



Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 11:17 AM JST

PDB ID : 8IPY
EMDB ID : EMD-35651
Title : human nuclear pre-60S ribosomal particle - State D'
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-03-15
Resolution : 3.20 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

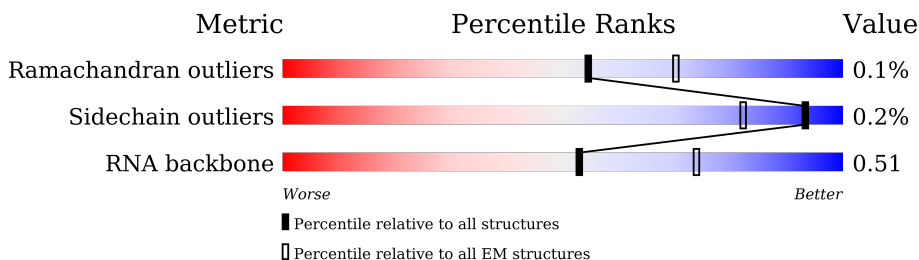
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






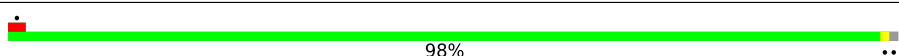
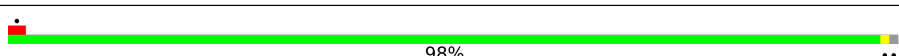
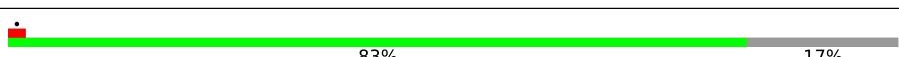
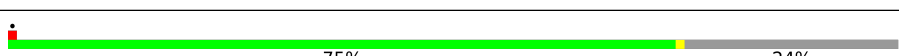
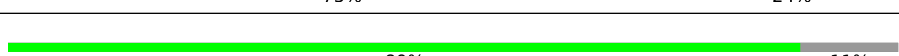
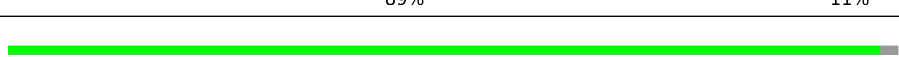
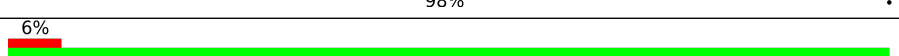
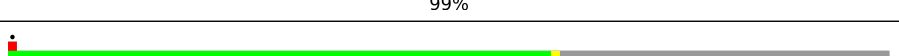
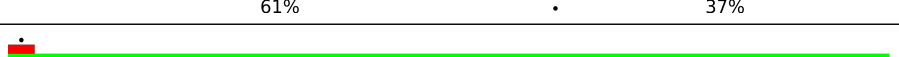
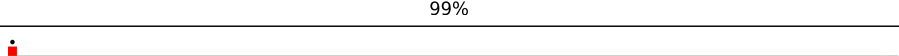
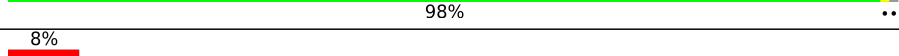
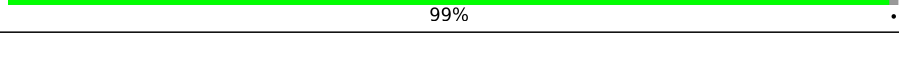


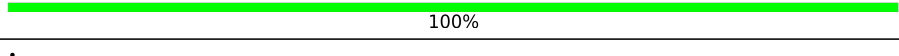
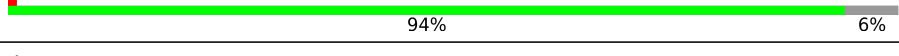
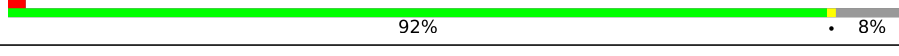
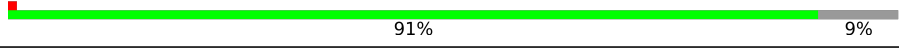
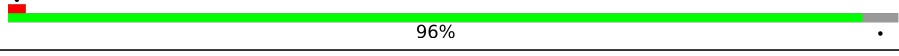
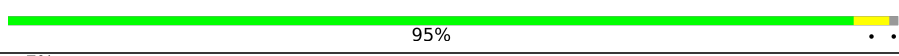

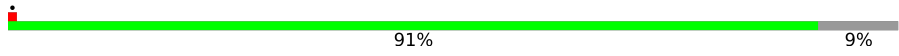
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | N | 687 | |
| 2 | 2 | 5054 | |
| 3 | 6 | 245 | |
| 4 | 7 | 163 | |
| 5 | 8 | 156 | |
| 6 | 9 | 134 | |
| 7 | A | 159 | |
| 8 | B | 403 | |


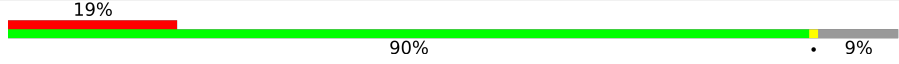
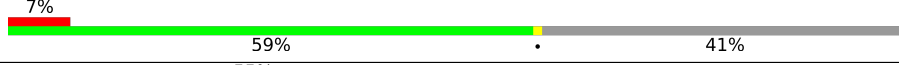
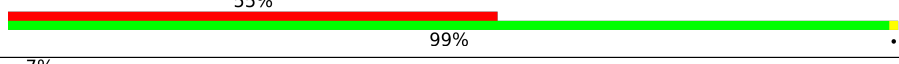

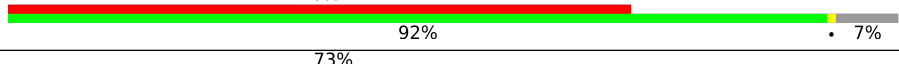
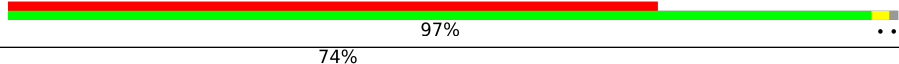

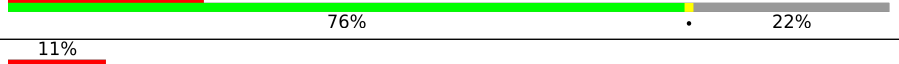
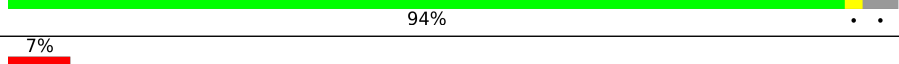
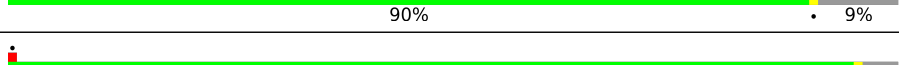
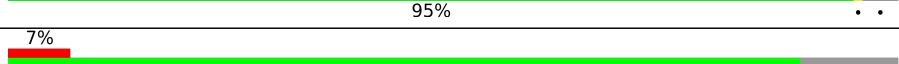


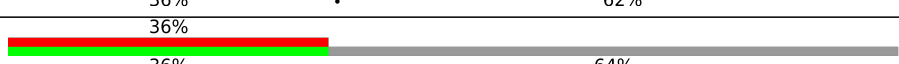
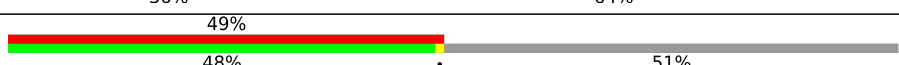

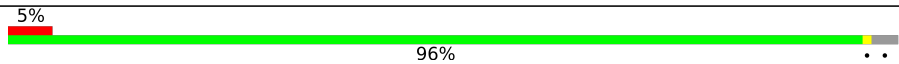
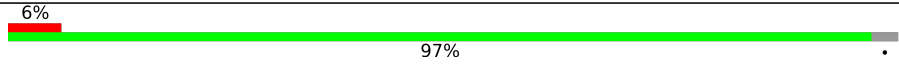
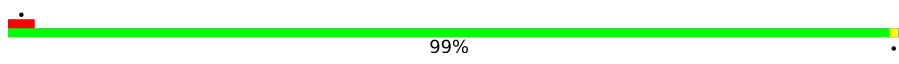
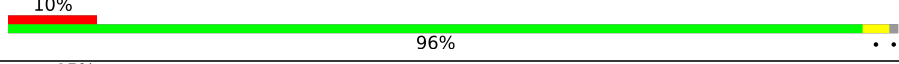
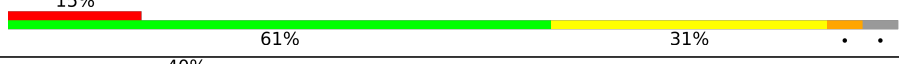
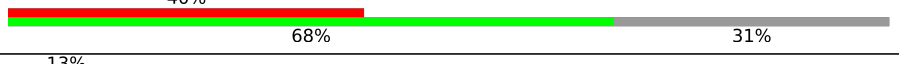
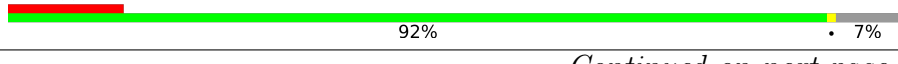

