | 47 | U | 3.6 |
| 22 | Y | 91 | GLU | 3.6 |
| 35 | b | 129 | GLU | 3.6 |
| 59 | z | 434 | ARG | 3.6 |
| 56 | w | 45 | U | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 17 | T | 38 | ASN | 3.6 |
| 56 | w | 10 | G | 3.6 |
| 40 | g | 85 | TYR | 3.6 |
| 23 | Z | 94 | GLU | 3.5 |
| 34 | a | 153 | G | 3.5 |
| 3 | C | 30 | LYS | 3.5 |
| 9 | J | 68 | LEU | 3.5 |
| 1 | A | 681 | G | 3.5 |
| 1 | A | 1218 | A | 3.5 |
| 10 | K | 119 | ASP | 3.5 |
| 34 | a | 1011 | C | 3.5 |
| 35 | b | 227 | GLY | 3.5 |
| 34 | a | 76 | G | 3.5 |
| 34 | a | 89 | G | 3.5 |
| 58 | y | 45 | U | 3.5 |
| 10 | K | 132 | ARG | 3.5 |
| 10 | K | 84 | LEU | 3.5 |
| 1 | A | 1759 | U | 3.5 |
| 1 | A | 2189 | G | 3.5 |
| 34 | a | 158 | C | 3.5 |
| 56 | w | 73 | A | 3.5 |
| 59 | z | 394 | ALA | 3.5 |
| 1 | A | 1773 | C | 3.4 |
| 3 | C | 55 | ASP | 3.4 |
| 9 | J | 4 | LYS | 3.4 |
| 59 | z | -3 | GLU | 3.4 |
| 34 | a | 1016 | G | 3.4 |
| 59 | z | 515 | THR | 3.4 |
| 36 | c | 132 | ARG | 3.4 |
| 57 | x | 47 | U | 3.4 |
| 1 | A | 942 | C | 3.4 |
| 9 | J | 104 | ILE | 3.4 |
| 34 | a | 1018 | A | 3.4 |
| 3 | C | 37 | PHE | 3.4 |
| 28 | 4 | 46 | GLN | 3.4 |
| 56 | w | 44 | G | 3.4 |
| 9 | J | 124 | ALA | 3.4 |
| 59 | z | 586 | ALA | 3.4 |
| 37 | d | 47 | ARG | 3.4 |
| 9 | J | 120 | LYS | 3.4 |
| 57 | x | 1 | C | 3.4 |
| 55 | v | 14 | A | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | C | 54 | SER | 3.3 |
| 1 | A | 385 | U | 3.3 |
| 1 | A | 1126 | U | 3.3 |
| 34 | a | 707 | U | 3.3 |
| 10 | K | 90 | LYS | 3.3 |
| 1 | A | 2187 | G | 3.3 |
| 10 | K | 51 | ALA | 3.3 |
| 56 | w | 6 | G | 3.3 |
| 58 | y | 28 | G | 3.3 |
| 9 | J | 84 | GLU | 3.3 |
| 9 | J | 90 | ALA | 3.3 |
| 10 | K | 97 | GLY | 3.3 |
| 10 | K | 27 | LEU | 3.3 |
| 43 | j | 79 | ARG | 3.3 |
| 34 | a | 210 | U | 3.3 |
| 46 | m | 34 | LEU | 3.3 |
| 1 | A | 2815 | G | 3.3 |
| 9 | J | 25 | PHE | 3.3 |
| 35 | b | 236 | TYR | 3.3 |
| 3 | C | 178 | ALA | 3.3 |
| 10 | K | 32 | ALA | 3.3 |
| 58 | y | 22 | G | 3.3 |
| 34 | a | 1007 | C | 3.3 |
| 6 | F | 15 | SER | 3.3 |
| 10 | K | 65 | PHE | 3.3 |
| 1 | A | 2135 | A | 3.3 |
| 35 | b | 228 | GLY | 3.3 |
| 1 | A | 386 | G | 3.2 |
| 1 | A | 2121 | G | 3.2 |
| 34 | a | 824 | C | 3.2 |
| 58 | y | 46 | G | 3.2 |
| 1 | A | 2120 | U | 3.2 |
| 35 | b | 231 | GLU | 3.2 |
| 59 | z | 380 | VAL | 3.2 |
| 1 | A | 296 | C | 3.2 |
| 3 | C | 181 | PRO | 3.2 |
| 1 | A | 2186 | G | 3.2 |
| 3 | C | 163 | PHE | 3.2 |
| 9 | J | 24 | PHE | 3.2 |
| 35 | b | 229 | VAL | 3.2 |
| 1 | A | 1553 | A | 3.2 |
| 10 | K | 56 | GLU | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 57 | x | 17 | C | 3.2 |
| 10 | K | 22 | PRO | 3.2 |
| 28 | 4 | 45 | GLY | 3.2 |
| 28 | 4 | 52 | THR | 3.2 |
| 43 | j | 36 | GLY | 3.2 |
| 35 | b | 136 | VAL | 3.1 |
| 46 | m | 56 | LEU | 3.1 |
| 1 | A | 928 | G | 3.1 |
| 9 | J | 96 | PHE | 3.1 |
| 59 | z | 526 | GLU | 3.1 |
| 1 | A | 1636 | G | 3.1 |
| 34 | a | 212 | G | 3.1 |
| 56 | w | 1 | G | 3.1 |
| 3 | C | 22 | ILE | 3.1 |
| 43 | j | 32 | ALA | 3.1 |
| 56 | w | 23 | A | 3.1 |
| 59 | z | 289 | SER | 3.1 |
| 34 | a | 1009 | C | 3.1 |
| 10 | K | 85 | GLU | 3.1 |
| 40 | g | 84 | ASN | 3.1 |
| 1 | A | 2153 | U | 3.1 |
| 1 | A | 1637 | C | 3.1 |
| 3 | C | 183 | GLU | 3.1 |
| 9 | J | 70 | GLU | 3.1 |
| 46 | m | 40 | ASN | 3.1 |
| 1 | A | 2133 | G | 3.1 |
| 10 | K | 21 | PRO | 3.1 |
| 3 | C | 203 | GLY | 3.1 |
| 43 | j | 72 | VAL | 3.1 |
| 3 | C | 63 | SER | 3.1 |
| 58 | y | 10 | G | 3.1 |
| 9 | J | 51 | LEU | 3.1 |
| 43 | j | 33 | GLN | 3.1 |
| 57 | x | 17(A) | U | 3.0 |
| 35 | b | 120 | ALA | 3.0 |
| 3 | C | 201 | PRO | 3.0 |
| 3 | C | 224 | ILE | 3.0 |
| 10 | K | 19 | PRO | 3.0 |
| 3 | C | 53 | ARG | 3.0 |
| 3 | C | 162 | GLU | 3.0 |
| 6 | F | 16 | GLY | 3.0 |
| 52 | s | 27 | GLU | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 43 | j | 26 | ALA | 3.0 |
| 1 | A | 270 | U | 3.0 |
| 13 | P | 141 | ALA | 3.0 |
| 42 | i | 84 | ALA | 3.0 |
| 22 | Y | 61 | ILE | 3.0 |
| 1 | A | 1221 | A | 3.0 |
| 1 | A | 1772 | C | 2.9 |
| 3 | C | 171 | ILE | 2.9 |
| 3 | C | 207 | THR | 2.9 |
| 34 | a | 979 | A | 2.9 |
| 46 | m | 48 | LEU | 2.9 |
| 40 | g | 155 | ARG | 2.9 |
| 40 | g | 156 | TRP | 2.9 |
| 26 | 2 | 18 | PRO | 2.9 |
| 1 | A | 1135 | U | 2.9 |
| 58 | y | 57 | G | 2.9 |
| 25 | 1 | 81 | LYS | 2.9 |
| 35 | b | 156 | LYS | 2.9 |
| 45 | l | 18 | VAL | 2.9 |
| 1 | A | 2138 | A | 2.9 |
| 40 | g | 50 | ILE | 2.9 |
| 20 | W | 1 | MET | 2.9 |
| 1 | A | 1136 | G | 2.9 |
| 3 | C | 204 | ALA | 2.9 |
| 9 | J | 119 | ALA | 2.9 |
| 35 | b | 131 | PRO | 2.9 |
| 1 | A | 924 | A | 2.9 |
| 1 | A | 941 | A | 2.9 |
| 59 | z | -11 | LEU | 2.9 |
| 56 | w | 61 | C | 2.9 |
| 10 | K | 81 | ALA | 2.9 |
| 1 | A | 1776 | G | 2.9 |
| 35 | b | 223 | ILE | 2.9 |
| 51 | r | 25 | THR | 2.9 |
| 7 | G | 148 | MET | 2.9 |
| 3 | C | 25 | ALA | 2.9 |
| 58 | y | 13 | C | 2.9 |
| 5 | E | 88 | GLY | 2.9 |
| 27 | 3 | 36 | VAL | 2.9 |
| 1 | A | 1635 | U | 2.9 |
| 35 | b | 144 | ARG | 2.9 |
| 10 | K | 24 | GLY | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 59 | z | 510 | ARG | 2.9 |
| 1 | A | 287 | U | 2.8 |
| 43 | j | 35 | SER | 2.8 |
| 1 | A | 2159 | C | 2.8 |
| 56 | w | 72 | C | 2.8 |
| 35 | b | 61 | LEU | 2.8 |
| 46 | m | 53 | VAL | 2.8 |
| 3 | C | 65 | PRO | 2.8 |
| 52 | s | 46 | GLY | 2.8 |
| 8 | H | 111 | HIS | 2.8 |
| 58 | y | 56 | C | 2.8 |
| 8 | H | 20 | ALA | 2.8 |
| 9 | J | 69 | PRO | 2.8 |
| 34 | a | 70 | G | 2.8 |
| 56 | w | 53 | G | 2.8 |
| 10 | K | 108 | ALA | 2.8 |
| 10 | K | 75 | SER | 2.8 |
| 7 | G | 58 | GLN | 2.8 |
| 1 | A | 2816 | G | 2.8 |
| 1 | A | 2803 | C | 2.8 |
| 48 | o | 4 | THR | 2.8 |
| 9 | J | 125 | LEU | 2.8 |
| 3 | C | 60 | GLY | 2.8 |
| 53 | t | 47 | GLY | 2.8 |
| 38 | e | 108 | ALA | 2.8 |
| 35 | b | 48 | MET | 2.8 |
| 1 | A | 945 | A | 2.8 |
| 1 | A | 2177 | G | 2.8 |
| 10 | K | 109 | LYS | 2.8 |
| 16 | S | 81 | GLY | 2.8 |
| 3 | C | 16 | PRO | 2.7 |
| 21 | X | 68 | ARG | 2.7 |
| 59 | z | 599 | ALA | 2.7 |
| 34 | a | 159 | U | 2.7 |
| 56 | w | 63 | G | 2.7 |
| 28 | 4 | 48 | ARG | 2.7 |
| 40 | g | 52 | GLU | 2.7 |
| 1 | A | 2211 | G | 2.7 |
| 3 | C | 166 | ASP | 2.7 |
| 39 | f | 17 | SER | 2.7 |
| 1 | A | 378 | G | 2.7 |
| 1 | A | 697 | G | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | J | 13 | LEU | 2.7 |
| 1 | A | 312 | A | 2.7 |
| 3 | C | 179 | SER | 2.7 |
| 59 | z | 39 | ARG | 2.7 |
| 9 | J | 126 | ALA | 2.7 |
| 1 | A | 1761 | G | 2.7 |
| 46 | m | 54 | VAL | 2.7 |
| 59 | z | 436 | VAL | 2.7 |
| 59 | z | 392 | ASN | 2.7 |
| 37 | d | 168 | ARG | 2.7 |
| 49 | p | 48 | TRP | 2.7 |
| 31 | 7 | 45 | ALA | 2.6 |
| 34 | a | 88 | C | 2.6 |
| 58 | y | 23 | A | 2.6 |
| 1 | A | 1216 | G | 2.6 |
| 13 | P | 98 | GLU | 2.6 |
| 3 | C | 59 | ARG | 2.6 |
| 37 | d | 86 | LYS | 2.6 |
| 59 | z | 582 | LYS | 2.6 |
| 1 | A | 1090 | A | 2.6 |
| 22 | Y | 52 | SER | 2.6 |
| 34 | a | 91 | G | 2.6 |
| 3 | C | 197 | GLU | 2.6 |
| 3 | C | 23 | ASP | 2.6 |
| 56 | w | 75 | C | 2.6 |
| 1 | A | 2154 | G | 2.6 |
| 43 | j | 96 | ILE | 2.6 |
| 9 | J | 19 | ARG | 2.6 |
| 36 | c | 92 | ALA | 2.6 |
| 44 | k | 126 | ARG | 2.6 |
| 58 | y | 42 | C | 2.6 |
| 9 | J | 107 | VAL | 2.6 |
| 35 | b | 230 | VAL | 2.6 |
| 59 | z | 592 | VAL | 2.6 |
| 1 | A | 2190 | A | 2.6 |
| 56 | w | 76 | A | 2.6 |
| 39 | f | 24 | GLU | 2.6 |
| 59 | z | 565 | GLY | 2.6 |
| 8 | H | 112 | PRO | 2.6 |
| 34 | a | 998 | C | 2.6 |
| 22 | Y | 90 | LEU | 2.6 |
| 25 | 1 | 80 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | K | 129 | GLY | 2.6 |
| 1 | A | 8 | U | 2.5 |
| 59 | z | 290 | PRO | 2.5 |
| 1 | A | 925 | G | 2.5 |
| 1 | A | 311 | C | 2.5 |
| 10 | K | 106 | GLU | 2.5 |
| 1 | A | 271 | U | 2.5 |
| 59 | z | 420 | TYR | 2.5 |
| 8 | H | 99 | VAL | 2.5 |
| 49 | p | 80 | PHE | 2.5 |
| 4 | D | 2 | ALA | 2.5 |
| 10 | K | 74 | ALA | 2.5 |
| 36 | c | 50 | ALA | 2.5 |
| 5 | E | 71 | GLY | 2.5 |
| 42 | i | 93 | ARG | 2.5 |
| 43 | j | 17 | ASP | 2.5 |
| 31 | 7 | 49 | ARG | 2.5 |
| 40 | g | 79 | ARG | 2.5 |
| 59 | z | 246 | THR | 2.5 |
| 1 | A | 310 | C | 2.5 |
| 59 | z | 225 | GLY | 2.5 |
| 46 | m | 52 | GLU | 2.5 |
| 34 | a | 1006 | C | 2.5 |
| 10 | K | 133 | SER | 2.5 |
| 35 | b | 235 | SER | 2.5 |
| 14 | Q | 59 | ARG | 2.5 |
| 43 | j | 89 | ASP | 2.5 |
| 21 | X | 92 | LEU | 2.5 |
| 34 | a | 155 | A | 2.5 |
| 10 | K | 67 | PHE | 2.5 |
| 1 | A | 1217 | G | 2.5 |
| 1 | A | 1127 | U | 2.4 |
| 56 | w | 21 | A | 2.4 |
| 3 | C | 31 | GLU | 2.4 |
| 8 | H | 47 | GLU | 2.4 |
| 56 | w | 74 | C | 2.4 |
| 52 | s | 59 | PRO | 2.4 |
| 1 | A | 1459 | G | 2.4 |
| 23 | Z | 16 | SER | 2.4 |
| 3 | C | 9 | ALA | 2.4 |
| 37 | d | 149 | ALA | 2.4 |
| 1 | A | 161 | G | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 34 | a | 1001 | G | 2.4 |
| 43 | j | 25 | GLU | 2.4 |
| 59 | z | 395 | ASP | 2.4 |
| 59 | z | 523 | LYS | 2.4 |
| 28 | 4 | 60 | GLN | 2.4 |
| 56 | w | 68 | C | 2.4 |
| 34 | a | 1156 | G | 2.4 |
| 28 | 4 | 51 | ASP | 2.4 |
| 34 | a | 706 | A | 2.4 |
| 3 | C | 58 | VAL | 2.4 |
| 9 | J | 67 | GLY | 2.4 |
| 56 | w | 13 | C | 2.4 |
| 28 | 4 | 61 | ARG | 2.4 |
| 39 | f | 36 | ARG | 2.4 |
| 1 | A | 1144 | G | 2.4 |
| 1 | A | 1899 | G | 2.4 |