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 9 | D | 427 |  |
| 10 | E | 115 |  |
| 11 | G | 266 |  |
| 12 | H | 123 |  |
| 13 | I | 192 |  |
| 14 | J | 260 |  |
| 15 | L | 148 |  |
| 16 | M | 97 |  |
| 17 | P | 51 |  |
| 18 | Q | 211 |  |
| 19 | S | 215 |  |
| 20 | U | 204 |  |
| 21 | V | 203 |  |
| 22 | X | 92 |  |
| 23 | Z | 188 |  |
| 24 | a | 196 |  |
| 25 | b | 176 |  |
| 26 | e | 140 |  |
| 27 | h | 145 |  |
| 28 | l | 137 |  |
| 29 | m | 257 |  |
| 30 | n | 110 |  |
| 31 | o | 288 |  |
| 32 | p | 248 |  |
| 33 | r | 360 |  |


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 34 | u | 549 |  |
| 35 | v | 239 |  |
| 36 | w | 731 |  |
| 37 | y | 165 |  |
| 38 | z | 129 |  |
| 39 | C | 178 |  |
| 40 | R | 297 |  |
| 41 | W | 485 |  |
| 42 | T | 160 |  |
| 43 | 4 | 634 |  |
| 44 | Y | 184 |  |
| 45 | k | 135 |  |
| 46 | j | 125 |  |
| 47 | d | 128 |  |
| 48 | t | 293 |  |
| 49 | x | 160 |  |
| 50 | c | 490 |  |
| 51 | 1 | 255 |  |
| 52 | K | 105 |  |
| 53 | F | 117 |  |
| 54 | i | 136 |  |
| 55 | O | 70 |  |
| 56 | 3 | 120 |  |
| 57 | q | 588 |  |
| 58 | g | 156 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 59 | f | 478 |  <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '32%', a green segment in the middle labeled '53%', and a grey segment on the right labeled '46%'. A small black dot is located at the end of the green segment.</p> |

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 163715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein SDA1 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | N | 332 | 2719 | 1762 | 461 | 475 | 21 | 0 | 0 |

- Molecule 2 is a RNA chain called 28S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| | | | Total | C | N | O | P | | |
| 2 | 2 | 3485 | 74812 | 33355 | 13680 | 24293 | 3484 | 0 | 0 |

- Molecule 3 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | 6 | 244 | 1852 | 1149 | 318 | 372 | 13 | 0 | 0 |

- Molecule 4 is a protein called Probable ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | 7 | 135 | 1159 | 737 | 225 | 187 | 10 | 0 | 0 |

- Molecule 5 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| | | | Total | C | N | O | P | | |
| 5 | 8 | 156 | 3315 | 1481 | 585 | 1094 | 155 | 0 | 0 |

- Molecule 6 is a protein called Zinc finger protein 593.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | 9 | 86 | 711 | 433 | 154 | 121 | 3 | 0 | 0 |

- Molecule 7 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 7 | A | 45 | 352 | 221 | 76 | 52 | 3 | 0 | 0 |

- Molecule 8 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | B | 402 | 3244 | 2065 | 609 | 556 | 14 | 1 | 0 |

- Molecule 9 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 9 | D | 358 | 2853 | 1797 | 570 | 473 | 13 | 0 | 0 |

- Molecule 10 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 10 | E | 98 | 764 | 485 | 135 | 138 | 6 | 0 | 0 |

- Molecule 11 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 11 | G | 241 | 1927 | 1228 | 371 | 324 | 4 | 0 | 0 |

- Molecule 12 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 12 | H | 122 | 1015 | 641 | 205 | 168 | 1 | 0 | 0 |

- Molecule 13 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 13 | I | 190 | 1518 | 956 | 284 | 272 | 6 | 0 | 0 |

- Molecule 14 is a protein called Ribosome biogenesis protein NSA2 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14 | J | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1772 | 1134 | 334 | 296 | 8 | | |

- Molecule 15 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | L | 112 | Total | C | N | O | S | 0 | 0 |
| | | | 877 | 557 | 172 | 145 | 3 | | |

- Molecule 16 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | M | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 705 | 434 | 155 | 111 | 5 | | |

- Molecule 17 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17 | P | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 281 | 98 | 64 | 1 | | |

- Molecule 18 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18 | Q | 210 | Total | C | N | O | S | 0 | 0 |
| | | | 1701 | 1064 | 352 | 281 | 4 | | |

- Molecule 19 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | S | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1111 | 713 | 213 | 178 | 7 | | |

- Molecule 20 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20 | U | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1701 | 1072 | 359 | 266 | 4 | | |

- Molecule 21 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21 | V | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1063 | 321 | 261 | 5 | | |

- Molecule 22 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | X | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 708 | 445 | 136 | 120 | 7 | | |

- Molecule 23 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | Z | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1223 | 768 | 247 | 203 | 5 | | |

- Molecule 24 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | a | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1239 | 772 | 266 | 192 | 9 | | |

- Molecule 25 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 25 | b | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1461 | 930 | 284 | 236 | 11 | | |

- Molecule 26 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | e | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 618 | 184 | 172 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | h | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1115 | 700 | 226 | 186 | 3 | | |

- Molecule 28 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 28 | l | 125 | 1002 | 622 | 207 | 168 | 5 | 0 | 0 |

- Molecule 29 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 29 | m | 248 | 1898 | 1189 | 389 | 314 | 6 | 0 | 0 |

- Molecule 30 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 30 | n | 109 | 876 | 555 | 174 | 144 | 3 | 0 | 0 |

- Molecule 31 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 31 | o | 235 | 1897 | 1217 | 360 | 316 | 4 | 0 | 0 |

- Molecule 32 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 32 | p | 225 | 1878 | 1207 | 361 | 301 | 9 | 1 | 0 |

- Molecule 33 is a protein called Coiled-coil domain-containing protein 86.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 33 | r | 82 | 723 | 442 | 158 | 121 | 2 | 0 | 0 |

- Molecule 34 is a protein called Guanine nucleotide-binding protein-like 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 34 | u | 67 | 569 | 357 | 119 | 90 | 3 | 0 | 0 |

- Molecule 35 is a protein called mRNA turnover protein 4 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 35 | v | 217 | 1771 | 1129 | 311 | 320 | 11 | 0 | 0 |

- Molecule 36 is a protein called G Protein Nucleolar 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 36 | w | 433 | 3472 | 2201 | 615 | 643 | 13 | 0 | 0 |

- Molecule 37 is a protein called 60S ribosomal protein L12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 37 | y | 165 | 1250 | 779 | 232 | 234 | 5 | 0 | 0 |

- Molecule 38 is a protein called Protein LLP homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 38 | z | 67 | 581 | 363 | 128 | 88 | 2 | 0 | 0 |

- Molecule 39 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 39 | C | 165 | 1319 | 836 | 245 | 233 | 5 | 0 | 0 |

- Molecule 40 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 40 | R | 293 | 2382 | 1507 | 434 | 427 | 14 | 0 | 0 |

- Molecule 41 is a protein called Notchless protein homolog 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 41 | W | 388 | 3018 | 1889 | 556 | 562 | 11 | 0 | 0 |

- Molecule 42 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | T | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1001 | 632 | 194 | 171 | 4 | | |

- Molecule 43 is a protein called GTP-binding protein 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43 | 4 | 611 | Total | C | N | O | S | 0 | 0 |
| | | | 5016 | 3151 | 918 | 920 | 27 | | |

- Molecule 44 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | Y | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1355 | 848 | 260 | 238 | 9 | | |

- Molecule 45 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | k | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1064 | 673 | 220 | 166 | 5 | | |

- Molecule 46 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | j | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 918 | 578 | 178 | 160 | 2 | | |

- Molecule 47 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47 | d | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 542 | 149 | 157 | 2 | | |

- Molecule 48 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | t | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 928 | 601 | 157 | 167 | 3 | | |

- Molecule 49 is a RNA chain called ITS2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|---|-----|----|---------|-------|
| 49 | x | 57 | Total | C | N | O | P | 0 | 0 |
| | | | 684 | 285 | 1 | 341 | 57 | | |

- Molecule 50 is a protein called Ribosomal L1 domain-containing protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50 | c | 239 | Total | C | N | O | S | 0 | 0 |
| | | | 1924 | 1232 | 338 | 348 | 6 | | |

- Molecule 51 is a protein called 60S ribosomal protein L7-like 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51 | 1 | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1897 | 1226 | 357 | 310 | 4 | | |

- Molecule 52 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52 | K | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 832 | 521 | 177 | 129 | 5 | | |

- Molecule 53 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | F | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 897 | 560 | 185 | 146 | 6 | | |

- Molecule 54 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54 | i | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1107 | 714 | 208 | 182 | 3 | | |

- Molecule 55 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 55 | O | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 569 | 366 | 103 | 99 | 1 | | |

- Molecule 56 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | P | | |
| 56 | 3 | 115 | 2453 | 1093 | 437 | 808 | 115 | 0 | 0 |

- Molecule 57 is a protein called Pescadillo homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 57 | q | 404 | 3317 | 2140 | 582 | 582 | 13 | 0 | 0 |

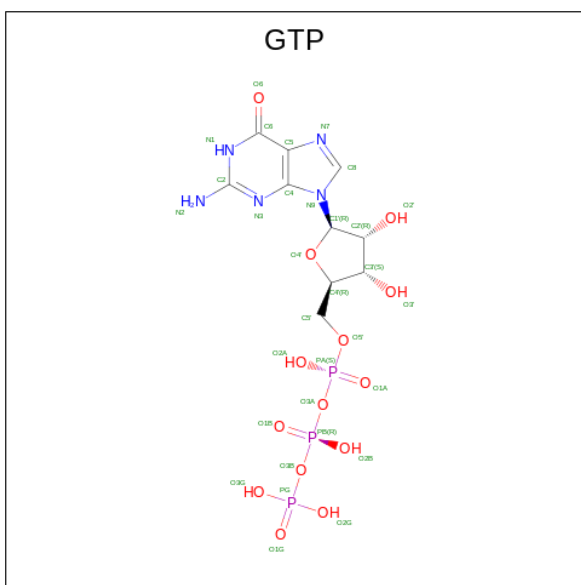
- Molecule 58 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 58 | g | 145 | 1170 | 750 | 222 | 197 | 1 | 0 | 0 |