| 1 | A | 2169 | G | 2.4 |
| 7 | G | 60 | LEU | 2.4 |
| 10 | K | 131 | ALA | 2.4 |
| 59 | z | 146 | LEU | 2.4 |
| 49 | p | 52 | ASP | 2.4 |
| 1 | A | 2134 | U | 2.4 |
| 34 | a | 90 | U | 2.4 |
| 34 | a | 1008 | C | 2.4 |
| 59 | z | 387 | GLU | 2.4 |
| 48 | o | 9 | GLN | 2.4 |
| 43 | j | 73 | ASP | 2.4 |
| 35 | b | 38 | GLY | 2.4 |
| 58 | y | 29 | G | 2.4 |
| 14 | Q | 5 | ARG | 2.4 |
| 1 | A | 1771 | C | 2.3 |
| 11 | N | 132 | ALA | 2.3 |
| 36 | c | 41 | GLY | 2.3 |
| 9 | J | 83 | TYR | 2.3 |
| 10 | K | 91 | PRO | 2.3 |
| 52 | s | 47 | HIS | 2.3 |
| 1 | A | 931 | C | 2.3 |
| 1 | A | 2132 | C | 2.3 |
| 3 | C | 45 | ALA | 2.3 |
| 6 | F | 13 | SER | 2.3 |
| 28 | 4 | 23 | GLU | 2.3 |
| 46 | m | 49 | THR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 679 | G | 2.3 |
| 59 | z | 398 | ASP | 2.3 |
| 1 | A | 1465 | U | 2.3 |
| 3 | C | 211 | SER | 2.3 |
| 9 | J | 108 | LYS | 2.3 |
| 35 | b | 63 | MET | 2.3 |
| 1 | A | 2212 | G | 2.3 |
| 34 | a | 1114 | G | 2.3 |
| 59 | z | 239 | VAL | 2.3 |
| 59 | z | 521 | VAL | 2.3 |
| 34 | a | 1432 | A | 2.3 |
| 44 | k | 76 | GLY | 2.3 |
| 35 | b | 124 | SER | 2.3 |
| 59 | z | 396 | LEU | 2.3 |
| 35 | b | 237 | ALA | 2.3 |
| 59 | z | 291 | TYR | 2.3 |
| 59 | z | 319 | ALA | 2.3 |
| 34 | a | 5 | U | 2.3 |
| 7 | G | 150 | ASP | 2.3 |
| 9 | J | 73 | GLY | 2.3 |
| 26 | 2 | 8 | LYS | 2.3 |
| 1 | A | 2179 | A | 2.3 |
| 9 | J | 115 | GLN | 2.3 |
| 46 | m | 63 | THR | 2.3 |
| 34 | a | 1023 | U | 2.3 |
| 59 | z | -50 | VAL | 2.3 |
| 1 | A | 680 | C | 2.3 |
| 7 | G | 146 | TYR | 2.3 |
| 43 | j | 87 | THR | 2.3 |
| 1 | A | 1555 | A | 2.3 |
| 19 | V | 51 | VAL | 2.3 |
| 1 | A | 637 | U | 2.2 |
| 56 | w | 60 | U | 2.2 |
| 3 | C | 226 | PRO | 2.2 |
| 35 | b | 138 | LEU | 2.2 |
| 8 | H | 102 | ALA | 2.2 |
| 1 | A | 308 | C | 2.2 |
| 5 | E | 59 | VAL | 2.2 |
| 39 | f | 25 | ILE | 2.2 |
| 28 | 4 | 59 | PHE | 2.2 |
| 1 | A | 2127 | G | 2.2 |
| 59 | z | 322 | LYS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | 3 | 58 | VAL | 2.2 |
| 25 | 1 | 83 | GLU | 2.2 |
| 27 | 3 | 60 | GLU | 2.2 |
| 59 | z | 237 | PHE | 2.2 |
| 49 | p | 74 | LEU | 2.2 |
| 59 | z | 195 | PRO | 2.2 |
| 43 | j | 18 | ALA | 2.2 |
| 1 | A | 1760 | G | 2.2 |
| 1 | A | 2203 | G | 2.2 |
| 7 | G | 145 | THR | 2.2 |
| 49 | p | 19 | ILE | 2.2 |
| 59 | z | 360 | ARG | 2.2 |
| 8 | H | 168 | PRO | 2.2 |
| 37 | d | 84 | LYS | 2.2 |
| 22 | Y | 59 | GLY | 2.2 |
| 34 | a | 1112 | C | 2.2 |
| 46 | m | 51 | ALA | 2.2 |
| 1 | A | 2131 | G | 2.2 |
| 34 | a | 71 | G | 2.2 |
| 3 | C | 41 | VAL | 2.2 |
| 59 | z | 537 | ILE | 2.2 |
| 9 | J | 30 | GLN | 2.2 |
| 1 | A | 1551 | C | 2.2 |
| 1 | A | 1142 | U | 2.1 |
| 59 | z | -7 | LYS | 2.1 |
| 34 | a | 163 | G | 2.1 |
| 3 | C | 192 | PHE | 2.1 |
| 40 | g | 62 | PHE | 2.1 |
| 1 | A | 384 | G | 2.1 |
| 3 | C | 13 | LYS | 2.1 |
| 1 | A | 387 | A | 2.1 |
| 59 | z | 37 | SER | 2.1 |
| 44 | k | 75 | TYR | 2.1 |
| 37 | d | 187 | ARG | 2.1 |
| 52 | s | 38 | SER | 2.1 |
| 39 | f | 14 | LEU | 2.1 |
| 52 | s | 42 | PRO | 2.1 |
| 34 | a | 999 | U | 2.1 |
| 34 | a | 1109 | U | 2.1 |
| 34 | a | 1433 | C | 2.1 |
| 9 | J | 40 | LEU | 2.1 |
| 21 | X | 69 | TYR | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2155 | A | 2.1 |
| 34 | a | 976 | G | 2.1 |
| 34 | a | 1509 | A | 2.1 |
| 59 | z | 593 | PRO | 2.1 |
| 3 | C | 33 | ALA | 2.1 |
| 33 | 9 | 12 | ASP | 2.1 |
| 59 | z | 524 | LEU | 2.1 |
| 5 | E | 204 | ALA | 2.1 |
| 36 | c | 160 | ALA | 2.1 |
| 14 | Q | 60 | ARG | 2.1 |
| 59 | z | 233 | THR | 2.1 |
| 3 | C | 180 | PHE | 2.1 |
| 1 | A | 33 | C | 2.1 |
| 59 | z | 502 | ASP | 2.1 |
| 22 | Y | 19 | LYS | 2.1 |
| 35 | b | 125 | PRO | 2.1 |
| 40 | g | 58 | PRO | 2.1 |
| 1 | A | 638 | G | 2.0 |
| 1 | A | 1143 | A | 2.1 |
| 35 | b | 79 | ASP | 2.1 |
| 59 | z | -49 | ASP | 2.1 |
| 1 | A | 2226 | G | 2.0 |
| 59 | z | 542 | GLY | 2.1 |
| 59 | z | 564 | GLY | 2.1 |
| 3 | C | 66 | HIS | 2.0 |
| 9 | J | 80 | VAL | 2.0 |
| 34 | a | 188 | C | 2.0 |
| 40 | g | 51 | GLN | 2.0 |
| 13 | P | 110 | TYR | 2.0 |
| 23 | Z | 92 | SER | 2.0 |
| 37 | d | 143 | GLY | 2.0 |
| 59 | z | 171 | GLY | 2.0 |
| 59 | z | -52 | GLN | 2.0 |
| 59 | z | 435 | LEU | 2.0 |
| 3 | C | 174 | PRO | 2.0 |
| 7 | G | 5 | VAL | 2.0 |
| 36 | c | 141 | VAL | 2.0 |
| 43 | j | 34 | VAL | 2.0 |
| 1 | A | 2206 | C | 2.0 |
| 17 | T | 108 | ARG | 2.0 |
| 41 | h | 122 | ARG | 2.0 |
| 46 | m | 35 | GLU | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 38 | e | 21 | ALA | 2.0 |
| 10 | K | 83 | GLY | 2.0 |
| 33 | 9 | 11 | CYS | 2.0 |
| 38 | e | 116 | THR | 2.0 |
| 10 | K | 89 | HIS | 2.0 |
| 5 | E | 87 | GLU | 2.0 |
| 11 | N | 9 | VAL | 2.0 |
| 35 | b | 127 | ILE | 2.0 |
| 1 | A | 571 | A | 2.0 |
| 1 | A | 2901 | G | 2.0 |
| 9 | J | 62 | ALA | 2.0 |
| 34 | a | 1146 | C | 2.0 |
| 51 | r | 76 | LEU | 2.0 |
| 27 | 3 | 59 | VAL | 2.0 |
| 52 | s | 45 | VAL | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 56 | PSU | w | 55 | 20/21 | 0.67 | 0.31 | 96,105,110,111 | 13 |
| 56 | 5MU | w | 54 | 21/22 | 0.68 | 0.48 | 94,99,101,104 | 14 |
| 58 | PSU | y | 39 | 20/21 | 0.78 | 0.23 | 85,93,96,96 | 8 |
| 56 | 7MG | w | 46 | 24/25 | 0.79 | 0.23 | 91,97,102,104 | 13 |
| 58 | PSU | y | 32 | 20/21 | 0.82 | 0.20 | 92,98,106,108 | 11 |
| 58 | PSU | y | 55 | 20/21 | 0.82 | 0.21 | 68,75,84,88 | 11 |
| 58 | MIA | y | 37 | 22/30 | 0.83 | 0.18 | 75,84,87,89 | 8 |
| 58 | 4SU | y | 8 | 20/21 | 0.83 | 0.20 | 78,95,101,102 | 10 |
| 56 | 4SU | w | 8 | 20/21 | 0.83 | 0.24 | 86,92,95,95 | 12 |
| 58 | 5MU | y | 54 | 21/22 | 0.87 | 0.24 | 67,72,82,83 | 11 |
| 56 | PSU | w | 32 | 20/21 | 0.93 | 0.15 | 54,61,66,72 | 2 |
| 56 | PSU | w | 39 | 20/21 | 0.94 | 0.27 | 54,63,69,70 | 7 |
| 56 | MIA | w | 37 | 27/30 | 0.94 | 0.24 | 42,47,52,52 | 8 |
| 57 | 5MU | x | 54 | 21/22 | 0.94 | 0.20 | 40,51,55,61 | 10 |
| 57 | PSU | x | 55 | 20/21 | 0.95 | 0.18 | 39,51,54,57 | 7 |
| 57 | 4SU | x | 8 | 20/21 | 0.96 | 0.16 | 41,49,54,54 | 7 |
| 57 | 5MC | x | 32 | 21/22 | 0.96 | 0.18 | 33,40,44,46 | 4 |

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | a | 1614 | 1/1 | 0.29 | 0.67 | 75,75,75,75 | 0 |
| 60 | MG | a | 1705 | 1/1 | 0.38 | 0.37 | 72,72,72,72 | 0 |
| 60 | MG | B | 206 | 1/1 | 0.39 | 0.37 | 86,86,86,86 | 0 |
| 60 | MG | A | 3234 | 1/1 | 0.44 | 0.54 | 61,61,61,61 | 0 |
| 60 | MG | a | 1676 | 1/1 | 0.46 | 0.24 | 58,58,58,58 | 0 |
| 60 | MG | A | 3208 | 1/1 | 0.49 | 0.34 | 60,60,60,60 | 0 |
| 60 | MG | A | 3252 | 1/1 | 0.49 | 0.18 | 76,76,76,76 | 0 |
| 60 | MG | V | 202 | 1/1 | 0.51 | 0.55 | 73,73,73,73 | 0 |
| 60 | MG | A | 3155 | 1/1 | 0.51 | 0.28 | 65,65,65,65 | 0 |
| 60 | MG | A | 3283 | 1/1 | 0.53 | 0.53 | 41,41,41,41 | 0 |
| 60 | MG | A | 3057 | 1/1 | 0.54 | 0.38 | 72,72,72,72 | 0 |
| 60 | MG | a | 1638 | 1/1 | 0.54 | 0.42 | 53,53,53,53 | 0 |
| 60 | MG | A | 3586 | 1/1 | 0.55 | 0.52 | 75,75,75,75 | 0 |
| 60 | MG | a | 1661 | 1/1 | 0.56 | 0.19 | 69,69,69,69 | 0 |
| 60 | MG | a | 1701 | 1/1 | 0.58 | 0.18 | 66,66,66,66 | 0 |
| 60 | MG | A | 3274 | 1/1 | 0.59 | 0.23 | 66,66,66,66 | 0 |
| 60 | MG | A | 3169 | 1/1 | 0.59 | 0.45 | 44,44,44,44 | 1 |
| 60 | MG | A | 3394 | 1/1 | 0.59 | 0.30 | 81,81,81,81 | 0 |
| 60 | MG | A | 3098 | 1/1 | 0.60 | 0.24 | 61,61,61,61 | 0 |
| 60 | MG | A | 3267 | 1/1 | 0.60 | 0.45 | 64,64,64,64 | 0 |
| 60 | MG | a | 1604 | 1/1 | 0.61 | 0.25 | 64,64,64,64 | 0 |
| 60 | MG | A | 3295 | 1/1 | 0.62 | 0.36 | 58,58,58,58 | 0 |
| 60 | MG | a | 1689 | 1/1 | 0.62 | 0.24 | 74,74,74,74 | 0 |
| 60 | MG | A | 3006 | 1/1 | 0.62 | 0.38 | 52,52,52,52 | 1 |
| 60 | MG | A | 3117 | 1/1 | 0.62 | 0.30 | 48,48,48,48 | 0 |
| 60 | MG | x | 109 | 1/1 | 0.62 | 0.17 | 77,77,77,77 | 0 |
| 60 | MG | B | 204 | 1/1 | 0.63 | 0.24 | 63,63,63,63 | 0 |
| 60 | MG | A | 3094 | 1/1 | 0.63 | 0.54 | 55,55,55,55 | 0 |
| 60 | MG | a | 1662 | 1/1 | 0.64 | 0.33 | 53,53,53,53 | 0 |
| 60 | MG | B | 215 | 1/1 | 0.64 | 0.28 | 75,75,75,75 | 1 |
| 60 | MG | A | 3525 | 1/1 | 0.64 | 0.24 | 37,37,37,37 | 0 |
| 60 | MG | A | 3092 | 1/1 | 0.65 | 0.27 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3278 | 1/1 | 0.65 | 0.24 | 56,56,56,56 | 0 |
| 60 | MG | A | 3236 | 1/1 | 0.65 | 0.63 | 47,47,47,47 | 1 |
| 60 | MG | A | 3557 | 1/1 | 0.66 | 0.28 | 70,70,70,70 | 0 |
| 60 | MG | A | 3606 | 1/1 | 0.66 | 0.26 | 56,56,56,56 | 0 |
| 60 | MG | A | 3066 | 1/1 | 0.67 | 0.32 | 58,58,58,58 | 0 |
| 60 | MG | A | 3135 | 1/1 | 0.67 | 0.14 | 59,59,59,59 | 0 |
| 60 | MG | A | 3199 | 1/1 | 0.67 | 0.24 | 45,45,45,45 | 0 |
| 60 | MG | A | 3585 | 1/1 | 0.67 | 0.25 | 46,46,46,46 | 0 |
| 60 | MG | A | 3055 | 1/1 | 0.68 | 0.22 | 47,47,47,47 | 0 |
| 60 | MG | A | 3624 | 1/1 | 0.68 | 0.60 | 63,63,63,63 | 0 |
| 60 | MG | A | 3265 | 1/1 | 0.69 | 0.24 | 64,64,64,64 | 0 |
| 60 | MG | A | 3237 | 1/1 | 0.69 | 0.43 | 43,43,43,43 | 1 |
| 60 | MG | A | 3151 | 1/1 | 0.69 | 0.18 | 72,72,72,72 | 0 |
| 60 | MG | R | 202 | 1/1 | 0.70 | 0.19 | 62,62,62,62 | 0 |
| 60 | MG | a | 1666 | 1/1 | 0.70 | 0.44 | 68,68,68,68 | 0 |
| 60 | MG | A | 3014 | 1/1 | 0.70 | 0.32 | 37,37,37,37 | 0 |
| 60 | MG | A | 3335 | 1/1 | 0.70 | 0.35 | 59,59,59,59 | 1 |
| 60 | MG | A | 3154 | 1/1 | 0.70 | 0.33 | 67,67,67,67 | 0 |
| 60 | MG | B | 209 | 1/1 | 0.70 | 0.32 | 60,60,60,60 | 0 |
| 60 | MG | a | 1779 | 1/1 | 0.70 | 0.34 | 55,55,55,55 | 0 |
| 60 | MG | A | 3050 | 1/1 | 0.70 | 0.42 | 60,60,60,60 | 0 |
| 60 | MG | a | 1615 | 1/1 | 0.71 | 0.41 | 54,54,54,54 | 0 |
| 60 | MG | a | 1636 | 1/1 | 0.71 | 0.42 | 59,59,59,59 | 0 |
| 60 | MG | a | 1698 | 1/1 | 0.71 | 0.22 | 49,49,49,49 | 0 |
| 60 | MG | A | 3054 | 1/1 | 0.71 | 0.27 | 48,48,48,48 | 0 |
| 60 | MG | A | 3197 | 1/1 | 0.71 | 0.33 | 48,48,48,48 | 1 |
| 60 | MG | B | 211 | 1/1 | 0.71 | 0.28 | 69,69,69,69 | 0 |
| 60 | MG | A | 3255 | 1/1 | 0.71 | 0.39 | 94,94,94,94 | 0 |
| 60 | MG | A | 3022 | 1/1 | 0.72 | 0.29 | 59,59,59,59 | 0 |
| 60 | MG | A | 3179 | 1/1 | 0.72 | 0.25 | 61,61,61,61 | 0 |
| 60 | MG | A | 3127 | 1/1 | 0.72 | 0.33 | 24,24,24,24 | 1 |
| 60 | MG | A | 3602 | 1/1 | 0.72 | 0.34 | 48,48,48,48 | 0 |
| 60 | MG | A | 3049 | 1/1 | 0.72 | 0.32 | 68,68,68,68 | 0 |
| 60 | MG | A | 3243 | 1/1 | 0.72 | 0.22 | 52,52,52,52 | 0 |
| 60 | MG | x | 106 | 1/1 | 0.72 | 0.45 | 56,56,56,56 | 1 |
| 60 | MG | A | 3277 | 1/1 | 0.72 | 0.41 | 47,47,47,47 | 1 |
| 60 | MG | a | 1641 | 1/1 | 0.73 | 0.34 | 68,68,68,68 | 0 |
| 60 | MG | A | 3242 | 1/1 | 0.73 | 0.41 | 61,61,61,61 | 0 |
| 60 | MG | a | 1703 | 1/1 | 0.73 | 0.24 | 57,57,57,57 | 1 |
| 60 | MG | A | 3577 | 1/1 | 0.73 | 0.42 | 60,60,60,60 | 0 |
| 60 | MG | A | 3492 | 1/1 | 0.73 | 0.38 | 64,64,64,64 | 1 |
| 60 | MG | A | 3100 | 1/1 | 0.73 | 0.50 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3591 | 1/1 | 0.73 | 0.34 | 39,39,39,39 | 1 |
| 60 | MG | a | 1663 | 1/1 | 0.74 | 0.29 | 60,60,60,60 | 0 |
| 60 | MG | A | 3607 | 1/1 | 0.74 | 0.15 | 54,54,54,54 | 0 |
| 60 | MG | A | 3144 | 1/1 | 0.74 | 0.42 | 51,51,51,51 | 0 |
| 60 | MG | a | 1686 | 1/1 | 0.74 | 0.24 | 61,61,61,61 | 0 |
| 60 | MG | A | 3630 | 1/1 | 0.74 | 0.38 | 34,34,34,34 | 1 |
| 60 | MG | A | 3052 | 1/1 | 0.74 | 0.26 | 51,51,51,51 | 1 |
| 60 | MG | A | 3099 | 1/1 | 0.74 | 0.28 | 51,51,51,51 | 0 |
| 60 | MG | A | 3223 | 1/1 | 0.74 | 0.42 | 52,52,52,52 | 0 |
| 60 | MG | A | 3227 | 1/1 | 0.74 | 0.34 | 63,63,63,63 | 0 |
| 60 | MG | a | 1643 | 1/1 | 0.74 | 0.46 | 58,58,58,58 | 0 |
| 60 | MG | A | 3228 | 1/1 | 0.74 | 0.31 | 49,49,49,49 | 0 |
| 60 | MG | A | 3527 | 1/1 | 0.74 | 0.29 | 45,45,45,45 | 0 |
| 60 | MG | A | 3563 | 1/1 | 0.75 | 0.26 | 46,46,46,46 | 0 |
| 60 | MG | A | 3371 | 1/1 | 0.75 | 0.24 | 40,40,40,40 | 0 |
| 60 | MG | P | 202 | 1/1 | 0.75 | 0.40 | 59,59,59,59 | 0 |
| 60 | MG | A | 3097 | 1/1 | 0.75 | 0.29 | 56,56,56,56 | 0 |
| 60 | MG | A | 3342 | 1/1 | 0.75 | 0.30 | 58,58,58,58 | 0 |
| 60 | MG | A | 3610 | 1/1 | 0.75 | 0.24 | 62,62,62,62 | 0 |
| 60 | MG | a | 1660 | 1/1 | 0.75 | 0.36 | 53,53,53,53 | 0 |
| 60 | MG | a | 1665 | 1/1 | 0.76 | 0.52 | 47,47,47,47 | 1 |
| 60 | MG | a | 1606 | 1/1 | 0.76 | 0.12 | 48,48,48,48 | 0 |
| 60 | MG | A | 3521 | 1/1 | 0.76 | 0.23 | 35,35,35,35 | 1 |
| 60 | MG | A | 3282 | 1/1 | 0.76 | 0.29 | 68,68,68,68 | 0 |
| 60 | MG | A | 3358 | 1/1 | 0.76 | 0.32 | 46,46,46,46 | 1 |
| 60 | MG | a | 1691 | 1/1 | 0.76 | 0.29 | 53,53,53,53 | 0 |
| 60 | MG | A | 3536 | 1/1 | 0.76 | 0.31 | 57,57,57,57 | 0 |
| 60 | MG | A | 3157 | 1/1 | 0.76 | 0.54 | 40,40,40,40 | 1 |
| 60 | MG | A | 3064 | 1/1 | 0.76 | 0.14 | 58,58,58,58 | 0 |
| 60 | MG | A | 3465 | 1/1 | 0.76 | 0.10 | 59,59,59,59 | 0 |
| 60 | MG | A | 3217 | 1/1 | 0.76 | 0.56 | 56,56,56,56 | 1 |
| 60 | MG | 0 | 102 | 1/1 | 0.76 | 0.26 | 47,47,47,47 | 0 |
| 60 | MG | x | 108 | 1/1 | 0.76 | 0.26 | 55,55,55,55 | 0 |
| 60 | MG | B | 201 | 1/1 | 0.76 | 0.47 | 53,53,53,53 | 1 |
| 60 | MG | a | 1772 | 1/1 | 0.77 | 0.35 | 62,62,62,62 | 0 |
| 60 | MG | A | 3456 | 1/1 | 0.77 | 0.28 | 46,46,46,46 | 1 |
| 60 | MG | e | 201 | 1/1 | 0.77 | 0.15 | 78,78,78,78 | 0 |
| 60 | MG | A | 3402 | 1/1 | 0.77 | 0.35 | 36,36,36,36 | 0 |
| 60 | MG | A | 3449 | 1/1 | 0.77 | 0.31 | 29,29,29,29 | 1 |
| 60 | MG | A | 3517 | 1/1 | 0.77 | 0.21 | 85,85,85,85 | 0 |
| 60 | MG | a | 1761 | 1/1 | 0.78 | 0.25 | 55,55,55,55 | 1 |
| 60 | MG | A | 3235 | 1/1 | 0.78 | 0.20 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60 | MG | A | 3391 | 1/1 | 0.78 | 0.41 | 56,56,56,56 | 0 |
| 60 | MG | A | 3060 | 1/1 | 0.78 | 0.13 | 54,54,54,54 | 0 |
| 60 | MG | A | 3599 | 1/1 | 0.78 | 0.20 | 45,45,45,45 | 0 |
| 60 | MG | A | 3253 | 1/1 | 0.78 | 0.14 | 67,67,67,67 | 0 |
| 60 | MG | A | 3579 | 1/1 | 0.78 | 0.25 | 50,50,50,50 | 0 |
| 60 | MG | A | 3037 | 1/1 | 0.79 | 0.18 | 44,44,44,44 | 0 |
| 60 | MG | A | 3361 | 1/1 | 0.79 | 0.18 | 64,64,64,64 | 0 |
| 60 | MG | A | 3142 | 1/1 | 0.79 | 0.23 | 57,57,57,57 | 0 |
| 60 | MG | A | 3004 | 1/1 | 0.79 | 0.41 | 40,40,40,40 | 1 |
| 60 | MG | A | 3085 | 1/1 | 0.79 | 0.24 | 70,70,70,70 | 0 |
| 60 | MG | A | 3121 | 1/1 | 0.79 | 0.34 | 38,38,38,38 | 1 |
| 60 | MG | A | 3420 | 1/1 | 0.79 | 0.16 | 55,55,55,55 | 0 |
| 60 | MG | A | 3124 | 1/1 | 0.79 | 0.25 | 32,32,32,32 | 1 |
| 60 | MG | A | 3087 | 1/1 | 0.79 | 0.14 | 41,41,41,41 | 0 |
| 60 | MG | A | 3333 | 1/1 | 0.79 | 0.24 | 61,61,61,61 | 1 |
| 60 | MG | A | 3130 | 1/1 | 0.79 | 0.30 | 55,55,55,55 | 0 |
| 60 | MG | x | 103 | 1/1 | 0.79 | 0.10 | 62,62,62,62 | 0 |
| 60 | MG | A | 3172 | 1/1 | 0.79 | 0.39 | 49,49,49,49 | 0 |
| 60 | MG | A | 3518 | 1/1 | 0.79 | 0.19 | 39,39,39,39 | 0 |
| 60 | MG | A | 3344 | 1/1 | 0.79 | 0.11 | 70,70,70,70 | 0 |
| 60 | MG | A | 3305 | 1/1 | 0.80 | 0.40 | 38,38,38,38 | 0 |
| 60 | MG | F | 305 | 1/1 | 0.80 | 0.14 | 46,46,46,46 | 0 |
| 60 | MG | O | 201 | 1/1 | 0.80 | 0.23 | 55,55,55,55 | 0 |
| 60 | MG | a | 1664 | 1/1 | 0.80 | 0.26 | 62,62,62,62 | 0 |
| 60 | MG | P | 201 | 1/1 | 0.80 | 0.36 | 59,59,59,59 | 0 |
| 60 | MG | A | 3316 | 1/1 | 0.80 | 0.37 | 63,63,63,63 | 0 |
| 60 | MG | A | 3015 | 1/1 | 0.80 | 0.18 | 45,45,45,45 | 0 |
| 60 | MG | a | 1679 | 1/1 | 0.80 | 0.21 | 39,39,39,39 | 0 |
| 60 | MG | A | 3573 | 1/1 | 0.80 | 0.69 | 34,34,34,34 | 1 |
| 60 | MG | Z | 301 | 1/1 | 0.80 | 0.16 | 61,61,61,61 | 0 |
| 60 | MG | A | 3611 | 1/1 | 0.80 | 0.20 | 46,46,46,46 | 0 |
| 60 | MG | A | 3505 | 1/1 | 0.80 | 0.14 | 41,41,41,41 | 0 |
| 60 | MG | A | 3259 | 1/1 | 0.80 | 0.31 | 60,60,60,60 | 0 |
| 60 | MG | a | 1611 | 1/1 | 0.80 | 0.18 | 58,58,58,58 | 0 |
| 60 | MG | A | 3644 | 1/1 | 0.80 | 0.23 | 42,42,42,42 | 0 |
| 60 | MG | a | 1718 | 1/1 | 0.80 | 0.41 | 55,55,55,55 | 1 |
| 60 | MG | A | 3581 | 1/1 | 0.80 | 0.10 | 63,63,63,63 | 0 |
| 60 | MG | a | 1620 | 1/1 | 0.80 | 0.49 | 47,47,47,47 | 0 |
| 60 | MG | A | 3039 | 1/1 | 0.80 | 0.16 | 63,63,63,63 | 0 |
| 60 | MG | a | 1785 | 1/1 | 0.80 | 0.47 | 53,53,53,53 | 0 |
| 60 | MG | A | 3011 | 1/1 | 0.80 | 0.70 | 53,53,53,53 | 0 |
| 60 | MG | B | 207 | 1/1 | 0.80 | 0.15 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3122 | 1/1 | 0.80 | 0.31 | 51,51,51,51 | 1 |
| 60 | MG | a | 1648 | 1/1 | 0.80 | 0.27 | 58,58,58,58 | 0 |
| 60 | MG | A | 3453 | 1/1 | 0.80 | 0.14 | 57,57,57,57 | 0 |
| 60 | MG | A | 3244 | 1/1 | 0.81 | 0.19 | 53,53,53,53 | 0 |
| 60 | MG | A | 3438 | 1/1 | 0.81 | 0.13 | 77,77,77,77 | 0 |
| 60 | MG | A | 3141 | 1/1 | 0.81 | 0.32 | 42,42,42,42 | 1 |
| 60 | MG | a | 1625 | 1/1 | 0.81 | 0.30 | 60,60,60,60 | 0 |
| 60 | MG | a | 1629 | 1/1 | 0.81 | 0.15 | 44,44,44,44 | 0 |
| 60 | MG | A | 3209 | 1/1 | 0.81 | 0.30 | 72,72,72,72 | 0 |
| 60 | MG | A | 3551 | 1/1 | 0.81 | 0.18 | 71,71,71,71 | 0 |
| 60 | MG | a | 1704 | 1/1 | 0.81 | 0.22 | 52,52,52,52 | 0 |
| 60 | MG | A | 3555 | 1/1 | 0.81 | 0.15 | 63,63,63,63 | 0 |
| 60 | MG | A | 3180 | 1/1 | 0.81 | 0.35 | 44,44,44,44 | 0 |
| 60 | MG | A | 3257 | 1/1 | 0.81 | 0.16 | 52,52,52,52 | 0 |
| 60 | MG | A | 3088 | 1/1 | 0.81 | 0.32 | 53,53,53,53 | 0 |
| 60 | MG | A | 3263 | 1/1 | 0.81 | 0.21 | 67,67,67,67 | 0 |
| 60 | MG | A | 3510 | 1/1 | 0.81 | 0.33 | 48,48,48,48 | 0 |
| 60 | MG | a | 1786 | 1/1 | 0.81 | 0.77 | 38,38,38,38 | 1 |
| 60 | MG | 6 | 101 | 1/1 | 0.81 | 0.35 | 42,42,42,42 | 1 |
| 60 | MG | a | 1603 | 1/1 | 0.81 | 0.29 | 67,67,67,67 | 0 |
| 60 | MG | A | 3511 | 1/1 | 0.81 | 0.33 | 50,50,50,50 | 0 |
| 60 | MG | A | 3068 | 1/1 | 0.81 | 0.38 | 69,69,69,69 | 0 |
| 60 | MG | A | 3200 | 1/1 | 0.81 | 0.18 | 39,39,39,39 | 0 |
| 60 | MG | A | 3249 | 1/1 | 0.82 | 0.41 | 72,72,72,72 | 0 |
| 60 | MG | A | 3212 | 1/1 | 0.82 | 0.13 | 46,46,46,46 | 0 |
| 60 | MG | A | 3270 | 1/1 | 0.82 | 0.19 | 51,51,51,51 | 0 |
| 60 | MG | A | 3597 | 1/1 | 0.82 | 0.34 | 47,47,47,47 | 0 |
| 60 | MG | A | 3132 | 1/1 | 0.82 | 0.42 | 43,43,43,43 | 1 |
| 60 | MG | A | 3556 | 1/1 | 0.82 | 0.29 | 35,35,35,35 | 1 |
| 60 | MG | a | 1725 | 1/1 | 0.82 | 0.30 | 51,51,51,51 | 0 |
| 60 | MG | A | 3604 | 1/1 | 0.82 | 0.17 | 64,64,64,64 | 0 |
| 60 | MG | A | 3170 | 1/1 | 0.82 | 0.25 | 33,33,33,33 | 0 |
| 60 | MG | A | 3150 | 1/1 | 0.82 | 0.17 | 54,54,54,54 | 0 |
| 60 | MG | a | 1782 | 1/1 | 0.82 | 0.58 | 62,62,62,62 | 0 |
| 60 | MG | a | 1616 | 1/1 | 0.82 | 0.21 | 54,54,54,54 | 0 |
| 60 | MG | a | 1675 | 1/1 | 0.82 | 0.60 | 61,61,61,61 | 0 |
| 60 | MG | A | 3029 | 1/1 | 0.82 | 0.30 | 48,48,48,48 | 0 |
| 60 | MG | A | 3519 | 1/1 | 0.82 | 0.17 | 48,48,48,48 | 0 |
| 60 | MG | A | 3167 | 1/1 | 0.82 | 0.37 | 51,51,51,51 | 0 |