- Molecule 59 is a protein called Ribosome biogenesis protein NOP53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 59 | f | 258 | 2137 | 1326 | 427 | 382 | 2 | 0 | 0 |

- Molecule 60 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



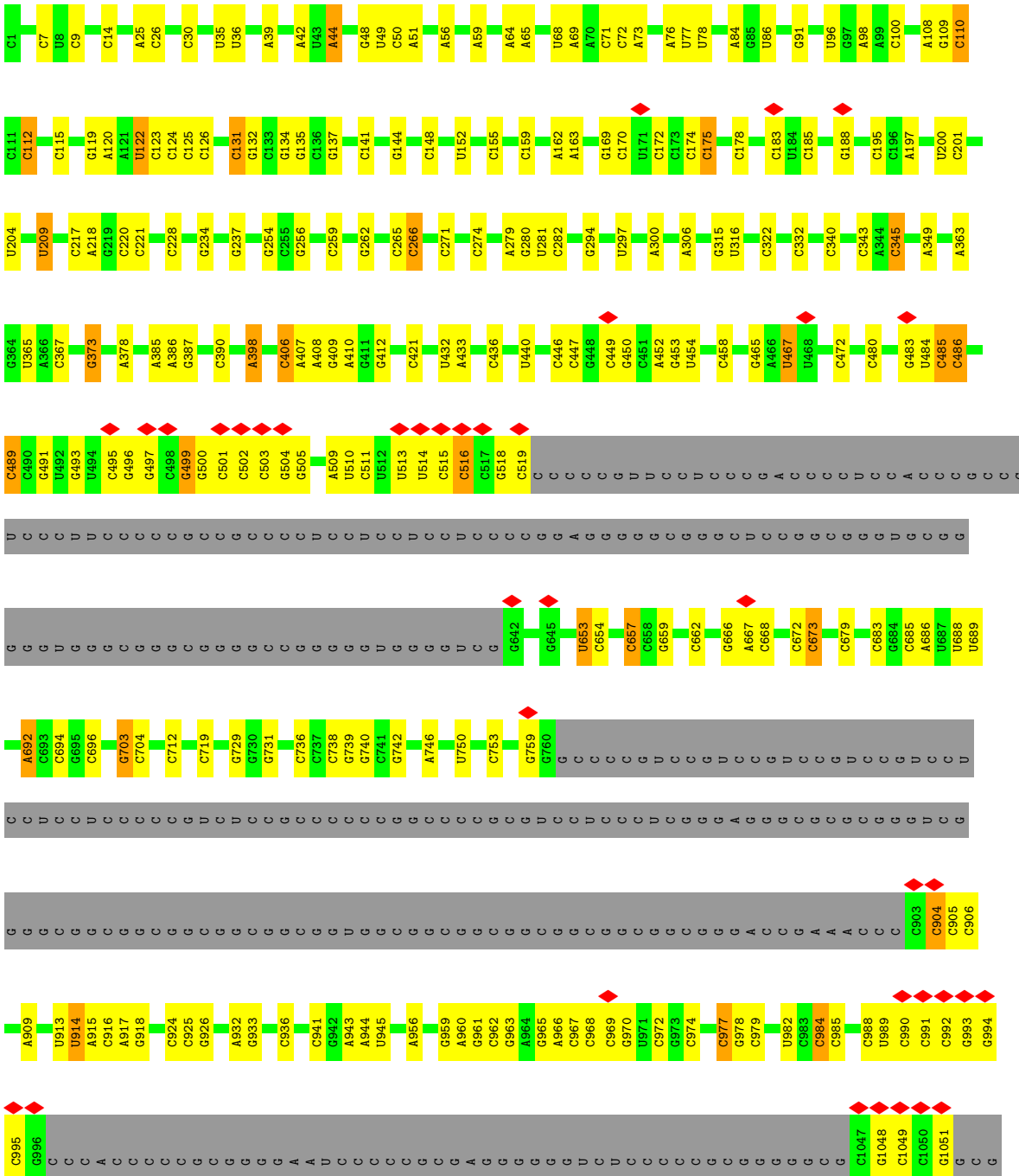
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 60 | w | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

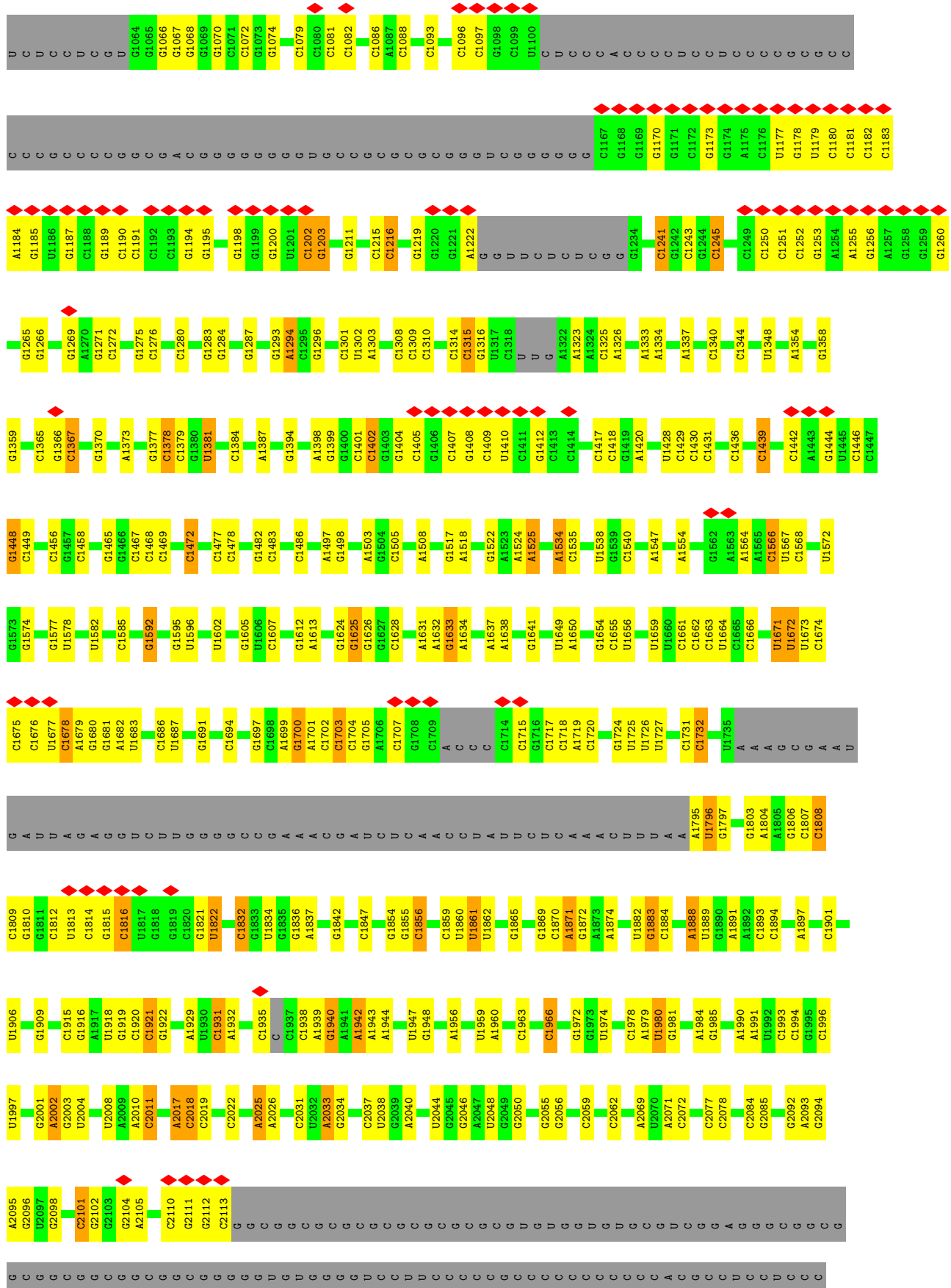
- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