| 60 | MG | A | 3284 | 1/1 | 0.82 | 0.28 | 39,39,39,39 | 1 |
| 60 | MG | A | 3639 | 1/1 | 0.82 | 0.29 | 36,36,36,36 | 0 |
| 60 | MG | z | 702 | 1/1 | 0.82 | 0.07 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3262 | 1/1 | 0.83 | 0.12 | 50,50,50,50 | 1 |
| 60 | MG | A | 3281 | 1/1 | 0.83 | 0.23 | 43,43,43,43 | 0 |
| 60 | MG | a | 1715 | 1/1 | 0.83 | 0.31 | 58,58,58,58 | 0 |
| 60 | MG | A | 3158 | 1/1 | 0.83 | 0.34 | 38,38,38,38 | 1 |
| 60 | MG | A | 3603 | 1/1 | 0.83 | 0.37 | 50,50,50,50 | 0 |
| 60 | MG | a | 1731 | 1/1 | 0.83 | 0.20 | 49,49,49,49 | 0 |
| 60 | MG | a | 1741 | 1/1 | 0.83 | 0.18 | 63,63,63,63 | 0 |
| 60 | MG | A | 3008 | 1/1 | 0.83 | 0.17 | 42,42,42,42 | 0 |
| 60 | MG | A | 3362 | 1/1 | 0.83 | 0.28 | 47,47,47,47 | 0 |
| 60 | MG | A | 3266 | 1/1 | 0.83 | 0.55 | 67,67,67,67 | 0 |
| 60 | MG | A | 3387 | 1/1 | 0.83 | 0.24 | 26,26,26,26 | 0 |
| 60 | MG | a | 1784 | 1/1 | 0.83 | 0.41 | 52,52,52,52 | 0 |
| 60 | MG | A | 3080 | 1/1 | 0.83 | 0.43 | 48,48,48,48 | 0 |
| 60 | MG | A | 3056 | 1/1 | 0.83 | 0.24 | 39,39,39,39 | 0 |
| 60 | MG | A | 3627 | 1/1 | 0.83 | 0.22 | 25,25,25,25 | 0 |
| 60 | MG | n | 101 | 1/1 | 0.83 | 0.66 | 64,64,64,64 | 0 |
| 60 | MG | A | 3106 | 1/1 | 0.83 | 0.28 | 46,46,46,46 | 1 |
| 60 | MG | A | 3275 | 1/1 | 0.83 | 0.29 | 55,55,55,55 | 1 |
| 60 | MG | a | 1642 | 1/1 | 0.83 | 0.38 | 70,70,70,70 | 0 |
| 60 | MG | A | 3040 | 1/1 | 0.83 | 0.36 | 31,31,31,31 | 1 |
| 60 | MG | z | 701 | 1/1 | 0.83 | 0.28 | 59,59,59,59 | 0 |
| 60 | MG | A | 3341 | 1/1 | 0.83 | 0.27 | 30,30,30,30 | 0 |
| 60 | MG | A | 3026 | 1/1 | 0.84 | 0.25 | 43,43,43,43 | 0 |
| 60 | MG | A | 3188 | 1/1 | 0.84 | 0.29 | 39,39,39,39 | 0 |
| 60 | MG | A | 3044 | 1/1 | 0.84 | 0.30 | 25,25,25,25 | 1 |
| 60 | MG | A | 3588 | 1/1 | 0.84 | 0.29 | 60,60,60,60 | 0 |
| 60 | MG | A | 3462 | 1/1 | 0.84 | 0.13 | 58,58,58,58 | 0 |
| 60 | MG | a | 1612 | 1/1 | 0.84 | 0.13 | 57,57,57,57 | 0 |
| 60 | MG | A | 3541 | 1/1 | 0.84 | 0.08 | 63,63,63,63 | 0 |
| 60 | MG | A | 3542 | 1/1 | 0.84 | 0.25 | 63,63,63,63 | 0 |
| 60 | MG | A | 3549 | 1/1 | 0.84 | 0.09 | 47,47,47,47 | 0 |
| 60 | MG | A | 3272 | 1/1 | 0.84 | 0.31 | 55,55,55,55 | 0 |
| 60 | MG | A | 3137 | 1/1 | 0.84 | 0.28 | 35,35,35,35 | 0 |
| 60 | MG | d | 301 | 1/1 | 0.84 | 0.56 | 59,59,59,59 | 0 |
| 60 | MG | A | 3260 | 1/1 | 0.84 | 0.32 | 44,44,44,44 | 1 |
| 60 | MG | a | 1635 | 1/1 | 0.84 | 0.26 | 55,55,55,55 | 0 |
| 60 | MG | A | 3089 | 1/1 | 0.84 | 0.15 | 58,58,58,58 | 0 |
| 60 | MG | A | 3002 | 1/1 | 0.84 | 0.09 | 58,58,58,58 | 0 |
| 60 | MG | A | 3572 | 1/1 | 0.84 | 0.21 | 58,58,58,58 | 0 |
| 60 | MG | A | 3418 | 1/1 | 0.84 | 0.34 | 48,48,48,48 | 0 |
| 60 | MG | A | 3264 | 1/1 | 0.84 | 0.28 | 23,23,23,23 | 1 |
| 60 | MG | A | 3143 | 1/1 | 0.84 | 0.22 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | a | 1669 | 1/1 | 0.85 | 0.27 | 60,60,60,60 | 0 |
| 60 | MG | a | 1674 | 1/1 | 0.85 | 0.43 | 50,50,50,50 | 0 |
| 60 | MG | A | 3081 | 1/1 | 0.85 | 0.35 | 56,56,56,56 | 0 |
| 60 | MG | A | 3206 | 1/1 | 0.85 | 0.31 | 50,50,50,50 | 0 |
| 60 | MG | A | 3546 | 1/1 | 0.85 | 0.13 | 53,53,53,53 | 0 |
| 60 | MG | a | 1601 | 1/1 | 0.85 | 0.53 | 68,68,68,68 | 0 |
| 60 | MG | A | 3353 | 1/1 | 0.85 | 0.22 | 60,60,60,60 | 0 |
| 60 | MG | a | 1690 | 1/1 | 0.85 | 0.14 | 69,69,69,69 | 0 |
| 60 | MG | A | 3458 | 1/1 | 0.85 | 0.24 | 38,38,38,38 | 0 |
| 60 | MG | a | 1693 | 1/1 | 0.85 | 0.32 | 39,39,39,39 | 0 |
| 60 | MG | A | 3552 | 1/1 | 0.85 | 0.12 | 48,48,48,48 | 0 |
| 60 | MG | a | 1609 | 1/1 | 0.85 | 0.55 | 51,51,51,51 | 0 |
| 60 | MG | A | 3280 | 1/1 | 0.85 | 0.33 | 46,46,46,46 | 0 |
| 60 | MG | A | 3082 | 1/1 | 0.85 | 0.31 | 43,43,43,43 | 1 |
| 60 | MG | A | 3084 | 1/1 | 0.85 | 0.11 | 56,56,56,56 | 0 |
| 60 | MG | A | 3072 | 1/1 | 0.85 | 0.17 | 46,46,46,46 | 0 |
| 60 | MG | A | 3568 | 1/1 | 0.85 | 0.24 | 61,61,61,61 | 0 |
| 60 | MG | A | 3059 | 1/1 | 0.85 | 0.22 | 37,37,37,37 | 1 |
| 60 | MG | A | 3183 | 1/1 | 0.85 | 0.25 | 21,21,21,21 | 0 |
| 60 | MG | A | 3574 | 1/1 | 0.85 | 0.18 | 39,39,39,39 | 0 |
| 60 | MG | A | 3250 | 1/1 | 0.85 | 0.28 | 64,64,64,64 | 0 |
| 60 | MG | a | 1763 | 1/1 | 0.85 | 0.27 | 34,34,34,34 | 1 |
| 60 | MG | a | 1767 | 1/1 | 0.85 | 0.12 | 45,45,45,45 | 0 |
| 60 | MG | A | 3225 | 1/1 | 0.85 | 0.29 | 54,54,54,54 | 0 |
| 60 | MG | A | 3118 | 1/1 | 0.85 | 0.23 | 64,64,64,64 | 0 |
| 60 | MG | B | 212 | 1/1 | 0.85 | 0.18 | 52,52,52,52 | 0 |
| 60 | MG | A | 3520 | 1/1 | 0.85 | 0.36 | 55,55,55,55 | 0 |
| 60 | MG | A | 3161 | 1/1 | 0.85 | 0.29 | 34,34,34,34 | 1 |
| 60 | MG | a | 1644 | 1/1 | 0.85 | 0.17 | 46,46,46,46 | 0 |
| 60 | MG | F | 306 | 1/1 | 0.85 | 0.33 | 46,46,46,46 | 0 |
| 60 | MG | G | 202 | 1/1 | 0.85 | 0.10 | 48,48,48,48 | 0 |
| 60 | MG | A | 3423 | 1/1 | 0.85 | 0.20 | 73,73,73,73 | 0 |
| 60 | MG | A | 3433 | 1/1 | 0.85 | 0.20 | 27,27,27,27 | 1 |
| 60 | MG | A | 3528 | 1/1 | 0.85 | 0.51 | 51,51,51,51 | 0 |
| 60 | MG | A | 3531 | 1/1 | 0.85 | 0.41 | 55,55,55,55 | 0 |
| 60 | MG | A | 3148 | 1/1 | 0.85 | 0.30 | 47,47,47,47 | 0 |
| 60 | MG | W | 201 | 1/1 | 0.85 | 0.29 | 59,59,59,59 | 0 |
| 60 | MG | a | 1667 | 1/1 | 0.85 | 0.21 | 55,55,55,55 | 0 |
| 60 | MG | A | 3350 | 1/1 | 0.86 | 0.12 | 59,59,59,59 | 0 |
| 60 | MG | A | 3043 | 1/1 | 0.86 | 0.24 | 39,39,39,39 | 0 |
| 60 | MG | A | 3356 | 1/1 | 0.86 | 0.40 | 50,50,50,50 | 0 |
| 60 | MG | a | 1640 | 1/1 | 0.86 | 0.62 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3429 | 1/1 | 0.86 | 0.29 | 45,45,45,45 | 0 |
| 60 | MG | A | 3067 | 1/1 | 0.86 | 0.18 | 34,34,34,34 | 0 |
| 60 | MG | A | 3182 | 1/1 | 0.86 | 0.41 | 43,43,43,43 | 0 |
| 60 | MG | a | 1721 | 1/1 | 0.86 | 0.08 | 41,41,41,41 | 0 |
| 60 | MG | A | 3441 | 1/1 | 0.86 | 0.56 | 52,52,52,52 | 0 |
| 60 | MG | A | 3443 | 1/1 | 0.86 | 0.28 | 41,41,41,41 | 0 |
| 60 | MG | A | 3448 | 1/1 | 0.86 | 0.43 | 60,60,60,60 | 0 |
| 60 | MG | a | 1752 | 1/1 | 0.86 | 0.35 | 43,43,43,43 | 0 |
| 60 | MG | A | 3633 | 1/1 | 0.86 | 0.31 | 30,30,30,30 | 0 |
| 60 | MG | A | 3576 | 1/1 | 0.86 | 0.12 | 59,59,59,59 | 0 |
| 60 | MG | A | 3063 | 1/1 | 0.86 | 0.29 | 49,49,49,49 | 0 |
| 60 | MG | A | 3530 | 1/1 | 0.86 | 0.42 | 38,38,38,38 | 1 |
| 60 | MG | A | 3111 | 1/1 | 0.86 | 0.23 | 46,46,46,46 | 0 |
| 60 | MG | A | 3384 | 1/1 | 0.86 | 0.23 | 39,39,39,39 | 0 |
| 60 | MG | A | 3540 | 1/1 | 0.86 | 0.10 | 57,57,57,57 | 0 |
| 60 | MG | A | 3024 | 1/1 | 0.86 | 0.28 | 40,40,40,40 | 0 |
| 60 | MG | A | 3258 | 1/1 | 0.86 | 0.41 | 41,41,41,41 | 0 |
| 60 | MG | A | 3247 | 1/1 | 0.86 | 0.23 | 46,46,46,46 | 1 |
| 60 | MG | A | 3271 | 1/1 | 0.86 | 0.48 | 71,71,71,71 | 0 |
| 60 | MG | f | 201 | 1/1 | 0.86 | 0.19 | 53,53,53,53 | 0 |
| 60 | MG | B | 216 | 1/1 | 0.86 | 0.11 | 53,53,53,53 | 0 |
| 60 | MG | a | 1681 | 1/1 | 0.86 | 0.16 | 55,55,55,55 | 0 |
| 60 | MG | D | 304 | 1/1 | 0.86 | 0.32 | 36,36,36,36 | 1 |
| 60 | MG | F | 302 | 1/1 | 0.86 | 0.27 | 32,32,32,32 | 1 |
| 60 | MG | a | 1627 | 1/1 | 0.86 | 0.28 | 47,47,47,47 | 0 |
| 60 | MG | A | 3404 | 1/1 | 0.86 | 0.27 | 35,35,35,35 | 0 |
| 60 | MG | a | 1631 | 1/1 | 0.86 | 0.43 | 42,42,42,42 | 0 |
| 60 | MG | A | 3450 | 1/1 | 0.87 | 0.33 | 58,58,58,58 | 0 |
| 60 | MG | U | 201 | 1/1 | 0.87 | 0.33 | 30,30,30,30 | 1 |
| 60 | MG | A | 3110 | 1/1 | 0.87 | 0.27 | 25,25,25,25 | 1 |
| 60 | MG | A | 3343 | 1/1 | 0.87 | 0.09 | 64,64,64,64 | 0 |
| 60 | MG | a | 1672 | 1/1 | 0.87 | 0.23 | 41,41,41,41 | 0 |
| 60 | MG | A | 3133 | 1/1 | 0.87 | 0.26 | 36,36,36,36 | 1 |
| 60 | MG | a | 1632 | 1/1 | 0.87 | 0.36 | 42,42,42,42 | 0 |
| 60 | MG | A | 3075 | 1/1 | 0.87 | 0.14 | 60,60,60,60 | 1 |
| 60 | MG | A | 3436 | 1/1 | 0.87 | 0.21 | 43,43,43,43 | 0 |
| 60 | MG | a | 1775 | 1/1 | 0.87 | 0.18 | 53,53,53,53 | 1 |
| 60 | MG | 7 | 101 | 1/1 | 0.87 | 0.14 | 63,63,63,63 | 0 |
| 60 | MG | A | 3580 | 1/1 | 0.87 | 0.35 | 43,43,43,43 | 0 |
| 60 | MG | a | 1602 | 1/1 | 0.87 | 0.28 | 57,57,57,57 | 0 |
| 60 | MG | A | 3612 | 1/1 | 0.87 | 0.10 | 62,62,62,62 | 0 |
| 60 | MG | A | 3320 | 1/1 | 0.87 | 0.21 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3354 | 1/1 | 0.87 | 0.30 | 53,53,53,53 | 0 |
| 60 | MG | a | 1694 | 1/1 | 0.87 | 0.15 | 41,41,41,41 | 0 |
| 60 | MG | A | 3153 | 1/1 | 0.87 | 0.24 | 45,45,45,45 | 0 |
| 60 | MG | a | 1653 | 1/1 | 0.87 | 0.42 | 61,61,61,61 | 0 |
| 60 | MG | A | 3559 | 1/1 | 0.87 | 0.27 | 38,38,38,38 | 1 |
| 60 | MG | A | 3073 | 1/1 | 0.87 | 0.21 | 32,32,32,32 | 0 |
| 60 | MG | A | 3642 | 1/1 | 0.87 | 0.21 | 38,38,38,38 | 1 |
| 60 | MG | a | 1709 | 1/1 | 0.87 | 0.12 | 36,36,36,36 | 0 |
| 60 | MG | A | 3291 | 1/1 | 0.87 | 0.40 | 55,55,55,55 | 0 |
| 60 | MG | A | 3571 | 1/1 | 0.87 | 0.30 | 38,38,38,38 | 1 |
| 60 | MG | A | 3339 | 1/1 | 0.88 | 0.12 | 54,54,54,54 | 0 |
| 60 | MG | A | 3001 | 1/1 | 0.88 | 0.20 | 51,51,51,51 | 0 |
| 60 | MG | A | 3224 | 1/1 | 0.88 | 0.20 | 34,34,34,34 | 0 |
| 60 | MG | A | 3012 | 1/1 | 0.88 | 0.30 | 60,60,60,60 | 0 |
| 60 | MG | A | 3246 | 1/1 | 0.88 | 0.29 | 66,66,66,66 | 0 |
| 60 | MG | A | 3152 | 1/1 | 0.88 | 0.10 | 48,48,48,48 | 0 |
| 60 | MG | A | 3351 | 1/1 | 0.88 | 0.37 | 33,33,33,33 | 0 |
| 60 | MG | A | 3164 | 1/1 | 0.88 | 0.32 | 31,31,31,31 | 0 |
| 60 | MG | A | 3229 | 1/1 | 0.88 | 0.26 | 39,39,39,39 | 0 |
| 60 | MG | A | 3532 | 1/1 | 0.88 | 0.20 | 41,41,41,41 | 0 |
| 60 | MG | a | 1713 | 1/1 | 0.88 | 0.45 | 43,43,43,43 | 0 |
| 60 | MG | F | 303 | 1/1 | 0.88 | 0.20 | 53,53,53,53 | 0 |
| 60 | MG | F | 304 | 1/1 | 0.88 | 0.70 | 28,28,28,28 | 1 |
| 60 | MG | A | 3025 | 1/1 | 0.88 | 0.28 | 51,51,51,51 | 1 |
| 60 | MG | A | 3592 | 1/1 | 0.88 | 0.48 | 41,41,41,41 | 1 |
| 60 | MG | A | 3038 | 1/1 | 0.88 | 0.21 | 29,29,29,29 | 0 |
| 60 | MG | A | 3297 | 1/1 | 0.88 | 0.28 | 35,35,35,35 | 1 |
| 60 | MG | a | 1742 | 1/1 | 0.88 | 0.18 | 58,58,58,58 | 0 |
| 60 | MG | A | 3299 | 1/1 | 0.88 | 0.32 | 35,35,35,35 | 0 |
| 60 | MG | a | 1759 | 1/1 | 0.88 | 0.13 | 53,53,53,53 | 0 |
| 60 | MG | A | 3544 | 1/1 | 0.88 | 0.33 | 53,53,53,53 | 0 |
| 60 | MG | a | 1654 | 1/1 | 0.88 | 0.16 | 50,50,50,50 | 0 |
| 60 | MG | a | 1657 | 1/1 | 0.88 | 0.14 | 57,57,57,57 | 0 |
| 60 | MG | A | 3254 | 1/1 | 0.88 | 0.30 | 62,62,62,62 | 0 |
| 60 | MG | A | 3548 | 1/1 | 0.88 | 0.38 | 65,65,65,65 | 0 |
| 60 | MG | A | 3375 | 1/1 | 0.88 | 0.20 | 35,35,35,35 | 0 |
| 60 | MG | A | 3382 | 1/1 | 0.88 | 0.27 | 30,30,30,30 | 0 |
| 60 | MG | A | 3310 | 1/1 | 0.88 | 0.16 | 37,37,37,37 | 0 |
| 60 | MG | A | 3129 | 1/1 | 0.88 | 0.19 | 35,35,35,35 | 1 |
| 60 | MG | A | 3617 | 1/1 | 0.88 | 0.16 | 45,45,45,45 | 0 |
| 60 | MG | A | 3618 | 1/1 | 0.88 | 0.17 | 57,57,57,57 | 0 |
| 60 | MG | A | 3620 | 1/1 | 0.88 | 0.18 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3496 | 1/1 | 0.88 | 0.31 | 33,33,33,33 | 1 |
| 60 | MG | A | 3502 | 1/1 | 0.88 | 0.14 | 44,44,44,44 | 0 |
| 60 | MG | A | 3221 | 1/1 | 0.88 | 0.30 | 49,49,49,49 | 0 |
| 60 | MG | A | 3560 | 1/1 | 0.88 | 0.20 | 58,58,58,58 | 0 |
| 60 | MG | A | 3328 | 1/1 | 0.88 | 0.17 | 62,62,62,62 | 0 |
| 60 | MG | A | 3239 | 1/1 | 0.88 | 0.49 | 51,51,51,51 | 0 |
| 60 | MG | A | 3514 | 1/1 | 0.88 | 0.15 | 69,69,69,69 | 0 |
| 60 | MG | A | 3276 | 1/1 | 0.88 | 0.20 | 51,51,51,51 | 1 |
| 60 | MG | A | 3041 | 1/1 | 0.89 | 0.26 | 38,38,38,38 | 0 |
| 60 | MG | A | 3251 | 1/1 | 0.89 | 0.15 | 46,46,46,46 | 0 |
| 60 | MG | A | 3160 | 1/1 | 0.89 | 0.45 | 57,57,57,57 | 0 |
| 60 | MG | A | 3226 | 1/1 | 0.89 | 0.29 | 45,45,45,45 | 0 |
| 60 | MG | A | 3190 | 1/1 | 0.89 | 0.49 | 58,58,58,58 | 0 |
| 60 | MG | A | 3191 | 1/1 | 0.89 | 0.22 | 51,51,51,51 | 0 |
| 60 | MG | A | 3196 | 1/1 | 0.89 | 0.20 | 51,51,51,51 | 0 |
| 60 | MG | A | 3537 | 1/1 | 0.89 | 0.16 | 45,45,45,45 | 0 |
| 60 | MG | D | 303 | 1/1 | 0.89 | 0.24 | 24,24,24,24 | 1 |
| 60 | MG | A | 3231 | 1/1 | 0.89 | 0.24 | 68,68,68,68 | 0 |
| 60 | MG | A | 3146 | 1/1 | 0.89 | 0.09 | 72,72,72,72 | 0 |
| 60 | MG | A | 3593 | 1/1 | 0.89 | 0.08 | 70,70,70,70 | 0 |
| 60 | MG | A | 3016 | 1/1 | 0.89 | 0.38 | 59,59,59,59 | 0 |
| 60 | MG | A | 3289 | 1/1 | 0.89 | 0.19 | 59,59,59,59 | 0 |
| 60 | MG | A | 3545 | 1/1 | 0.89 | 0.42 | 42,42,42,42 | 0 |
| 60 | MG | A | 3290 | 1/1 | 0.89 | 0.20 | 56,56,56,56 | 0 |
| 60 | MG | H | 201 | 1/1 | 0.89 | 0.18 | 62,62,62,62 | 0 |
| 60 | MG | a | 1732 | 1/1 | 0.89 | 0.17 | 54,54,54,54 | 0 |
| 60 | MG | A | 3112 | 1/1 | 0.89 | 0.27 | 44,44,44,44 | 0 |
| 60 | MG | A | 3201 | 1/1 | 0.89 | 0.48 | 45,45,45,45 | 0 |
| 60 | MG | A | 3550 | 1/1 | 0.89 | 0.39 | 65,65,65,65 | 0 |
| 60 | MG | a | 1758 | 1/1 | 0.89 | 0.49 | 72,72,72,72 | 0 |
| 60 | MG | a | 1656 | 1/1 | 0.89 | 0.10 | 60,60,60,60 | 0 |
| 60 | MG | A | 3474 | 1/1 | 0.89 | 0.34 | 44,44,44,44 | 0 |
| 60 | MG | a | 1659 | 1/1 | 0.89 | 0.27 | 55,55,55,55 | 0 |
| 60 | MG | a | 1765 | 1/1 | 0.89 | 0.13 | 55,55,55,55 | 0 |
| 60 | MG | A | 3374 | 1/1 | 0.89 | 0.22 | 54,54,54,54 | 0 |
| 60 | MG | V | 201 | 1/1 | 0.89 | 0.40 | 55,55,55,55 | 0 |
| 60 | MG | A | 3554 | 1/1 | 0.89 | 0.16 | 67,67,67,67 | 0 |
| 60 | MG | A | 3296 | 1/1 | 0.89 | 0.20 | 31,31,31,31 | 0 |
| 60 | MG | A | 3083 | 1/1 | 0.89 | 0.18 | 51,51,51,51 | 0 |
| 60 | MG | A | 3065 | 1/1 | 0.89 | 0.29 | 64,64,64,64 | 0 |
| 60 | MG | A | 3101 | 1/1 | 0.89 | 0.23 | 47,47,47,47 | 0 |
| 60 | MG | A | 3625 | 1/1 | 0.89 | 0.11 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3102 | 1/1 | 0.89 | 0.31 | 55,55,55,55 | 0 |
| 60 | MG | A | 3268 | 1/1 | 0.89 | 0.27 | 52,52,52,52 | 0 |
| 60 | MG | a | 1673 | 1/1 | 0.89 | 0.24 | 60,60,60,60 | 0 |
| 60 | MG | A | 3319 | 1/1 | 0.89 | 0.21 | 43,43,43,43 | 0 |
| 60 | MG | A | 3636 | 1/1 | 0.89 | 0.32 | 37,37,37,37 | 1 |
| 60 | MG | A | 3269 | 1/1 | 0.89 | 0.20 | 64,64,64,64 | 0 |
| 60 | MG | a | 1677 | 1/1 | 0.89 | 0.20 | 63,63,63,63 | 0 |
| 60 | MG | A | 3071 | 1/1 | 0.89 | 0.15 | 61,61,61,61 | 0 |
| 60 | MG | A | 3181 | 1/1 | 0.89 | 0.40 | 49,49,49,49 | 0 |
| 60 | MG | A | 3109 | 1/1 | 0.89 | 0.30 | 25,25,25,25 | 1 |
| 60 | MG | A | 3589 | 1/1 | 0.90 | 0.14 | 42,42,42,42 | 0 |
| 60 | MG | A | 3047 | 1/1 | 0.90 | 0.18 | 29,29,29,29 | 0 |
| 60 | MG | a | 1650 | 1/1 | 0.90 | 0.47 | 47,47,47,47 | 0 |
| 60 | MG | 0 | 101 | 1/1 | 0.90 | 0.23 | 39,39,39,39 | 0 |
| 60 | MG | A | 3220 | 1/1 | 0.90 | 0.29 | 45,45,45,45 | 0 |
| 60 | MG | a | 1717 | 1/1 | 0.90 | 0.63 | 54,54,54,54 | 0 |
| 60 | MG | 5 | 102 | 1/1 | 0.90 | 0.39 | 58,58,58,58 | 0 |
| 60 | MG | A | 3240 | 1/1 | 0.90 | 0.08 | 56,56,56,56 | 0 |
| 60 | MG | A | 3163 | 1/1 | 0.90 | 0.11 | 26,26,26,26 | 0 |
| 60 | MG | A | 3042 | 1/1 | 0.90 | 0.38 | 40,40,40,40 | 0 |
| 60 | MG | A | 3332 | 1/1 | 0.90 | 0.13 | 53,53,53,53 | 0 |
| 60 | MG | A | 3119 | 1/1 | 0.90 | 0.18 | 68,68,68,68 | 0 |
| 60 | MG | A | 3107 | 1/1 | 0.90 | 0.21 | 55,55,55,55 | 0 |
| 60 | MG | A | 3336 | 1/1 | 0.90 | 0.10 | 52,52,52,52 | 0 |
| 60 | MG | A | 3338 | 1/1 | 0.90 | 0.29 | 20,20,20,20 | 0 |
| 60 | MG | A | 3609 | 1/1 | 0.90 | 0.21 | 31,31,31,31 | 0 |
| 60 | MG | A | 3010 | 1/1 | 0.90 | 0.36 | 32,32,32,32 | 1 |
| 60 | MG | E | 304 | 1/1 | 0.90 | 0.20 | 35,35,35,35 | 0 |
| 60 | MG | A | 3003 | 1/1 | 0.90 | 0.24 | 32,32,32,32 | 0 |
| 60 | MG | A | 3535 | 1/1 | 0.90 | 0.26 | 55,55,55,55 | 0 |
| 60 | MG | a | 1770 | 1/1 | 0.90 | 0.35 | 56,56,56,56 | 0 |
| 60 | MG | A | 3613 | 1/1 | 0.90 | 0.31 | 67,67,67,67 | 0 |
| 60 | MG | a | 1622 | 1/1 | 0.90 | 0.21 | 36,36,36,36 | 0 |
| 60 | MG | A | 3468 | 1/1 | 0.90 | 0.18 | 37,37,37,37 | 1 |
| 60 | MG | a | 1626 | 1/1 | 0.90 | 0.42 | 52,52,52,52 | 0 |
| 60 | MG | A | 3471 | 1/1 | 0.90 | 0.13 | 65,65,65,65 | 0 |
| 60 | MG | A | 3090 | 1/1 | 0.90 | 0.21 | 43,43,43,43 | 0 |
| 60 | MG | a | 1683 | 1/1 | 0.90 | 0.40 | 58,58,58,58 | 0 |
| 60 | MG | A | 3480 | 1/1 | 0.90 | 0.34 | 41,41,41,41 | 0 |
| 60 | MG | A | 3202 | 1/1 | 0.90 | 0.09 | 36,36,36,36 | 0 |
| 60 | MG | A | 3079 | 1/1 | 0.90 | 0.17 | 18,18,18,18 | 0 |
| 60 | MG | A | 3232 | 1/1 | 0.90 | 0.20 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | R | 201 | 1/1 | 0.90 | 0.45 | 50,50,50,50 | 0 |
| 60 | MG | A | 3114 | 1/1 | 0.90 | 0.39 | 42,42,42,42 | 0 |
| 60 | MG | a | 1697 | 1/1 | 0.90 | 0.21 | 34,34,34,34 | 0 |
| 60 | MG | A | 3159 | 1/1 | 0.90 | 0.18 | 45,45,45,45 | 1 |
| 60 | MG | A | 3638 | 1/1 | 0.90 | 0.23 | 38,38,38,38 | 0 |
| 60 | MG | A | 3147 | 1/1 | 0.90 | 0.24 | 50,50,50,50 | 0 |
| 60 | MG | E | 301 | 1/1 | 0.91 | 0.17 | 33,33,33,33 | 0 |
| 60 | MG | a | 1687 | 1/1 | 0.91 | 0.29 | 29,29,29,29 | 0 |
| 60 | MG | E | 303 | 1/1 | 0.91 | 0.31 | 32,32,32,32 | 1 |
| 60 | MG | A | 3406 | 1/1 | 0.91 | 0.06 | 74,74,74,74 | 0 |
| 60 | MG | F | 301 | 1/1 | 0.91 | 0.20 | 44,44,44,44 | 0 |
| 60 | MG | A | 3499 | 1/1 | 0.91 | 0.19 | 36,36,36,36 | 0 |
| 60 | MG | a | 1628 | 1/1 | 0.91 | 0.20 | 45,45,45,45 | 0 |
| 60 | MG | A | 3321 | 1/1 | 0.91 | 0.17 | 49,49,49,49 | 0 |
| 60 | MG | a | 1630 | 1/1 | 0.91 | 0.31 | 44,44,44,44 | 0 |
| 60 | MG | A | 3045 | 1/1 | 0.91 | 0.35 | 20,20,20,20 | 0 |
| 60 | MG | A | 3245 | 1/1 | 0.91 | 0.18 | 45,45,45,45 | 0 |
| 60 | MG | A | 3256 | 1/1 | 0.91 | 0.50 | 62,62,62,62 | 0 |
| 60 | MG | A | 3334 | 1/1 | 0.91 | 0.37 | 57,57,57,57 | 0 |
| 60 | MG | a | 1706 | 1/1 | 0.91 | 0.11 | 48,48,48,48 | 0 |
| 60 | MG | A | 3435 | 1/1 | 0.91 | 0.33 | 51,51,51,51 | 0 |
| 60 | MG | a | 1712 | 1/1 | 0.91 | 0.25 | 54,54,54,54 | 0 |
| 60 | MG | N | 201 | 1/1 | 0.91 | 0.24 | 42,42,42,42 | 0 |
| 60 | MG | A | 3091 | 1/1 | 0.91 | 0.21 | 49,49,49,49 | 0 |
| 60 | MG | A | 3562 | 1/1 | 0.91 | 0.16 | 67,67,67,67 | 0 |
| 60 | MG | A | 3437 | 1/1 | 0.91 | 0.21 | 30,30,30,30 | 1 |
| 60 | MG | Q | 202 | 1/1 | 0.91 | 0.21 | 33,33,33,33 | 0 |
| 60 | MG | a | 1647 | 1/1 | 0.91 | 0.10 | 35,35,35,35 | 0 |
| 60 | MG | a | 1730 | 1/1 | 0.91 | 0.45 | 53,53,53,53 | 0 |
| 60 | MG | A | 3365 | 1/1 | 0.91 | 0.16 | 35,35,35,35 | 0 |
| 60 | MG | A | 3370 | 1/1 | 0.91 | 0.38 | 39,39,39,39 | 0 |
| 60 | MG | a | 1736 | 1/1 | 0.91 | 0.07 | 46,46,46,46 | 0 |
| 60 | MG | a | 1740 | 1/1 | 0.91 | 0.24 | 58,58,58,58 | 0 |
| 60 | MG | a | 1651 | 1/1 | 0.91 | 0.13 | 64,64,64,64 | 0 |
| 60 | MG | A | 3524 | 1/1 | 0.91 | 0.19 | 49,49,49,49 | 1 |
| 60 | MG | a | 1747 | 1/1 | 0.91 | 0.11 | 38,38,38,38 | 0 |
| 60 | MG | a | 1751 | 1/1 | 0.91 | 0.14 | 59,59,59,59 | 0 |
| 60 | MG | A | 3176 | 1/1 | 0.91 | 0.13 | 37,37,37,37 | 0 |