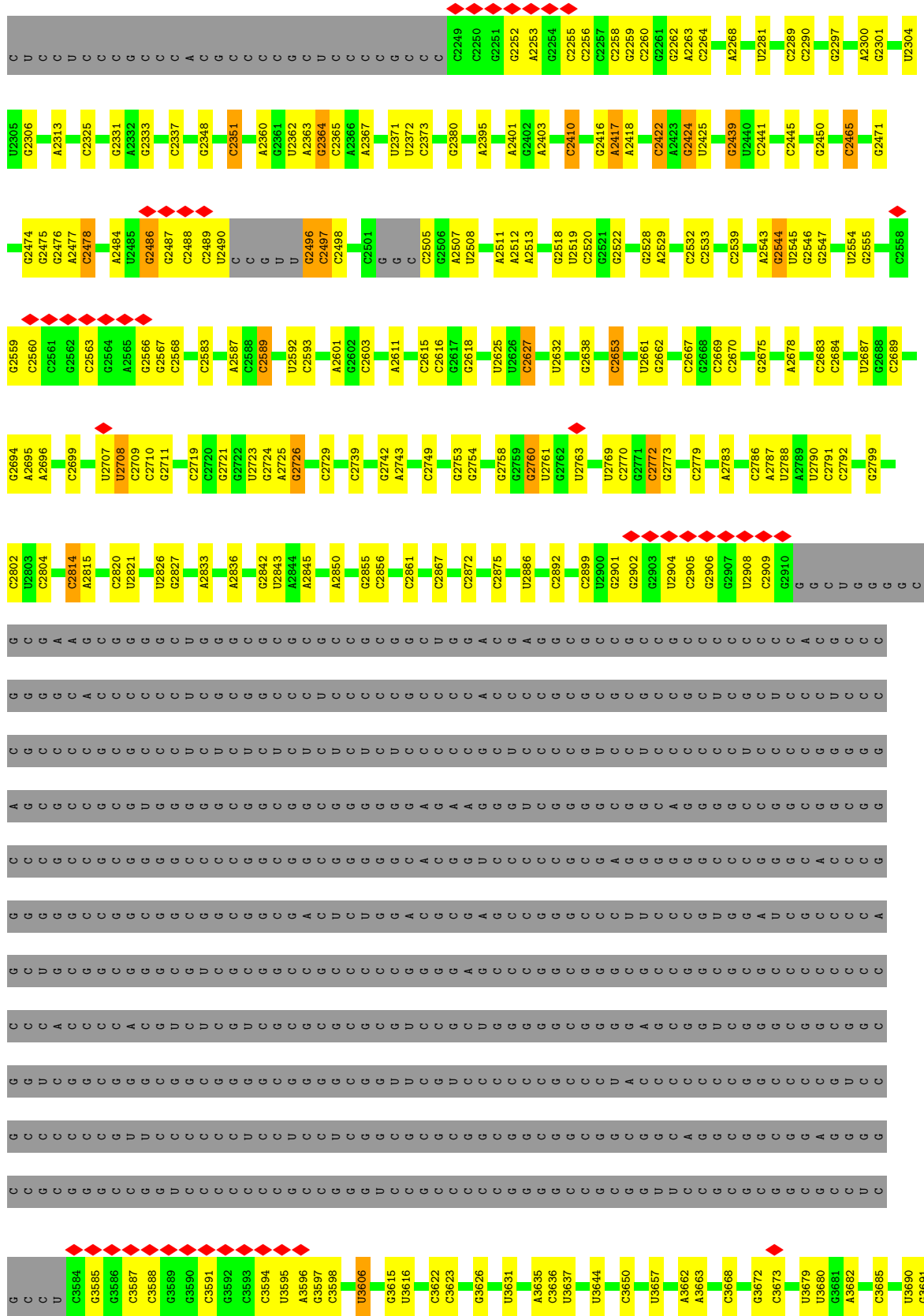
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Mg | |
| 61 | w | 1 | 1 | 1 | 0 |

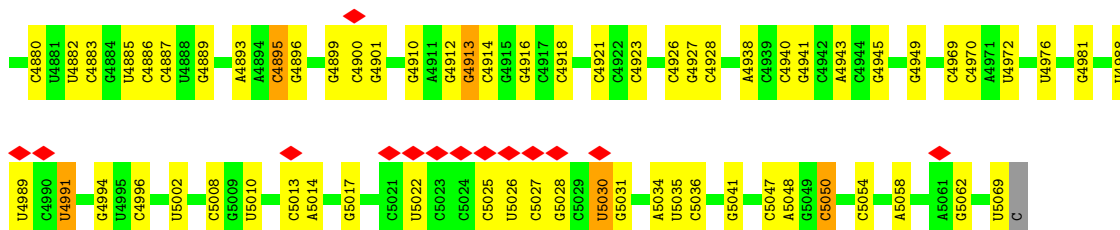
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | ASP | GLY | THR | ARG | LEU | ALA | THR | ALA | LEU | GLY | LYS | THR | ASP | ARG | LYS | ARG | GLY | PHE | VAL | ARG | LYS | LYS | THR | LYS | ASN | PRO | PHE | SER | SER | SER | THR | ASN | LYS | GLY | LYS | LYS | GLN | LYS | ASN | PHE | MET | MET | MET | ARG | TYR | SER | GLN | ASN | VAL | ARG | LYS | LYS | ASN | LYS | ARG | SER | |
| PHE | ARG | GLU | LYS | GLN | LEU | ALA | LEU | LEU | LEU | LYS | LYS | LYS | ARG | ASP | ALA | ALA | LEU | LEU | LYS | LYS | THR | ARG | LYS | LYS | THR | ASN | PRO | PHE | SER | SER | SER | THR | ASN | LYS | GLY | LYS | LYS | GLN | LYS | ASN | PHE | MET | MET | MET | ARG | TYR | SER | GLN | ASN | VAL | ARG | LYS | LYS | ASN | LYS | ARG | SER |

● Molecule 2: 28S rRNA

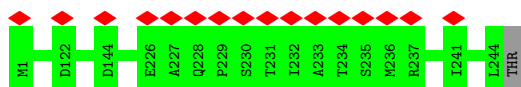




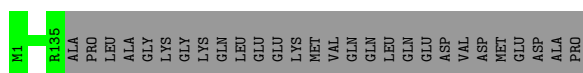
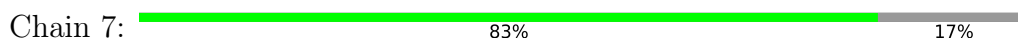




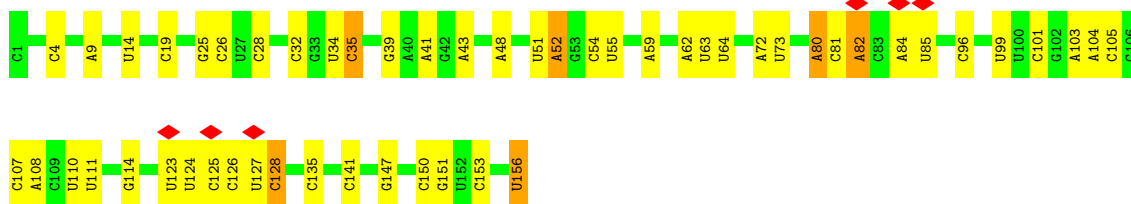
• Molecule 3: Eukaryotic translation initiation factor 6



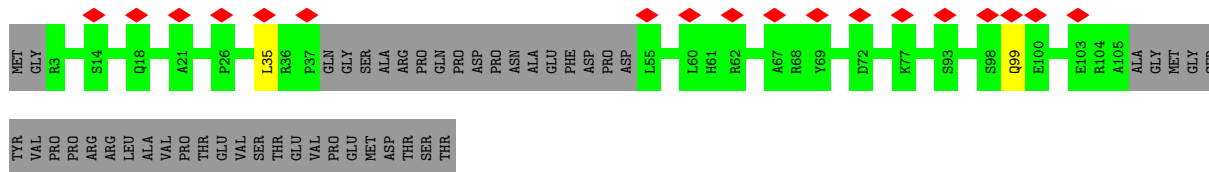
• Molecule 4: Probable ribosome biogenesis protein RLP24



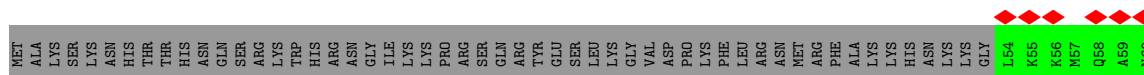
• Molecule 5: 5.8S rRNA



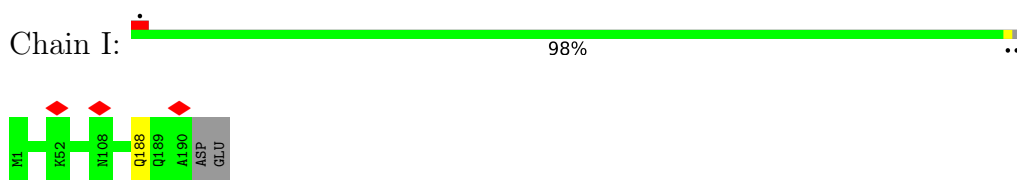
• Molecule 6: Zinc finger protein 593



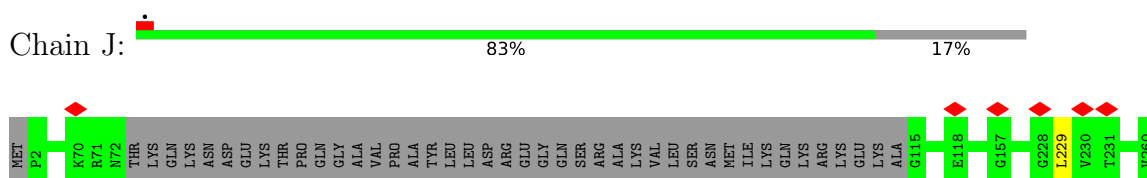
• Molecule 7: 60S ribosomal protein L29



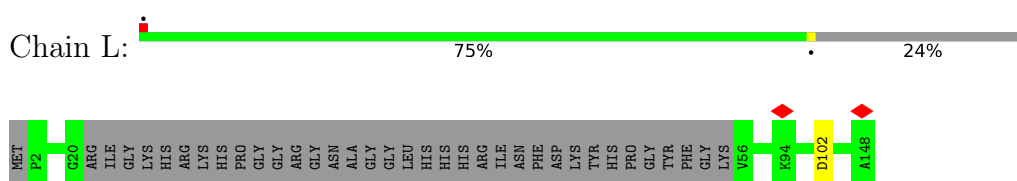
- Molecule 13: 60S ribosomal protein L9



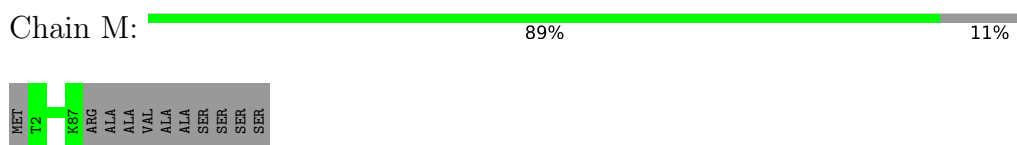
- Molecule 14: Ribosome biogenesis protein NSA2 homolog