| 60 | MG | A | 3165 | 1/1 | 0.91 | 0.34 | 42,42,42,42 | 0 |
| 60 | MG | A | 3218 | 1/1 | 0.91 | 0.65 | 52,52,52,52 | 0 |
| 60 | MG | A | 3311 | 1/1 | 0.91 | 0.20 | 41,41,41,41 | 0 |
| 60 | MG | a | 1762 | 1/1 | 0.91 | 0.15 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3578 | 1/1 | 0.91 | 0.18 | 60,60,60,60 | 0 |
| 60 | MG | A | 3312 | 1/1 | 0.91 | 0.18 | 40,40,40,40 | 0 |
| 60 | MG | A | 3385 | 1/1 | 0.91 | 0.16 | 35,35,35,35 | 0 |
| 60 | MG | a | 1769 | 1/1 | 0.91 | 0.12 | 58,58,58,58 | 0 |
| 60 | MG | A | 3315 | 1/1 | 0.91 | 0.16 | 37,37,37,37 | 0 |
| 60 | MG | A | 3460 | 1/1 | 0.91 | 0.13 | 41,41,41,41 | 0 |
| 60 | MG | 8 | 101 | 1/1 | 0.91 | 0.21 | 35,35,35,35 | 0 |
| 60 | MG | 9 | 101 | 1/1 | 0.91 | 0.31 | 50,50,50,50 | 0 |
| 60 | MG | A | 3461 | 1/1 | 0.91 | 0.22 | 40,40,40,40 | 0 |
| 60 | MG | a | 1783 | 1/1 | 0.91 | 0.39 | 60,60,60,60 | 0 |
| 60 | MG | B | 205 | 1/1 | 0.91 | 0.15 | 52,52,52,52 | 0 |
| 60 | MG | A | 3058 | 1/1 | 0.91 | 0.21 | 59,59,59,59 | 0 |
| 60 | MG | A | 3392 | 1/1 | 0.91 | 0.17 | 42,42,42,42 | 0 |
| 60 | MG | a | 1787 | 1/1 | 0.91 | 0.90 | 40,40,40,40 | 1 |
| 60 | MG | A | 3346 | 1/1 | 0.91 | 0.21 | 57,57,57,57 | 0 |
| 60 | MG | A | 3400 | 1/1 | 0.91 | 0.35 | 42,42,42,42 | 0 |
| 60 | MG | A | 3203 | 1/1 | 0.91 | 0.26 | 52,52,52,52 | 0 |
| 60 | MG | A | 3403 | 1/1 | 0.91 | 0.20 | 37,37,37,37 | 0 |
| 60 | MG | n | 102 | 1/1 | 0.91 | 0.32 | 28,28,28,28 | 0 |
| 60 | MG | v | 101 | 1/1 | 0.91 | 0.36 | 35,35,35,35 | 1 |
| 60 | MG | A | 3598 | 1/1 | 0.91 | 0.18 | 29,29,29,29 | 0 |
| 60 | MG | a | 1680 | 1/1 | 0.91 | 0.33 | 60,60,60,60 | 0 |
| 60 | MG | A | 3035 | 1/1 | 0.91 | 0.40 | 30,30,30,30 | 1 |
| 60 | MG | a | 1682 | 1/1 | 0.91 | 0.20 | 45,45,45,45 | 0 |
| 60 | MG | A | 3493 | 1/1 | 0.91 | 0.25 | 48,48,48,48 | 1 |
| 60 | MG | a | 1685 | 1/1 | 0.91 | 0.16 | 46,46,46,46 | 0 |
| 60 | MG | a | 1695 | 1/1 | 0.92 | 0.41 | 40,40,40,40 | 0 |
| 60 | MG | D | 302 | 1/1 | 0.92 | 0.19 | 43,43,43,43 | 0 |
| 60 | MG | A | 3095 | 1/1 | 0.92 | 0.10 | 32,32,32,32 | 0 |
| 60 | MG | A | 3359 | 1/1 | 0.92 | 0.16 | 63,63,63,63 | 0 |
| 60 | MG | A | 3442 | 1/1 | 0.92 | 0.44 | 60,60,60,60 | 0 |
| 60 | MG | A | 3233 | 1/1 | 0.92 | 0.12 | 56,56,56,56 | 0 |
| 60 | MG | A | 3103 | 1/1 | 0.92 | 0.17 | 44,44,44,44 | 0 |
| 60 | MG | A | 3115 | 1/1 | 0.92 | 0.33 | 27,27,27,27 | 1 |
| 60 | MG | a | 1637 | 1/1 | 0.92 | 0.41 | 54,54,54,54 | 0 |
| 60 | MG | A | 3538 | 1/1 | 0.92 | 0.27 | 39,39,39,39 | 0 |
| 60 | MG | a | 1639 | 1/1 | 0.92 | 0.15 | 48,48,48,48 | 0 |
| 60 | MG | A | 3367 | 1/1 | 0.92 | 0.15 | 40,40,40,40 | 0 |
| 60 | MG | A | 3317 | 1/1 | 0.92 | 0.09 | 52,52,52,52 | 0 |
| 60 | MG | A | 3104 | 1/1 | 0.92 | 0.17 | 25,25,25,25 | 0 |
| 60 | MG | a | 1719 | 1/1 | 0.92 | 0.20 | 48,48,48,48 | 0 |
| 60 | MG | A | 3543 | 1/1 | 0.92 | 0.26 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3166 | 1/1 | 0.92 | 0.17 | 40,40,40,40 | 0 |
| 60 | MG | A | 3219 | 1/1 | 0.92 | 0.20 | 50,50,50,50 | 0 |
| 60 | MG | A | 3377 | 1/1 | 0.92 | 0.29 | 26,26,26,26 | 0 |
| 60 | MG | A | 3379 | 1/1 | 0.92 | 0.15 | 36,36,36,36 | 0 |
| 60 | MG | A | 3326 | 1/1 | 0.92 | 0.17 | 32,32,32,32 | 0 |
| 60 | MG | A | 3194 | 1/1 | 0.92 | 0.12 | 63,63,63,63 | 0 |
| 60 | MG | A | 3329 | 1/1 | 0.92 | 0.21 | 33,33,33,33 | 1 |
| 60 | MG | A | 3614 | 1/1 | 0.92 | 0.19 | 39,39,39,39 | 0 |
| 60 | MG | A | 3076 | 1/1 | 0.92 | 0.27 | 33,33,33,33 | 1 |
| 60 | MG | A | 3388 | 1/1 | 0.92 | 0.19 | 31,31,31,31 | 0 |
| 60 | MG | A | 3488 | 1/1 | 0.92 | 0.24 | 41,41,41,41 | 0 |
| 60 | MG | A | 3623 | 1/1 | 0.92 | 0.35 | 57,57,57,57 | 0 |
| 60 | MG | A | 3390 | 1/1 | 0.92 | 0.13 | 36,36,36,36 | 0 |
| 60 | MG | A | 3222 | 1/1 | 0.92 | 0.15 | 39,39,39,39 | 0 |
| 60 | MG | A | 3626 | 1/1 | 0.92 | 0.26 | 30,30,30,30 | 1 |
| 60 | MG | A | 3288 | 1/1 | 0.92 | 0.24 | 45,45,45,45 | 0 |
| 60 | MG | A | 3136 | 1/1 | 0.92 | 0.27 | 32,32,32,32 | 0 |
| 60 | MG | A | 3631 | 1/1 | 0.92 | 0.42 | 24,24,24,24 | 1 |
| 60 | MG | a | 1768 | 1/1 | 0.92 | 0.36 | 43,43,43,43 | 0 |
| 60 | MG | A | 3632 | 1/1 | 0.92 | 0.26 | 35,35,35,35 | 1 |
| 60 | MG | a | 1670 | 1/1 | 0.92 | 0.10 | 57,57,57,57 | 0 |
| 60 | MG | a | 1671 | 1/1 | 0.92 | 0.22 | 48,48,48,48 | 0 |
| 60 | MG | a | 1773 | 1/1 | 0.92 | 0.14 | 58,58,58,58 | 0 |
| 60 | MG | A | 3034 | 1/1 | 0.92 | 0.43 | 59,59,59,59 | 0 |
| 60 | MG | A | 3634 | 1/1 | 0.92 | 0.14 | 42,42,42,42 | 1 |
| 60 | MG | A | 3635 | 1/1 | 0.92 | 0.35 | 29,29,29,29 | 1 |
| 60 | MG | A | 3504 | 1/1 | 0.92 | 0.21 | 25,25,25,25 | 0 |
| 60 | MG | A | 3108 | 1/1 | 0.92 | 0.36 | 60,60,60,60 | 0 |
| 60 | MG | A | 3569 | 1/1 | 0.92 | 0.18 | 41,41,41,41 | 0 |
| 60 | MG | a | 1678 | 1/1 | 0.92 | 0.23 | 36,36,36,36 | 0 |
| 60 | MG | a | 1605 | 1/1 | 0.92 | 0.27 | 54,54,54,54 | 0 |
| 60 | MG | A | 3292 | 1/1 | 0.92 | 0.42 | 47,47,47,47 | 0 |
| 60 | MG | A | 3293 | 1/1 | 0.92 | 0.26 | 48,48,48,48 | 0 |
| 60 | MG | A | 3021 | 1/1 | 0.92 | 0.19 | 34,34,34,34 | 0 |
| 60 | MG | A | 3414 | 1/1 | 0.92 | 0.09 | 47,47,47,47 | 0 |
| 60 | MG | A | 3248 | 1/1 | 0.92 | 0.34 | 48,48,48,48 | 1 |
| 60 | MG | A | 3028 | 1/1 | 0.92 | 0.11 | 57,57,57,57 | 0 |
| 60 | MG | A | 3125 | 1/1 | 0.92 | 0.30 | 22,22,22,22 | 1 |
| 60 | MG | A | 3300 | 1/1 | 0.92 | 0.28 | 42,42,42,42 | 0 |
| 60 | MG | A | 3204 | 1/1 | 0.92 | 0.35 | 39,39,39,39 | 0 |
| 60 | MG | A | 3306 | 1/1 | 0.92 | 0.28 | 33,33,33,33 | 0 |
| 60 | MG | A | 3307 | 1/1 | 0.92 | 0.17 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3009 | 1/1 | 0.92 | 0.14 | 52,52,52,52 | 0 |
| 60 | MG | A | 3466 | 1/1 | 0.93 | 0.22 | 49,49,49,49 | 0 |
| 60 | MG | A | 3409 | 1/1 | 0.93 | 0.16 | 35,35,35,35 | 0 |
| 60 | MG | A | 3048 | 1/1 | 0.93 | 0.15 | 35,35,35,35 | 0 |
| 60 | MG | A | 3189 | 1/1 | 0.93 | 0.31 | 50,50,50,50 | 0 |
| 60 | MG | A | 3476 | 1/1 | 0.93 | 0.09 | 58,58,58,58 | 0 |
| 60 | MG | A | 3019 | 1/1 | 0.93 | 0.31 | 20,20,20,20 | 0 |
| 60 | MG | A | 3482 | 1/1 | 0.93 | 0.25 | 38,38,38,38 | 0 |
| 60 | MG | G | 201 | 1/1 | 0.93 | 0.21 | 48,48,48,48 | 0 |
| 60 | MG | A | 3285 | 1/1 | 0.93 | 0.31 | 31,31,31,31 | 0 |
| 60 | MG | a | 1714 | 1/1 | 0.93 | 0.44 | 54,54,54,54 | 0 |
| 60 | MG | A | 3427 | 1/1 | 0.93 | 0.20 | 49,49,49,49 | 0 |
| 60 | MG | A | 3428 | 1/1 | 0.93 | 0.19 | 56,56,56,56 | 0 |
| 60 | MG | A | 3494 | 1/1 | 0.93 | 0.20 | 35,35,35,35 | 0 |
| 60 | MG | A | 3553 | 1/1 | 0.93 | 0.25 | 51,51,51,51 | 1 |
| 60 | MG | A | 3287 | 1/1 | 0.93 | 0.20 | 35,35,35,35 | 0 |
| 60 | MG | a | 1649 | 1/1 | 0.93 | 0.43 | 67,67,67,67 | 0 |
| 60 | MG | A | 3431 | 1/1 | 0.93 | 0.31 | 52,52,52,52 | 0 |
| 60 | MG | A | 3500 | 1/1 | 0.93 | 0.20 | 30,30,30,30 | 0 |
| 60 | MG | A | 3020 | 1/1 | 0.93 | 0.18 | 26,26,26,26 | 0 |
| 60 | MG | A | 3313 | 1/1 | 0.93 | 0.17 | 29,29,29,29 | 0 |
| 60 | MG | A | 3193 | 1/1 | 0.93 | 0.22 | 27,27,27,27 | 0 |
| 60 | MG | A | 3561 | 1/1 | 0.93 | 0.20 | 60,60,60,60 | 0 |
| 60 | MG | a | 1658 | 1/1 | 0.93 | 0.12 | 30,30,30,30 | 0 |
| 60 | MG | A | 3507 | 1/1 | 0.93 | 0.13 | 42,42,42,42 | 0 |
| 60 | MG | X | 101 | 1/1 | 0.93 | 0.25 | 50,50,50,50 | 0 |
| 60 | MG | A | 3508 | 1/1 | 0.93 | 0.11 | 68,68,68,68 | 0 |
| 60 | MG | a | 1753 | 1/1 | 0.93 | 0.32 | 46,46,46,46 | 0 |
| 60 | MG | a | 1754 | 1/1 | 0.93 | 0.12 | 42,42,42,42 | 0 |
| 60 | MG | a | 1755 | 1/1 | 0.93 | 0.08 | 40,40,40,40 | 0 |
| 60 | MG | A | 3566 | 1/1 | 0.93 | 0.44 | 55,55,55,55 | 0 |
| 60 | MG | A | 3381 | 1/1 | 0.93 | 0.16 | 56,56,56,56 | 0 |
| 60 | MG | 5 | 101 | 1/1 | 0.93 | 0.30 | 44,44,44,44 | 1 |
| 60 | MG | A | 3207 | 1/1 | 0.93 | 0.32 | 61,61,61,61 | 0 |
| 60 | MG | A | 3345 | 1/1 | 0.93 | 0.26 | 48,48,48,48 | 0 |
| 60 | MG | A | 3093 | 1/1 | 0.93 | 0.30 | 50,50,50,50 | 0 |
| 60 | MG | A | 3347 | 1/1 | 0.93 | 0.27 | 37,37,37,37 | 1 |
| 60 | MG | A | 3349 | 1/1 | 0.93 | 0.18 | 42,42,42,42 | 0 |
| 60 | MG | A | 3575 | 1/1 | 0.93 | 0.29 | 39,39,39,39 | 1 |
| 60 | MG | A | 3641 | 1/1 | 0.93 | 0.17 | 32,32,32,32 | 1 |
| 60 | MG | A | 3195 | 1/1 | 0.93 | 0.47 | 55,55,55,55 | 0 |
| 60 | MG | A | 3210 | 1/1 | 0.93 | 0.56 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60 | MG | A | 3452 | 1/1 | 0.93 | 0.07 | 69,69,69,69 | 0 |
| 60 | MG | a | 1777 | 1/1 | 0.93 | 0.28 | 32,32,32,32 | 1 |
| 60 | MG | a | 1778 | 1/1 | 0.93 | 0.26 | 53,53,53,53 | 0 |
| 60 | MG | A | 3211 | 1/1 | 0.93 | 0.23 | 50,50,50,50 | 0 |
| 60 | MG | A | 3455 | 1/1 | 0.93 | 0.27 | 28,28,28,28 | 0 |
| 60 | MG | A | 3325 | 1/1 | 0.93 | 0.14 | 23,23,23,23 | 0 |
| 60 | MG | A | 3583 | 1/1 | 0.93 | 0.21 | 46,46,46,46 | 0 |
| 60 | MG | A | 3457 | 1/1 | 0.93 | 0.18 | 24,24,24,24 | 0 |
| 60 | MG | A | 3156 | 1/1 | 0.93 | 0.19 | 26,26,26,26 | 0 |
| 60 | MG | A | 3149 | 1/1 | 0.93 | 0.08 | 54,54,54,54 | 0 |
| 60 | MG | a | 1617 | 1/1 | 0.93 | 0.38 | 47,47,47,47 | 0 |
| 60 | MG | a | 1619 | 1/1 | 0.93 | 0.27 | 32,32,32,32 | 0 |
| 60 | MG | A | 3007 | 1/1 | 0.93 | 0.21 | 35,35,35,35 | 0 |
| 60 | MG | A | 3134 | 1/1 | 0.93 | 0.19 | 25,25,25,25 | 0 |
| 60 | MG | a | 1623 | 1/1 | 0.93 | 0.22 | 46,46,46,46 | 1 |
| 60 | MG | A | 3463 | 1/1 | 0.93 | 0.68 | 48,48,48,48 | 0 |
| 60 | MG | x | 101 | 1/1 | 0.93 | 0.33 | 29,29,29,29 | 1 |