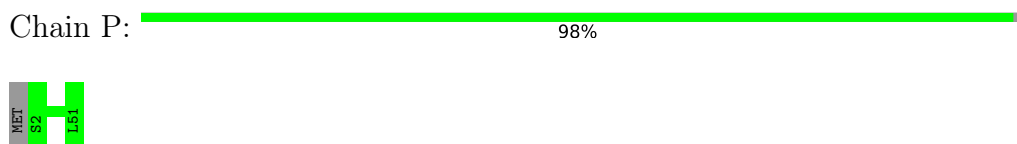
- Molecule 15: 60S ribosomal protein L27a



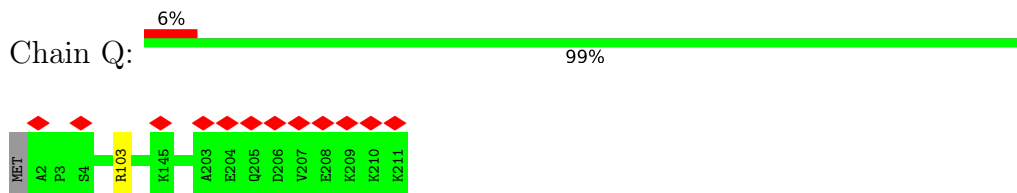
- Molecule 16: 60S ribosomal protein L37



- Molecule 17: 60S ribosomal protein L39

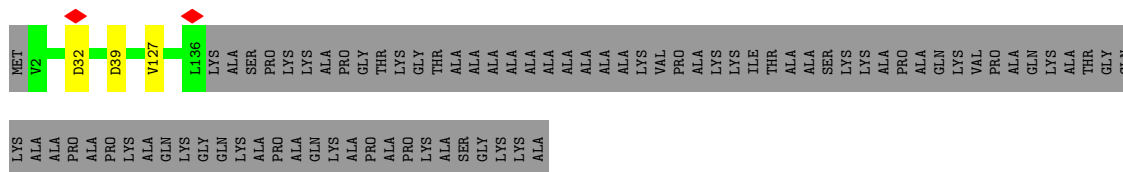


- Molecule 18: 60S ribosomal protein L13

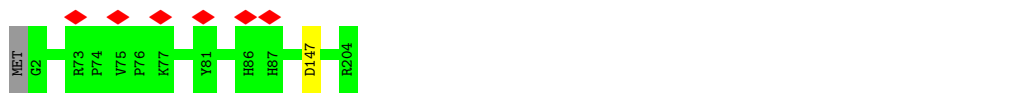


- Molecule 19: 60S ribosomal protein L14





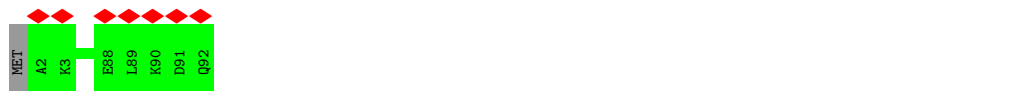
- Molecule 20: 60S ribosomal protein L15



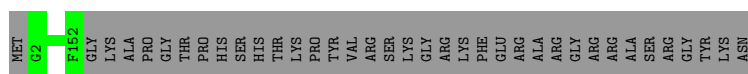
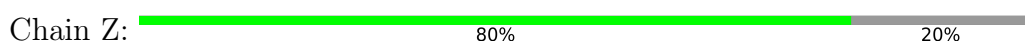
- Molecule 21: 60S ribosomal protein L13a



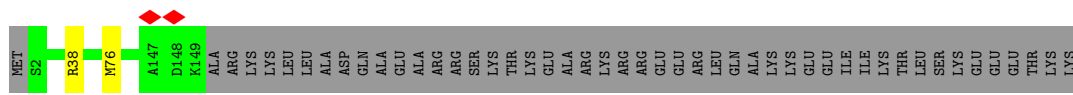
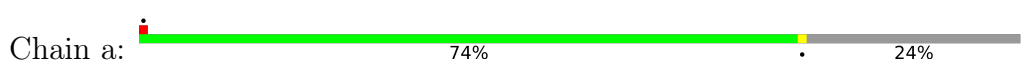
- Molecule 22: 60S ribosomal protein L37a



- Molecule 23: 60S ribosomal protein L18



- Molecule 24: 60S ribosomal protein L19

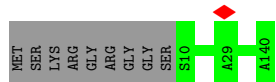


- Molecule 25: 60S ribosomal protein L18a

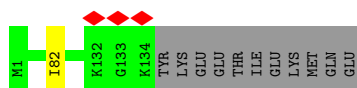
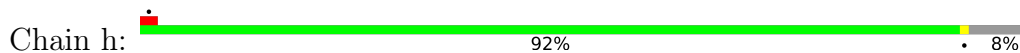


There are no outlier residues recorded for this chain.

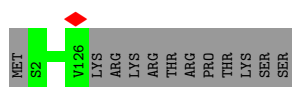
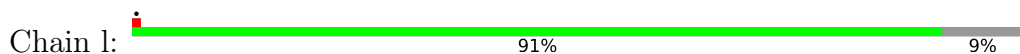
- Molecule 26: 60S ribosomal protein L23



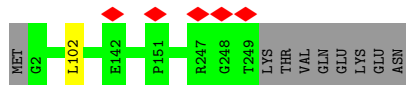
- Molecule 27: 60S ribosomal protein L26



- Molecule 28: 60S ribosomal protein L28



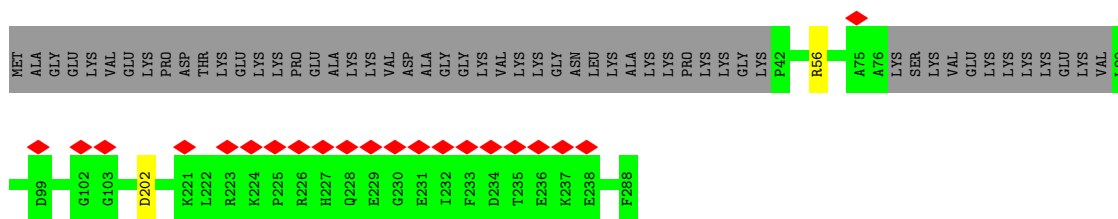
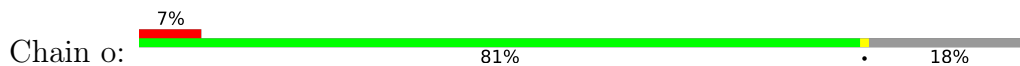
- Molecule 29: 60S ribosomal protein L8



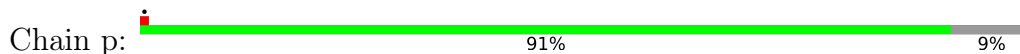
- Molecule 30: 60S ribosomal protein L35a

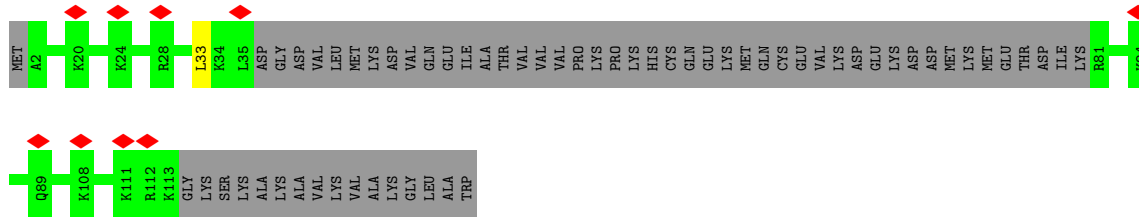


- Molecule 31: 60S ribosomal protein L6

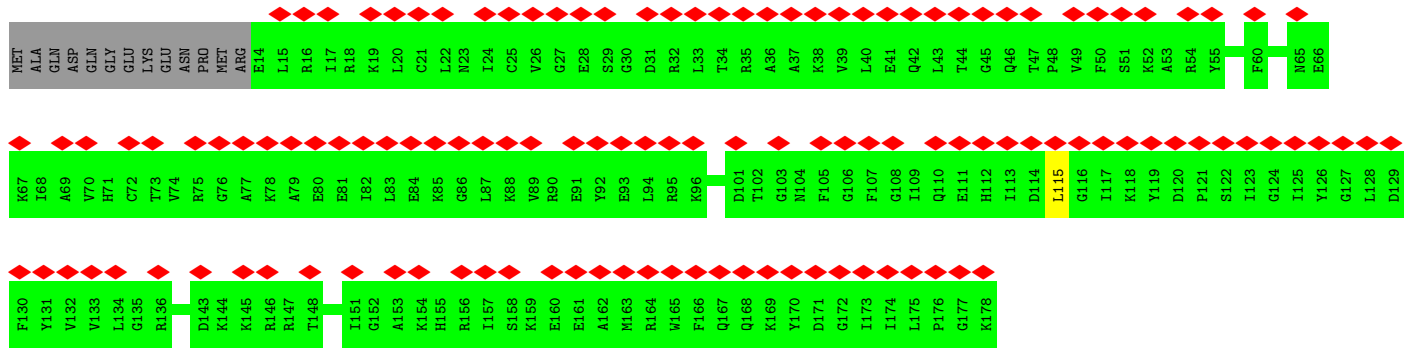


- Molecule 32: 60S ribosomal protein L7

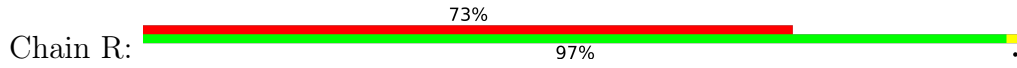




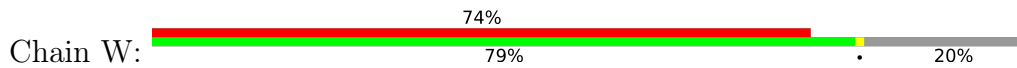
• Molecule 39: 60S ribosomal protein L11

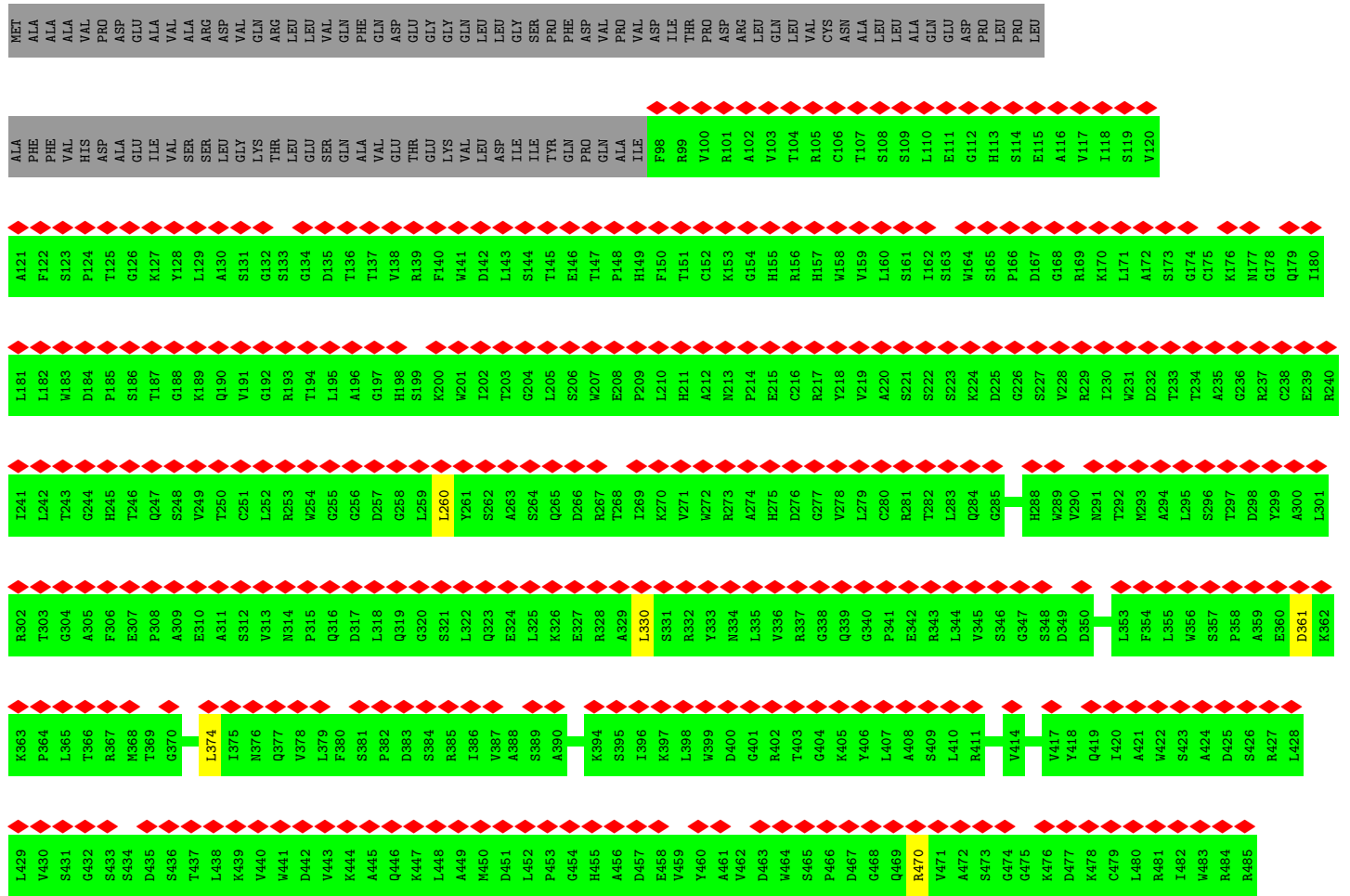


• Molecule 40: 60S ribosomal protein L5

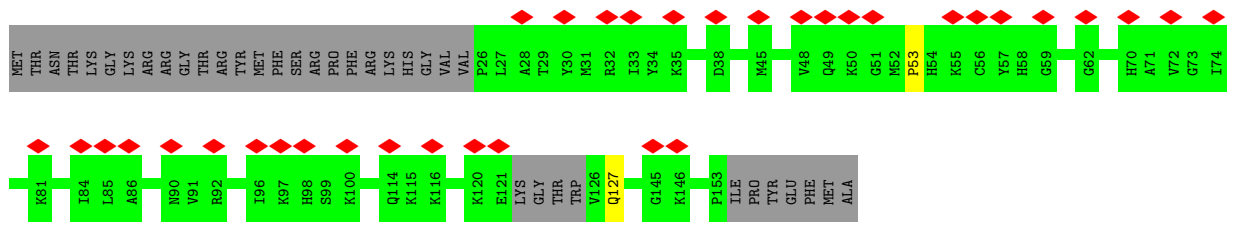
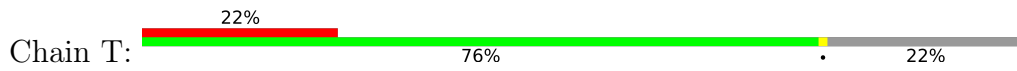


• Molecule 41: Notchless protein homolog 1

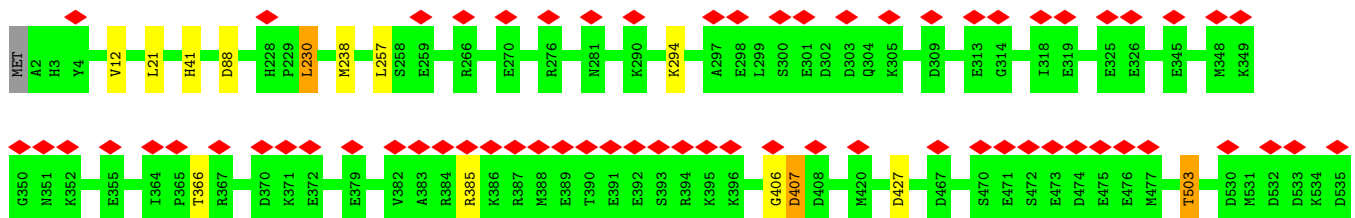




• Molecule 42: 60S ribosomal protein L21

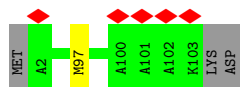


• Molecule 43: GTP-binding protein 4

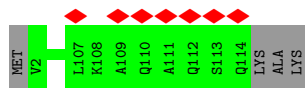




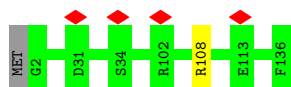
- Molecule 52: 60S ribosomal protein L36



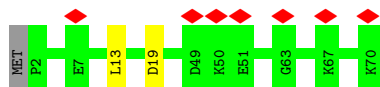
- Molecule 53: 60S ribosomal protein L34



- Molecule 54: 60S ribosomal protein L27



- Molecule 55: 60S ribosomal protein L38



- Molecule 56: 5S rRNA

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 26584 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 1.8 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 1800 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value | 0.211 | Depositor |
| Minimum map value | -0.074 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.006 | Depositor |
| Recommended contour level | 0.032 | Depositor |
| Map size (Å) | 548.0, 548.0, 548.0 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.37, 1.37, 1.37 | Depositor |