| 60 | MG | A | 3464 | 1/1 | 0.93 | 0.13 | 56,56,56,56 | 0 |
| 60 | MG | A | 3596 | 1/1 | 0.93 | 0.25 | 44,44,44,44 | 1 |
| 60 | MG | x | 107 | 1/1 | 0.93 | 0.09 | 69,69,69,69 | 0 |
| 60 | MG | D | 306 | 1/1 | 0.93 | 0.16 | 25,25,25,25 | 0 |
| 60 | MG | A | 3539 | 1/1 | 0.93 | 0.17 | 21,21,21,21 | 0 |
| 60 | MG | a | 1696 | 1/1 | 0.93 | 0.49 | 52,52,52,52 | 0 |
| 60 | MG | A | 3303 | 1/1 | 0.93 | 0.17 | 57,57,57,57 | 0 |
| 60 | MG | A | 3364 | 1/1 | 0.94 | 0.10 | 45,45,45,45 | 0 |
| 60 | MG | A | 3621 | 1/1 | 0.94 | 0.31 | 48,48,48,48 | 0 |
| 60 | MG | A | 3078 | 1/1 | 0.94 | 0.33 | 27,27,27,27 | 1 |
| 60 | MG | a | 1737 | 1/1 | 0.94 | 0.35 | 46,46,46,46 | 0 |
| 60 | MG | a | 1739 | 1/1 | 0.94 | 0.17 | 42,42,42,42 | 0 |
| 60 | MG | a | 1618 | 1/1 | 0.94 | 0.54 | 54,54,54,54 | 0 |
| 60 | MG | A | 3498 | 1/1 | 0.94 | 0.15 | 68,68,68,68 | 0 |
| 60 | MG | A | 3185 | 1/1 | 0.94 | 0.22 | 32,32,32,32 | 0 |
| 60 | MG | a | 1745 | 1/1 | 0.94 | 0.21 | 40,40,40,40 | 0 |
| 60 | MG | A | 3304 | 1/1 | 0.94 | 0.13 | 53,53,53,53 | 0 |
| 60 | MG | A | 3126 | 1/1 | 0.94 | 0.28 | 28,28,28,28 | 1 |
| 60 | MG | a | 1624 | 1/1 | 0.94 | 0.14 | 39,39,39,39 | 0 |
| 60 | MG | A | 3372 | 1/1 | 0.94 | 0.20 | 41,41,41,41 | 0 |
| 60 | MG | A | 3327 | 1/1 | 0.94 | 0.23 | 30,30,30,30 | 0 |
| 60 | MG | A | 3214 | 1/1 | 0.94 | 0.52 | 44,44,44,44 | 1 |
| 60 | MG | A | 3584 | 1/1 | 0.94 | 0.13 | 39,39,39,39 | 0 |
| 60 | MG | A | 3131 | 1/1 | 0.94 | 0.20 | 57,57,57,57 | 0 |
| 60 | MG | A | 3547 | 1/1 | 0.94 | 0.10 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3331 | 1/1 | 0.94 | 0.21 | 31,31,31,31 | 0 |
| 60 | MG | A | 3637 | 1/1 | 0.94 | 0.45 | 37,37,37,37 | 0 |
| 60 | MG | a | 1634 | 1/1 | 0.94 | 0.35 | 53,53,53,53 | 0 |
| 60 | MG | a | 1766 | 1/1 | 0.94 | 0.24 | 49,49,49,49 | 0 |
| 60 | MG | A | 3175 | 1/1 | 0.94 | 0.19 | 62,62,62,62 | 0 |
| 60 | MG | A | 3352 | 1/1 | 0.94 | 0.36 | 39,39,39,39 | 0 |
| 60 | MG | A | 3516 | 1/1 | 0.94 | 0.19 | 25,25,25,25 | 1 |
| 60 | MG | A | 3053 | 1/1 | 0.94 | 0.27 | 35,35,35,35 | 0 |
| 60 | MG | A | 3643 | 1/1 | 0.94 | 0.29 | 34,34,34,34 | 0 |
| 60 | MG | A | 3192 | 1/1 | 0.94 | 0.18 | 26,26,26,26 | 0 |
| 60 | MG | a | 1774 | 1/1 | 0.94 | 0.14 | 29,29,29,29 | 0 |
| 60 | MG | A | 3432 | 1/1 | 0.94 | 0.16 | 54,54,54,54 | 0 |
| 60 | MG | A | 3386 | 1/1 | 0.94 | 0.24 | 33,33,33,33 | 0 |
| 60 | MG | 0 | 103 | 1/1 | 0.94 | 0.08 | 53,53,53,53 | 0 |
| 60 | MG | A | 3469 | 1/1 | 0.94 | 0.12 | 48,48,48,48 | 0 |
| 60 | MG | A | 3523 | 1/1 | 0.94 | 0.28 | 31,31,31,31 | 0 |
| 60 | MG | A | 3205 | 1/1 | 0.94 | 0.17 | 53,53,53,53 | 0 |
| 60 | MG | 6 | 103 | 1/1 | 0.94 | 0.17 | 41,41,41,41 | 0 |
| 60 | MG | A | 3138 | 1/1 | 0.94 | 0.12 | 31,31,31,31 | 0 |
| 60 | MG | A | 3605 | 1/1 | 0.94 | 0.36 | 50,50,50,50 | 0 |
| 60 | MG | A | 3526 | 1/1 | 0.94 | 0.20 | 29,29,29,29 | 0 |
| 60 | MG | a | 1707 | 1/1 | 0.94 | 0.16 | 34,34,34,34 | 0 |
| 60 | MG | A | 3139 | 1/1 | 0.94 | 0.30 | 37,37,37,37 | 0 |
| 60 | MG | a | 1710 | 1/1 | 0.94 | 0.34 | 53,53,53,53 | 1 |
| 60 | MG | a | 1711 | 1/1 | 0.94 | 0.18 | 48,48,48,48 | 0 |
| 60 | MG | A | 3608 | 1/1 | 0.94 | 0.23 | 32,32,32,32 | 0 |
| 60 | MG | n | 103 | 1/1 | 0.94 | 0.31 | 55,55,55,55 | 0 |
| 60 | MG | A | 3478 | 1/1 | 0.94 | 0.34 | 50,50,50,50 | 0 |
| 60 | MG | v | 102 | 1/1 | 0.94 | 0.30 | 42,42,42,42 | 0 |
| 60 | MG | A | 3564 | 1/1 | 0.94 | 0.13 | 52,52,52,52 | 0 |
| 60 | MG | x | 102 | 1/1 | 0.94 | 0.07 | 77,77,77,77 | 0 |
| 60 | MG | A | 3140 | 1/1 | 0.94 | 0.19 | 48,48,48,48 | 0 |
| 60 | MG | x | 105 | 1/1 | 0.94 | 0.12 | 51,51,51,51 | 0 |
| 60 | MG | A | 3128 | 1/1 | 0.94 | 0.26 | 37,37,37,37 | 0 |
| 60 | MG | A | 3393 | 1/1 | 0.94 | 0.28 | 41,41,41,41 | 0 |
| 60 | MG | A | 3533 | 1/1 | 0.94 | 0.41 | 52,52,52,52 | 0 |
| 60 | MG | A | 3363 | 1/1 | 0.94 | 0.21 | 35,35,35,35 | 0 |
| 60 | MG | a | 1613 | 1/1 | 0.94 | 0.26 | 29,29,29,29 | 0 |
| 60 | MG | A | 3398 | 1/1 | 0.94 | 0.10 | 37,37,37,37 | 0 |
| 60 | MG | A | 3074 | 1/1 | 0.95 | 0.15 | 29,29,29,29 | 0 |
| 60 | MG | B | 218 | 1/1 | 0.95 | 0.27 | 49,49,49,49 | 0 |
| 60 | MG | A | 3426 | 1/1 | 0.95 | 0.15 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | a | 1668 | 1/1 | 0.95 | 0.18 | 30,30,30,30 | 0 |
| 60 | MG | A | 3357 | 1/1 | 0.95 | 0.48 | 36,36,36,36 | 0 |
| 60 | MG | A | 3522 | 1/1 | 0.95 | 0.21 | 28,28,28,28 | 0 |
| 60 | MG | D | 305 | 1/1 | 0.95 | 0.43 | 43,43,43,43 | 0 |
| 60 | MG | a | 1749 | 1/1 | 0.95 | 0.33 | 54,54,54,54 | 0 |
| 60 | MG | a | 1750 | 1/1 | 0.95 | 0.22 | 41,41,41,41 | 0 |
| 60 | MG | A | 3467 | 1/1 | 0.95 | 0.21 | 37,37,37,37 | 0 |
| 60 | MG | A | 3069 | 1/1 | 0.95 | 0.24 | 30,30,30,30 | 0 |
| 60 | MG | A | 3027 | 1/1 | 0.95 | 0.14 | 62,62,62,62 | 0 |
| 60 | MG | A | 3567 | 1/1 | 0.95 | 0.15 | 38,38,38,38 | 1 |
| 60 | MG | A | 3186 | 1/1 | 0.95 | 0.13 | 33,33,33,33 | 0 |
| 60 | MG | a | 1757 | 1/1 | 0.95 | 0.24 | 46,46,46,46 | 0 |
| 60 | MG | A | 3616 | 1/1 | 0.95 | 0.18 | 45,45,45,45 | 0 |
| 60 | MG | A | 3473 | 1/1 | 0.95 | 0.18 | 27,27,27,27 | 0 |
| 60 | MG | a | 1760 | 1/1 | 0.95 | 0.17 | 38,38,38,38 | 0 |
| 60 | MG | A | 3570 | 1/1 | 0.95 | 0.17 | 54,54,54,54 | 0 |
| 60 | MG | A | 3389 | 1/1 | 0.95 | 0.10 | 33,33,33,33 | 0 |
| 60 | MG | A | 3294 | 1/1 | 0.95 | 0.18 | 25,25,25,25 | 1 |
| 60 | MG | A | 3622 | 1/1 | 0.95 | 0.35 | 57,57,57,57 | 0 |
| 60 | MG | A | 3434 | 1/1 | 0.95 | 0.23 | 41,41,41,41 | 0 |
| 60 | MG | a | 1684 | 1/1 | 0.95 | 0.14 | 31,31,31,31 | 0 |
| 60 | MG | A | 3279 | 1/1 | 0.95 | 0.29 | 30,30,30,30 | 1 |
| 60 | MG | A | 3481 | 1/1 | 0.95 | 0.13 | 46,46,46,46 | 0 |
| 60 | MG | A | 3187 | 1/1 | 0.95 | 0.40 | 31,31,31,31 | 0 |
| 60 | MG | a | 1771 | 1/1 | 0.95 | 0.13 | 67,67,67,67 | 0 |
| 60 | MG | A | 3485 | 1/1 | 0.95 | 0.16 | 59,59,59,59 | 0 |
| 60 | MG | A | 3628 | 1/1 | 0.95 | 0.30 | 35,35,35,35 | 0 |
| 60 | MG | A | 3629 | 1/1 | 0.95 | 0.17 | 21,21,21,21 | 0 |
| 60 | MG | A | 3174 | 1/1 | 0.95 | 0.26 | 25,25,25,25 | 0 |
| 60 | MG | A | 3105 | 1/1 | 0.95 | 0.25 | 28,28,28,28 | 1 |
| 60 | MG | A | 3397 | 1/1 | 0.95 | 0.27 | 38,38,38,38 | 0 |
| 60 | MG | A | 3368 | 1/1 | 0.95 | 0.21 | 36,36,36,36 | 0 |
| 60 | MG | A | 3323 | 1/1 | 0.95 | 0.15 | 72,72,72,72 | 0 |
| 60 | MG | A | 3241 | 1/1 | 0.95 | 0.22 | 20,20,20,20 | 0 |
| 60 | MG | A | 3301 | 1/1 | 0.95 | 0.29 | 54,54,54,54 | 0 |
| 60 | MG | A | 3033 | 1/1 | 0.95 | 0.26 | 59,59,59,59 | 1 |
| 60 | MG | A | 3405 | 1/1 | 0.95 | 0.29 | 32,32,32,32 | 0 |
| 60 | MG | a | 1646 | 1/1 | 0.95 | 0.20 | 52,52,52,52 | 0 |
| 60 | MG | A | 3215 | 1/1 | 0.95 | 0.42 | 44,44,44,44 | 0 |
| 60 | MG | A | 3454 | 1/1 | 0.95 | 0.42 | 44,44,44,44 | 0 |
| 60 | MG | 0 | 104 | 1/1 | 0.95 | 0.40 | 36,36,36,36 | 1 |
| 60 | MG | l | 201 | 1/1 | 0.95 | 0.22 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3408 | 1/1 | 0.95 | 0.27 | 33,33,33,33 | 0 |
| 60 | MG | A | 3286 | 1/1 | 0.95 | 0.49 | 48,48,48,48 | 0 |
| 60 | MG | a | 1652 | 1/1 | 0.95 | 0.18 | 20,20,20,20 | 0 |
| 60 | MG | A | 3595 | 1/1 | 0.95 | 0.27 | 27,27,27,27 | 0 |
| 60 | MG | A | 3410 | 1/1 | 0.95 | 0.23 | 44,44,44,44 | 0 |
| 60 | MG | a | 1655 | 1/1 | 0.95 | 0.40 | 47,47,47,47 | 0 |
| 60 | MG | A | 3061 | 1/1 | 0.95 | 0.28 | 43,43,43,43 | 0 |
| 60 | MG | A | 3513 | 1/1 | 0.95 | 0.18 | 58,58,58,58 | 0 |
| 60 | MG | A | 3416 | 1/1 | 0.95 | 0.17 | 31,31,31,31 | 0 |
| 60 | MG | A | 3601 | 1/1 | 0.95 | 0.24 | 33,33,33,33 | 0 |
| 60 | MG | B | 208 | 1/1 | 0.95 | 0.08 | 64,64,64,64 | 0 |
| 60 | MG | A | 3515 | 1/1 | 0.95 | 0.28 | 47,47,47,47 | 0 |
| 60 | MG | A | 3417 | 1/1 | 0.95 | 0.28 | 43,43,43,43 | 0 |
| 60 | MG | A | 3123 | 1/1 | 0.95 | 0.22 | 30,30,30,30 | 1 |
| 60 | MG | A | 3168 | 1/1 | 0.95 | 0.22 | 23,23,23,23 | 0 |
| 61 | ZN | 4 | 501 | 1/1 | 0.95 | 0.06 | 79,79,79,79 | 0 |
| 61 | ZN | 6 | 102 | 1/1 | 0.95 | 0.25 | 72,72,72,72 | 0 |
| 62 | SF4 | d | 302 | 8/8 | 0.95 | 0.05 | 60,65,70,71 | 2 |
| 60 | MG | E | 302 | 1/1 | 0.96 | 0.29 | 32,32,32,32 | 0 |
| 60 | MG | A | 3230 | 1/1 | 0.96 | 0.26 | 40,40,40,40 | 0 |
| 60 | MG | a | 1756 | 1/1 | 0.96 | 0.15 | 52,52,52,52 | 0 |
| 60 | MG | a | 1692 | 1/1 | 0.96 | 0.25 | 41,41,41,41 | 0 |
| 60 | MG | A | 3529 | 1/1 | 0.96 | 0.12 | 59,59,59,59 | 0 |
| 60 | MG | A | 3495 | 1/1 | 0.96 | 0.16 | 35,35,35,35 | 0 |
| 60 | MG | A | 3030 | 1/1 | 0.96 | 0.18 | 33,33,33,33 | 0 |
| 60 | MG | A | 3298 | 1/1 | 0.96 | 0.20 | 34,34,34,34 | 0 |
| 60 | MG | A | 3366 | 1/1 | 0.96 | 0.15 | 19,19,19,19 | 1 |
| 60 | MG | A | 3337 | 1/1 | 0.96 | 0.29 | 48,48,48,48 | 0 |
| 60 | MG | a | 1700 | 1/1 | 0.96 | 0.25 | 50,50,50,50 | 0 |
| 60 | MG | A | 3077 | 1/1 | 0.96 | 0.31 | 24,24,24,24 | 1 |
| 60 | MG | A | 3412 | 1/1 | 0.96 | 0.21 | 44,44,44,44 | 0 |
| 60 | MG | A | 3440 | 1/1 | 0.96 | 0.13 | 45,45,45,45 | 0 |
| 60 | MG | A | 3640 | 1/1 | 0.96 | 0.14 | 30,30,30,30 | 1 |
| 60 | MG | A | 3506 | 1/1 | 0.96 | 0.33 | 41,41,41,41 | 0 |
| 60 | MG | A | 3116 | 1/1 | 0.96 | 0.24 | 47,47,47,47 | 0 |
| 60 | MG | O | 202 | 1/1 | 0.96 | 0.16 | 50,50,50,50 | 0 |
| 60 | MG | A | 3340 | 1/1 | 0.96 | 0.24 | 45,45,45,45 | 0 |
| 60 | MG | a | 1621 | 1/1 | 0.96 | 0.10 | 64,64,64,64 | 0 |