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: I4U, GTP, B8W, B8T, 2MG, B9H, P7G, UR3, E7G, B8K, B8Q, OMG, B9B, M7A, P4U, 5MU, 7MG, BGH, A2M, OMC, OMU, MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | N | 0.38 | 0/2772 | 0.73 | 4/3738 (0.1%) |
| 2 | 2 | 0.43 | 3/81923 (0.0%) | 1.38 | 1241/127714 (1.0%) |
| 3 | 6 | 0.31 | 0/1877 | 0.67 | 0/2554 |
| 4 | 7 | 0.36 | 0/1181 | 0.64 | 0/1563 |
| 5 | 8 | 0.43 | 0/3679 | 1.37 | 51/5732 (0.9%) |
| 6 | 9 | 0.31 | 0/723 | 0.83 | 2/961 (0.2%) |
| 7 | A | 0.27 | 0/354 | 0.74 | 0/465 |
| 8 | B | 0.32 | 0/3315 | 0.67 | 1/4435 (0.0%) |
| 9 | D | 0.29 | 0/2907 | 0.68 | 2/3905 (0.1%) |
| 10 | E | 0.32 | 0/774 | 0.77 | 2/1038 (0.2%) |
| 11 | G | 0.34 | 0/1960 | 0.69 | 1/2637 (0.0%) |
| 12 | H | 0.30 | 0/1023 | 0.62 | 0/1351 |
| 13 | I | 0.34 | 0/1537 | 0.72 | 1/2066 (0.0%) |
| 14 | J | 0.29 | 0/1808 | 0.58 | 1/2414 (0.0%) |
| 15 | L | 0.29 | 0/893 | 0.68 | 1/1193 (0.1%) |
| 16 | M | 0.31 | 0/720 | 0.69 | 0/952 |
| 17 | P | 0.30 | 0/454 | 0.65 | 0/599 |
| 18 | Q | 0.31 | 0/1732 | 0.67 | 0/2315 |
| 19 | S | 0.37 | 0/1133 | 0.70 | 3/1516 (0.2%) |
| 20 | U | 0.29 | 0/1746 | 0.67 | 1/2338 (0.0%) |
| 21 | V | 0.33 | 0/1682 | 0.67 | 2/2250 (0.1%) |
| 22 | X | 0.32 | 0/718 | 0.72 | 0/953 |
| 23 | Z | 0.31 | 0/1239 | 0.67 | 0/1658 |
| 24 | a | 0.30 | 0/1255 | 0.73 | 2/1662 (0.1%) |
| 25 | b | 0.32 | 0/1501 | 0.62 | 0/2013 |
| 26 | e | 0.31 | 0/993 | 0.69 | 0/1332 |
| 27 | h | 0.31 | 0/1132 | 0.67 | 1/1504 (0.1%) |
| 28 | l | 0.29 | 0/1017 | 0.68 | 0/1364 |
| 29 | m | 0.32 | 0/1936 | 0.72 | 1/2596 (0.0%) |
| 30 | n | 0.33 | 0/895 | 0.77 | 3/1198 (0.3%) |
| 31 | o | 0.31 | 0/1935 | 0.72 | 1/2596 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | p | 0.33 | 0/1916 | 0.63 | 0/2553 |
| 33 | r | 0.38 | 0/732 | 0.86 | 1/960 (0.1%) |
| 34 | u | 0.35 | 0/576 | 0.72 | 1/755 (0.1%) |
| 35 | v | 0.33 | 0/1806 | 0.70 | 2/2420 (0.1%) |
| 36 | w | 0.33 | 0/3541 | 0.63 | 3/4775 (0.1%) |
| 37 | y | 0.32 | 0/1269 | 0.72 | 1/1712 (0.1%) |
| 38 | z | 0.32 | 0/587 | 0.81 | 1/767 (0.1%) |
| 39 | C | 0.35 | 0/1341 | 0.72 | 1/1793 (0.1%) |
| 40 | R | 0.35 | 0/2428 | 0.77 | 6/3252 (0.2%) |
| 41 | W | 0.31 | 0/3093 | 0.72 | 4/4196 (0.1%) |
| 42 | T | 0.33 | 0/1018 | 0.71 | 1/1357 (0.1%) |
| 43 | 4 | 0.34 | 0/5099 | 0.75 | 9/6840 (0.1%) |
| 44 | Y | 0.29 | 0/1383 | 0.61 | 0/1856 |
| 45 | k | 0.29 | 0/1082 | 0.70 | 2/1443 (0.1%) |
| 46 | j | 0.30 | 0/933 | 0.66 | 0/1256 |
| 47 | d | 0.34 | 0/864 | 0.79 | 3/1160 (0.3%) |
| 48 | t | 0.37 | 0/955 | 0.73 | 2/1290 (0.2%) |
| 50 | c | 0.31 | 0/1956 | 0.65 | 3/2631 (0.1%) |
| 51 | l | 0.35 | 1/1933 (0.1%) | 0.70 | 3/2591 (0.1%) |
| 52 | K | 0.34 | 0/843 | 0.77 | 1/1115 (0.1%) |
| 53 | F | 0.28 | 0/907 | 0.69 | 0/1209 |
| 54 | i | 0.35 | 0/1130 | 0.67 | 0/1507 |
| 55 | O | 0.37 | 0/575 | 0.85 | 2/761 (0.3%) |
| 56 | 3 | 0.46 | 0/2739 | 1.49 | 59/4266 (1.4%) |
| 57 | q | 0.35 | 0/3395 | 0.67 | 1/4578 (0.0%) |
| 58 | g | 0.32 | 0/1191 | 0.67 | 1/1595 (0.1%) |
| 59 | f | 0.32 | 0/2169 | 0.74 | 3/2902 (0.1%) |
| All | All | 0.38 | 4/172275 (0.0%) | 1.13 | 1431/250152 (0.6%) |

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 |
|-----|-------|---------------------|---------------------|
| 7 | A | 0 | 1 |
| 8 | B | 0 | 1 |
| 11 | G | 0 | 2 |
| 30 | n | 0 | 1 |
| 33 | r | 0 | 1 |
| 34 | u | 0 | 1 |
| 42 | T | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 43 | 4 | 0 | 2 |
| 44 | Y | 0 | 1 |
| 48 | t | 0 | 1 |
| 51 | 1 | 0 | 1 |
| 59 | f | 0 | 1 |
| All | All | 0 | 14 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2 | 2 | 3876 | A | N9-C4 | 6.60 | 1.41 | 1.37 |
| 2 | 2 | 1795 | A | N9-C4 | 6.39 | 1.41 | 1.37 |
| 51 | 1 | 152 | PRO | CG-CD | -5.41 | 1.32 | 1.50 |
| 2 | 2 | 1929 | A | N9-C4 | 5.16 | 1.41 | 1.37 |