| 60 | MG | A | 3470 | 1/1 | 0.96 | 0.22 | 51,51,51,51 | 0 |
| 60 | MG | Q | 201 | 1/1 | 0.96 | 0.45 | 47,47,47,47 | 0 |
| 60 | MG | A | 3046 | 1/1 | 0.96 | 0.15 | 29,29,29,29 | 0 |
| 60 | MG | B | 203 | 1/1 | 0.96 | 0.07 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60 | MG | a | 1780 | 1/1 | 0.96 | 0.23 | 54,54,54,54 | 0 |
| 60 | MG | a | 1716 | 1/1 | 0.96 | 0.16 | 36,36,36,36 | 0 |
| 60 | MG | A | 3472 | 1/1 | 0.96 | 0.47 | 25,25,25,25 | 0 |
| 60 | MG | A | 3373 | 1/1 | 0.96 | 0.25 | 34,34,34,34 | 0 |
| 60 | MG | A | 3419 | 1/1 | 0.96 | 0.26 | 30,30,30,30 | 1 |
| 60 | MG | A | 3162 | 1/1 | 0.96 | 0.19 | 29,29,29,29 | 0 |
| 60 | MG | a | 1722 | 1/1 | 0.96 | 0.15 | 51,51,51,51 | 0 |
| 60 | MG | a | 1723 | 1/1 | 0.96 | 0.27 | 48,48,48,48 | 0 |
| 60 | MG | A | 3422 | 1/1 | 0.96 | 0.20 | 52,52,52,52 | 0 |
| 60 | MG | a | 1729 | 1/1 | 0.96 | 0.35 | 50,50,50,50 | 0 |
| 60 | MG | A | 3479 | 1/1 | 0.96 | 0.10 | 41,41,41,41 | 0 |
| 60 | MG | m | 201 | 1/1 | 0.96 | 0.22 | 38,38,38,38 | 1 |
| 60 | MG | A | 3619 | 1/1 | 0.96 | 0.30 | 16,16,16,16 | 0 |
| 60 | MG | a | 1633 | 1/1 | 0.96 | 0.21 | 32,32,32,32 | 0 |
| 60 | MG | a | 1735 | 1/1 | 0.96 | 0.15 | 37,37,37,37 | 0 |
| 60 | MG | A | 3395 | 1/1 | 0.96 | 0.29 | 51,51,51,51 | 0 |
| 60 | MG | B | 213 | 1/1 | 0.96 | 0.17 | 52,52,52,52 | 0 |
| 60 | MG | B | 214 | 1/1 | 0.96 | 0.07 | 59,59,59,59 | 0 |
| 60 | MG | A | 3330 | 1/1 | 0.96 | 0.34 | 37,37,37,37 | 1 |
| 60 | MG | A | 3005 | 1/1 | 0.96 | 0.17 | 31,31,31,31 | 1 |
| 60 | MG | A | 3360 | 1/1 | 0.96 | 0.19 | 54,54,54,54 | 0 |
| 60 | MG | a | 1743 | 1/1 | 0.96 | 0.31 | 45,45,45,45 | 0 |
| 60 | MG | A | 3023 | 1/1 | 0.96 | 0.17 | 34,34,34,34 | 0 |
| 60 | MG | a | 1746 | 1/1 | 0.96 | 0.09 | 49,49,49,49 | 0 |
| 60 | MG | A | 3489 | 1/1 | 0.96 | 0.26 | 27,27,27,27 | 0 |
| 60 | MG | A | 3490 | 1/1 | 0.96 | 0.12 | 40,40,40,40 | 0 |
| 60 | MG | A | 3113 | 1/1 | 0.96 | 0.25 | 29,29,29,29 | 1 |
| 61 | ZN | Y | 501 | 1/1 | 0.96 | 0.05 | 63,63,63,63 | 0 |
| 60 | MG | A | 3558 | 1/1 | 0.96 | 0.24 | 53,53,53,53 | 0 |
| 60 | MG | a | 1645 | 1/1 | 0.96 | 0.20 | 42,42,42,42 | 0 |
| 60 | MG | A | 3459 | 1/1 | 0.96 | 0.24 | 33,33,33,33 | 0 |
| 63 | GCP | z | 703 | 32/32 | 0.96 | 0.15 | 47,57,62,63 | 13 |
| 60 | MG | A | 3376 | 1/1 | 0.97 | 0.14 | 31,31,31,31 | 0 |
| 60 | MG | A | 3173 | 1/1 | 0.97 | 0.65 | 37,37,37,37 | 0 |
| 60 | MG | A | 3378 | 1/1 | 0.97 | 0.31 | 41,41,41,41 | 0 |
| 60 | MG | A | 3062 | 1/1 | 0.97 | 0.16 | 41,41,41,41 | 0 |
| 60 | MG | P | 203 | 1/1 | 0.97 | 0.28 | 45,45,45,45 | 1 |
| 60 | MG | B | 202 | 1/1 | 0.97 | 0.14 | 52,52,52,52 | 0 |
| 60 | MG | A | 3380 | 1/1 | 0.97 | 0.18 | 45,45,45,45 | 0 |
| 60 | MG | A | 3017 | 1/1 | 0.97 | 0.28 | 41,41,41,41 | 0 |
| 60 | MG | A | 3261 | 1/1 | 0.97 | 0.19 | 46,46,46,46 | 0 |
| 60 | MG | A | 3383 | 1/1 | 0.97 | 0.10 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3216 | 1/1 | 0.97 | 0.38 | 31,31,31,31 | 0 |
| 60 | MG | A | 3031 | 1/1 | 0.97 | 0.20 | 33,33,33,33 | 0 |
| 60 | MG | A | 3177 | 1/1 | 0.97 | 0.37 | 39,39,39,39 | 0 |
| 60 | MG | B | 210 | 1/1 | 0.97 | 0.13 | 44,44,44,44 | 0 |
| 60 | MG | a | 1776 | 1/1 | 0.97 | 0.25 | 52,52,52,52 | 0 |
| 60 | MG | A | 3411 | 1/1 | 0.97 | 0.15 | 39,39,39,39 | 0 |
| 60 | MG | A | 3439 | 1/1 | 0.97 | 0.25 | 50,50,50,50 | 0 |
| 60 | MG | a | 1726 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 60 | MG | a | 1728 | 1/1 | 0.97 | 0.13 | 33,33,33,33 | 0 |
| 60 | MG | a | 1781 | 1/1 | 0.97 | 0.23 | 46,46,46,46 | 0 |
| 60 | MG | A | 3302 | 1/1 | 0.97 | 0.15 | 22,22,22,22 | 0 |
| 60 | MG | A | 3413 | 1/1 | 0.97 | 0.13 | 35,35,35,35 | 0 |
| 60 | MG | A | 3178 | 1/1 | 0.97 | 0.40 | 56,56,56,56 | 0 |
| 60 | MG | A | 3582 | 1/1 | 0.97 | 0.19 | 21,21,21,21 | 1 |
| 60 | MG | a | 1733 | 1/1 | 0.97 | 0.28 | 51,51,51,51 | 0 |
| 60 | MG | B | 217 | 1/1 | 0.97 | 0.13 | 40,40,40,40 | 0 |
| 60 | MG | A | 3415 | 1/1 | 0.97 | 0.11 | 34,34,34,34 | 0 |
| 60 | MG | D | 301 | 1/1 | 0.97 | 0.26 | 21,21,21,21 | 0 |
| 60 | MG | a | 1738 | 1/1 | 0.97 | 0.17 | 35,35,35,35 | 0 |
| 60 | MG | A | 3445 | 1/1 | 0.97 | 0.26 | 42,42,42,42 | 1 |
| 60 | MG | A | 3475 | 1/1 | 0.97 | 0.15 | 41,41,41,41 | 0 |
| 60 | MG | m | 202 | 1/1 | 0.97 | 0.31 | 56,56,56,56 | 0 |
| 60 | MG | A | 3446 | 1/1 | 0.97 | 0.24 | 26,26,26,26 | 0 |
| 60 | MG | A | 3477 | 1/1 | 0.97 | 0.22 | 21,21,21,21 | 0 |
| 60 | MG | A | 3447 | 1/1 | 0.97 | 0.21 | 47,47,47,47 | 0 |
| 60 | MG | a | 1744 | 1/1 | 0.97 | 0.16 | 46,46,46,46 | 0 |
| 60 | MG | A | 3590 | 1/1 | 0.97 | 0.29 | 63,63,63,63 | 0 |
| 60 | MG | A | 3198 | 1/1 | 0.97 | 0.10 | 20,20,20,20 | 0 |
| 60 | MG | A | 3322 | 1/1 | 0.97 | 0.18 | 42,42,42,42 | 1 |
| 60 | MG | a | 1748 | 1/1 | 0.97 | 0.07 | 46,46,46,46 | 0 |
| 60 | MG | A | 3145 | 1/1 | 0.97 | 0.41 | 61,61,61,61 | 0 |
| 60 | MG | A | 3594 | 1/1 | 0.97 | 0.34 | 85,85,85,85 | 0 |
| 60 | MG | A | 3451 | 1/1 | 0.97 | 0.29 | 45,45,45,45 | 0 |
| 60 | MG | A | 3355 | 1/1 | 0.97 | 0.17 | 61,61,61,61 | 0 |
| 60 | MG | A | 3487 | 1/1 | 0.97 | 0.21 | 35,35,35,35 | 0 |
| 60 | MG | A | 3324 | 1/1 | 0.97 | 0.11 | 38,38,38,38 | 0 |
| 60 | MG | A | 3421 | 1/1 | 0.97 | 0.14 | 57,57,57,57 | 0 |
| 60 | MG | a | 1702 | 1/1 | 0.97 | 0.48 | 42,42,42,42 | 0 |
| 60 | MG | A | 3600 | 1/1 | 0.97 | 0.08 | 53,53,53,53 | 0 |
| 61 | ZN | 5 | 103 | 1/1 | 0.97 | 0.08 | 54,54,54,54 | 0 |
| 60 | MG | A | 3120 | 1/1 | 0.97 | 0.33 | 26,26,26,26 | 0 |
| 61 | ZN | 9 | 102 | 1/1 | 0.97 | 0.19 | 49,49,49,49 | 1 |

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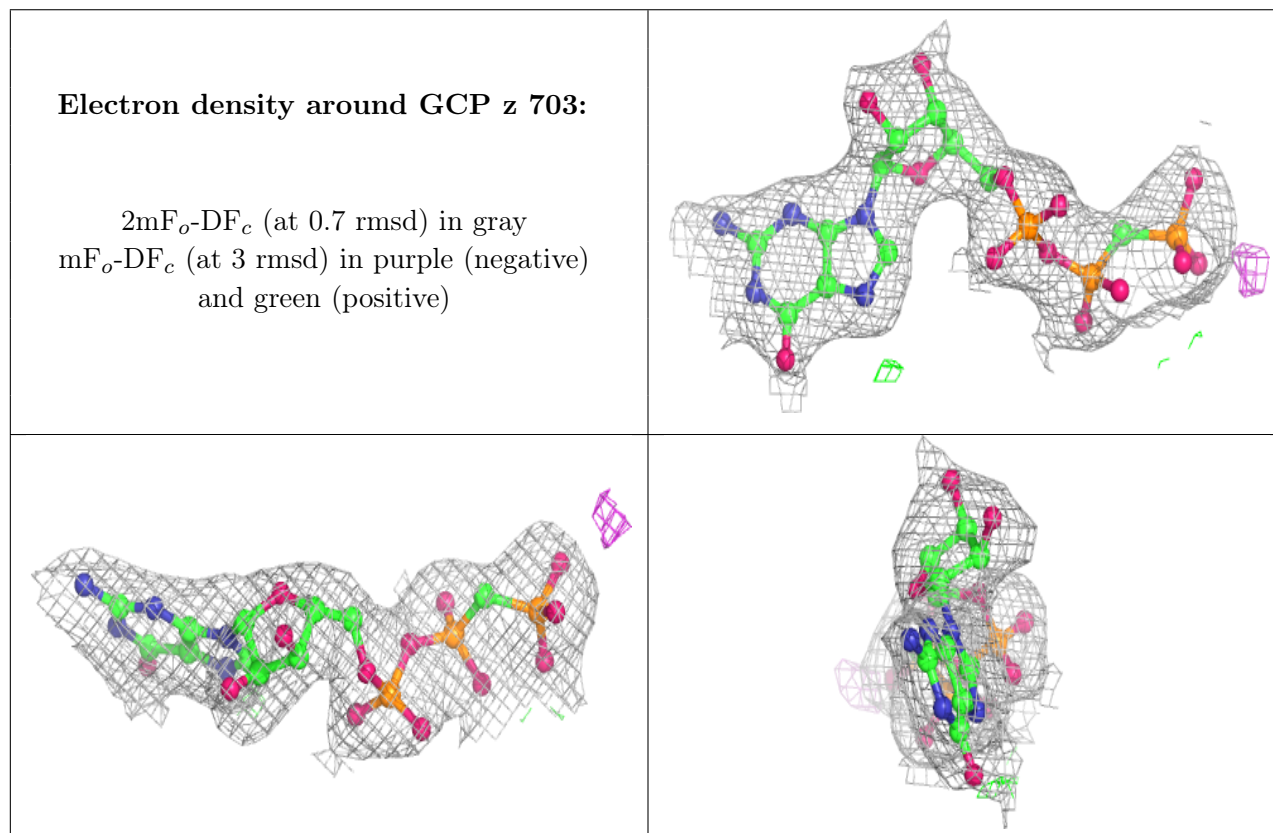
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3491 | 1/1 | 0.97 | 0.34 | 39,39,39,39 | 0 |
| 60 | MG | A | 3032 | 1/1 | 0.97 | 0.27 | 50,50,50,50 | 0 |
| 60 | MG | a | 1734 | 1/1 | 0.98 | 0.09 | 33,33,33,33 | 0 |
| 60 | MG | A | 3503 | 1/1 | 0.98 | 0.21 | 53,53,53,53 | 0 |
| 60 | MG | A | 3565 | 1/1 | 0.98 | 0.12 | 35,35,35,35 | 0 |
| 60 | MG | A | 3534 | 1/1 | 0.98 | 0.23 | 35,35,35,35 | 0 |
| 60 | MG | A | 3051 | 1/1 | 0.98 | 0.31 | 54,54,54,54 | 0 |
| 60 | MG | A | 3036 | 1/1 | 0.98 | 0.25 | 25,25,25,25 | 1 |
| 60 | MG | a | 1699 | 1/1 | 0.98 | 0.26 | 56,56,56,56 | 0 |
| 60 | MG | A | 3318 | 1/1 | 0.98 | 0.17 | 42,42,42,42 | 1 |
| 60 | MG | A | 3096 | 1/1 | 0.98 | 0.14 | 27,27,27,27 | 0 |
| 60 | MG | A | 3348 | 1/1 | 0.98 | 0.24 | 30,30,30,30 | 0 |
| 60 | MG | A | 3509 | 1/1 | 0.98 | 0.37 | 45,45,45,45 | 0 |
| 60 | MG | A | 3018 | 1/1 | 0.98 | 0.25 | 27,27,27,27 | 0 |
| 60 | MG | A | 3070 | 1/1 | 0.98 | 0.27 | 10,10,10,10 | 0 |
| 60 | MG | a | 1788 | 1/1 | 0.98 | 0.10 | 43,43,43,43 | 1 |
| 60 | MG | A | 3512 | 1/1 | 0.98 | 0.22 | 44,44,44,44 | 0 |
| 60 | MG | A | 3483 | 1/1 | 0.98 | 0.21 | 31,31,31,31 | 0 |
| 60 | MG | a | 1708 | 1/1 | 0.98 | 0.11 | 40,40,40,40 | 0 |
| 60 | MG | A | 3484 | 1/1 | 0.98 | 0.40 | 41,41,41,41 | 0 |
| 60 | MG | A | 3308 | 1/1 | 0.98 | 0.23 | 14,14,14,14 | 0 |
| 60 | MG | A | 3486 | 1/1 | 0.98 | 0.17 | 44,44,44,44 | 0 |
| 60 | MG | A | 3401 | 1/1 | 0.98 | 0.37 | 36,36,36,36 | 0 |
| 60 | MG | A | 3309 | 1/1 | 0.98 | 0.20 | 49,49,49,49 | 0 |
| 60 | MG | A | 3086 | 1/1 | 0.98 | 0.31 | 21,21,21,21 | 0 |
| 60 | MG | a | 1610 | 1/1 | 0.98 | 0.29 | 32,32,32,32 | 1 |
| 60 | MG | A | 3369 | 1/1 | 0.98 | 0.14 | 31,31,31,31 | 0 |
| 60 | MG | A | 3444 | 1/1 | 0.98 | 0.31 | 39,39,39,39 | 0 |
| 60 | MG | A | 3238 | 1/1 | 0.98 | 0.31 | 38,38,38,38 | 0 |
| 60 | MG | A | 3424 | 1/1 | 0.98 | 0.33 | 20,20,20,20 | 0 |
| 60 | MG | x | 104 | 1/1 | 0.98 | 0.30 | 43,43,43,43 | 0 |
| 60 | MG | a | 1720 | 1/1 | 0.98 | 0.22 | 48,48,48,48 | 0 |
| 60 | MG | A | 3587 | 1/1 | 0.98 | 0.28 | 23,23,23,23 | 1 |
| 60 | MG | A | 3425 | 1/1 | 0.98 | 0.28 | 54,54,54,54 | 0 |
| 60 | MG | a | 1764 | 1/1 | 0.98 | 0.49 | 37,37,37,37 | 0 |
| 60 | MG | A | 3013 | 1/1 | 0.98 | 0.23 | 24,24,24,24 | 0 |
| 60 | MG | A | 3407 | 1/1 | 0.98 | 0.17 | 30,30,30,30 | 0 |
| 60 | MG | A | 3497 | 1/1 | 0.98 | 0.25 | 38,38,38,38 | 1 |
| 60 | MG | a | 1727 | 1/1 | 0.98 | 0.13 | 49,49,49,49 | 0 |
| 60 | MG | a | 1688 | 1/1 | 0.98 | 0.22 | 32,32,32,32 | 0 |
| 60 | MG | A | 3171 | 1/1 | 0.98 | 0.19 | 31,31,31,31 | 0 |
| 60 | MG | A | 3314 | 1/1 | 0.98 | 0.09 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60 | MG | A | 3430 | 1/1 | 0.98 | 0.22 | 43,43,43,43 | 0 |
| 60 | MG | A | 3501 | 1/1 | 0.98 | 0.15 | 24,24,24,24 | 0 |
| 60 | MG | A | 3213 | 1/1 | 0.98 | 0.10 | 34,34,34,34 | 1 |
| 60 | MG | a | 1607 | 1/1 | 0.99 | 0.35 | 42,42,42,42 | 1 |
| 60 | MG | a | 1608 | 1/1 | 0.99 | 0.29 | 23,23,23,23 | 0 |
| 60 | MG | A | 3184 | 1/1 | 0.99 | 0.42 | 30,30,30,30 | 0 |
| 60 | MG | A | 3273 | 1/1 | 0.99 | 0.34 | 37,37,37,37 | 1 |
| 60 | MG | A | 3615 | 1/1 | 0.99 | 0.14 | 34,34,34,34 | 0 |
| 60 | MG | a | 1724 | 1/1 | 0.99 | 0.34 | 42,42,42,42 | 0 |
| 60 | MG | A | 3399 | 1/1 | 0.99 | 0.28 | 44,44,44,44 | 0 |
| 61 | ZN | n | 104 | 1/1 | 0.99 | 0.15 | 44,44,44,44 | 0 |
| 60 | MG | A | 3396 | 1/1 | 0.99 | 0.18 | 26,26,26,26 | 0 |
| 60 | MG | E | 305 | 1/1 | 0.99 | 0.16 | 23,23,23,23 | 1 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.