All (1431) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 2 | 2 | 1872 | G | OP1-P-OP2 | -27.26 | 78.71 | 119.60 |
| 2 | 2 | 1872 | G | O5'-P-OP1 | -25.34 | 80.30 | 110.70 |
| 2 | 2 | 1871 | A2M | OP2-P-O3' | -15.92 | 70.18 | 105.20 |
| 2 | 2 | 1872 | G | O5'-P-OP2 | 14.97 | 128.67 | 110.70 |
| 2 | 2 | 1871 | A2M | OP1-P-O3' | 14.70 | 137.55 | 105.20 |
| 2 | 2 | 4926 | C | N1-C2-O2 | 12.73 | 126.54 | 118.90 |
| 2 | 2 | 1216 | C | N1-C2-O2 | 12.27 | 126.26 | 118.90 |
| 2 | 2 | 753 | C | N1-C2-O2 | 12.17 | 126.20 | 118.90 |
| 56 | 3 | 78 | C | N1-C2-O2 | 11.84 | 126.00 | 118.90 |
| 2 | 2 | 4149 | C | N3-C2-O2 | -11.79 | 113.65 | 121.90 |
| 2 | 2 | 220 | C | N1-C2-O2 | 11.47 | 125.78 | 118.90 |
| 2 | 2 | 516 | C | N1-C2-O2 | 11.38 | 125.73 | 118.90 |
| 2 | 2 | 4926 | C | C6-N1-C2 | -11.26 | 115.80 | 120.30 |
| 2 | 2 | 100 | C | N1-C2-O2 | 11.21 | 125.63 | 118.90 |
| 2 | 2 | 4231 | C | N1-C2-O2 | 11.18 | 125.61 | 118.90 |
| 2 | 2 | 2820 | C | N1-C2-O2 | 11.17 | 125.60 | 118.90 |
| 2 | 2 | 100 | C | C2-N1-C1' | 10.98 | 130.88 | 118.80 |
| 2 | 2 | 4423 | U | C2-N1-C1' | 10.93 | 130.81 | 117.70 |
| 2 | 2 | 4423 | U | N1-C2-O2 | 10.87 | 130.41 | 122.80 |
| 2 | 2 | 753 | C | C2-N1-C1' | 10.76 | 130.64 | 118.80 |
| 2 | 2 | 1216 | C | C2-N1-C1' | 10.66 | 130.53 | 118.80 |
| 2 | 2 | 1994 | C | C2-N1-C1' | 10.65 | 130.52 | 118.80 |
| 2 | 2 | 4423 | U | N3-C2-O2 | -10.63 | 114.76 | 122.20 |
| 2 | 2 | 4926 | C | N3-C2-O2 | -10.63 | 114.46 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 2 | 2 | 4138 | C | N3-C2-O2 | -10.48 | 114.56 | 121.90 |
| 2 | 2 | 4284 | C | C5-C6-N1 | 10.45 | 126.22 | 121.00 |
| 56 | 3 | 78 | C | C6-N1-C2 | -10.42 | 116.13 | 120.30 |
| 2 | 2 | 4229 | U | C2-N1-C1' | 10.36 | 130.13 | 117.70 |
| 2 | 2 | 1994 | C | N1-C2-O2 | 10.33 | 125.10 | 118.90 |
| 2 | 2 | 77 | U | N3-C2-O2 | -10.27 | 115.01 | 122.20 |
| 2 | 2 | 3636 | C | C6-N1-C2 | -10.13 | 116.25 | 120.30 |
| 2 | 2 | 516 | C | N3-C2-O2 | -10.12 | 114.82 | 121.90 |
| 2 | 2 | 1966 | C | C6-N1-C2 | -10.07 | 116.27 | 120.30 |
| 56 | 3 | 78 | C | N3-C2-O2 | -10.03 | 114.88 | 121.90 |
| 2 | 2 | 4149 | C | C6-N1-C2 | -9.89 | 116.34 | 120.30 |
| 2 | 2 | 1671 | U | N1-C2-O2 | 9.84 | 129.68 | 122.80 |
| 2 | 2 | 4231 | C | C2-N1-C1' | 9.80 | 129.58 | 118.80 |
| 2 | 2 | 4426 | C | C6-N1-C2 | -9.78 | 116.39 | 120.30 |
| 2 | 2 | 1216 | C | N3-C2-O2 | -9.74 | 115.08 | 121.90 |
| 2 | 2 | 141 | C | C2-N1-C1' | 9.71 | 129.49 | 118.80 |
| 2 | 2 | 2627 | C | C6-N1-C2 | -9.69 | 116.42 | 120.30 |
| 2 | 2 | 4229 | U | N1-C2-O2 | 9.66 | 129.56 | 122.80 |
| 2 | 2 | 5035 | U | N3-C2-O2 | -9.63 | 115.46 | 122.20 |
| 2 | 2 | 753 | C | N3-C2-O2 | -9.60 | 115.18 | 121.90 |
| 2 | 2 | 4284 | C | C6-N1-C2 | -9.58 | 116.47 | 120.30 |
| 43 | 4 | 230 | LEU | CA-CB-CG | 9.56 | 137.28 | 115.30 |
| 2 | 2 | 2439 | G | C4-N9-C1' | 9.55 | 138.92 | 126.50 |
| 2 | 2 | 2351 | C | C6-N1-C2 | -9.54 | 116.48 | 120.30 |
| 2 | 2 | 220 | C | C6-N1-C2 | -9.49 | 116.50 | 120.30 |
| 2 | 2 | 3876 | A | C2-N3-C4 | 9.49 | 115.34 | 110.60 |
| 2 | 2 | 4926 | C | C2-N1-C1' | 9.45 | 129.20 | 118.80 |
| 2 | 2 | 4775 | C | N1-C2-O2 | 9.42 | 124.55 | 118.90 |
| 2 | 2 | 4758 | U | N1-C2-O2 | 9.36 | 129.35 | 122.80 |
| 2 | 2 | 4453 | C | N1-C2-O2 | 9.35 | 124.51 | 118.90 |
| 56 | 3 | 95 | C | C2-N1-C1' | 9.35 | 129.09 | 118.80 |
| 2 | 2 | 4709 | U | N1-C2-O2 | 9.33 | 129.33 | 122.80 |
| 2 | 2 | 2410 | C | C6-N1-C2 | -9.33 | 116.57 | 120.30 |
| 2 | 2 | 1671 | U | N3-C2-O2 | -9.32 | 115.67 | 122.20 |
| 2 | 2 | 4709 | U | N3-C2-O2 | -9.28 | 115.70 | 122.20 |
| 2 | 2 | 2627 | C | N1-C2-O2 | 9.28 | 124.47 | 118.90 |
| 2 | 2 | 4880 | C | N1-C2-O2 | 9.23 | 124.44 | 118.90 |
| 5 | 8 | 64 | U | N3-C2-O2 | -9.22 | 115.74 | 122.20 |
| 2 | 2 | 516 | C | C6-N1-C2 | -9.21 | 116.62 | 120.30 |
| 56 | 3 | 78 | C | C2-N1-C1' | 9.20 | 128.91 | 118.80 |
| 2 | 2 | 2820 | C | N3-C2-O2 | -9.18 | 115.48 | 121.90 |
| 2 | 2 | 100 | C | N3-C2-O2 | -9.16 | 115.48 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 4758 | U | N3-C2-O2 | -9.16 | 115.79 | 122.20 |
| 2 | 2 | 4758 | U | C2-N1-C1' | 9.11 | 128.63 | 117.70 |
| 2 | 2 | 4775 | C | C2-N1-C1' | 9.10 | 128.81 | 118.80 |
| 2 | 2 | 499 | G | C4-N9-C1' | 9.09 | 138.32 | 126.50 |
| 56 | 3 | 84 | U | C2-N1-C1' | 9.05 | 128.56 | 117.70 |
| 2 | 2 | 1795 | A | C2-N3-C4 | 9.00 | 115.10 | 110.60 |
| 2 | 2 | 4498 | U | C2-N1-C1' | 8.99 | 128.48 | 117.70 |
| 2 | 2 | 2478 | C | C2-N1-C1' | 8.98 | 128.67 | 118.80 |
| 2 | 2 | 4231 | C | N3-C2-O2 | -8.97 | 115.62 | 121.90 |
| 2 | 2 | 4149 | C | N1-C2-O2 | 8.93 | 124.26 | 118.90 |
| 2 | 2 | 2439 | G | C8-N9-C1' | -8.93 | 115.39 | 127.00 |
| 2 | 2 | 77 | U | N1-C2-O2 | 8.93 | 129.05 | 122.80 |
| 2 | 2 | 282 | C | N1-C2-O2 | 8.92 | 124.25 | 118.90 |
| 2 | 2 | 2262 | G | C4-N9-C1' | 8.91 | 138.09 | 126.50 |
| 2 | 2 | 963 | G | C4-N9-C1' | 8.91 | 138.08 | 126.50 |
| 2 | 2 | 1241 | C | N1-C2-O2 | 8.91 | 124.25 | 118.90 |
| 2 | 2 | 4682 | U | N3-C2-O2 | -8.88 | 115.98 | 122.20 |
| 2 | 2 | 985 | C | C6-N1-C2 | -8.88 | 116.75 | 120.30 |
| 2 | 2 | 220 | C | N3-C2-O2 | -8.87 | 115.69 | 121.90 |
| 2 | 2 | 2410 | C | C2-N1-C1' | 8.87 | 128.56 | 118.80 |
| 2 | 2 | 4229 | U | N3-C2-O2 | -8.87 | 116.00 | 122.20 |
| 2 | 2 | 3878 | C | N1-C2-O2 | 8.86 | 124.22 | 118.90 |
| 56 | 3 | 92 | C | C6-N1-C2 | -8.86 | 116.76 | 120.30 |
| 56 | 3 | 95 | C | N1-C2-O2 | 8.86 | 124.21 | 118.90 |
| 56 | 3 | 72 | U | O5'-P-OP1 | 8.84 | 121.31 | 110.70 |
| 2 | 2 | 4926 | C | C5-C6-N1 | 8.83 | 125.42 | 121.00 |
| 2 | 2 | 4864 | U | N1-C2-O2 | 8.82 | 128.98 | 122.80 |
| 2 | 2 | 2022 | C | N1-C2-O2 | 8.82 | 124.19 | 118.90 |
| 2 | 2 | 1963 | C | C6-N1-C2 | -8.82 | 116.77 | 120.30 |
| 2 | 2 | 499 | G | N3-C4-N9 | 8.78 | 131.27 | 126.00 |
| 2 | 2 | 4350 | C | C6-N1-C2 | -8.78 | 116.79 | 120.30 |
| 43 | 4 | 257 | LEU | CA-CB-CG | 8.76 | 135.45 | 115.30 |
| 51 | 1 | 152 | PRO | N-CD-CG | -8.68 | 90.18 | 103.20 |
| 2 | 2 | 4266 | G | N3-C4-C5 | -8.67 | 124.27 | 128.60 |
| 2 | 2 | 4864 | U | N3-C2-O2 | -8.66 | 116.14 | 122.20 |
| 2 | 2 | 1994 | C | N3-C2-O2 | -8.65 | 115.84 | 121.90 |
| 2 | 2 | 1081 | C | N3-C2-O2 | -8.64 | 115.85 | 121.90 |
| 2 | 2 | 35 | U | N3-C2-O2 | -8.64 | 116.15 | 122.20 |
| 2 | 2 | 1216 | C | C6-N1-C2 | -8.63 | 116.85 | 120.30 |
| 2 | 2 | 3772 | U | N3-C2-O2 | -8.59 | 116.19 | 122.20 |
| 2 | 2 | 96 | U | N3-C2-O2 | -8.58 | 116.19 | 122.20 |
| 2 | 2 | 178 | C | C6-N1-C2 | -8.57 | 116.87 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 3636 | C | N1-C2-O2 | 8.57 | 124.04 | 118.90 |
| 2 | 2 | 2262 | G | N3-C4-N9 | 8.54 | 131.12 | 126.00 |
| 2 | 2 | 2627 | C | C2-N1-C1' | 8.52 | 128.18 | 118.80 |
| 2 | 2 | 4275 | G | C4-N9-C1' | 8.51 | 137.56 | 126.50 |
| 56 | 3 | 92 | C | N1-C2-O2 | 8.51 | 124.01 | 118.90 |
| 2 | 2 | 4148 | C | N1-C2-O2 | 8.51 | 124.00 | 118.90 |
| 2 | 2 | 4158 | C | N3-C2-O2 | -8.50 | 115.95 | 121.90 |
| 2 | 2 | 1458 | C | N1-C2-O2 | 8.48 | 123.99 | 118.90 |
| 2 | 2 | 4887 | C | N1-C2-O2 | 8.47 | 123.98 | 118.90 |
| 2 | 2 | 35 | U | N1-C2-O2 | 8.47 | 128.73 | 122.80 |
| 2 | 2 | 50 | C | N1-C2-O2 | 8.46 | 123.98 | 118.90 |
| 9 | D | 319 | LEU | CA-CB-CG | 8.46 | 134.76 | 115.30 |
| 2 | 2 | 2478 | C | N1-C2-O2 | 8.44 | 123.96 | 118.90 |
| 2 | 2 | 141 | C | N1-C2-O2 | 8.44 | 123.96 | 118.90 |
| 2 | 2 | 1966 | C | C5-C6-N1 | 8.43 | 125.21 | 121.00 |
| 2 | 2 | 4068 | U | N3-C2-O2 | -8.42 | 116.31 | 122.20 |
| 2 | 2 | 4231 | C | C6-N1-C2 | -8.41 | 116.94 | 120.30 |
| 2 | 2 | 4266 | G | N3-C4-N9 | 8.41 | 131.04 | 126.00 |
| 2 | 2 | 220 | C | C5-C6-N1 | 8.40 | 125.20 | 121.00 |
| 2 | 2 | 390 | C | C6-N1-C2 | -8.40 | 116.94 | 120.30 |
| 2 | 2 | 4608 | G | C8-N9-C4 | -8.38 | 103.05 | 106.40 |
| 2 | 2 | 4885 | U | N3-C2-O2 | -8.38 | 116.33 | 122.20 |
| 2 | 2 | 4266 | G | C4-N9-C1' | 8.37 | 137.38 | 126.50 |
| 2 | 2 | 2262 | G | N3-C4-C5 | -8.37 | 124.42 | 128.60 |
| 2 | 2 | 112 | C | C6-N1-C2 | -8.36 | 116.96 | 120.30 |
| 2 | 2 | 472 | C | C6-N1-C2 | -8.35 | 116.96 | 120.30 |
| 2 | 2 | 4123 | C | N1-C2-O2 | 8.33 | 123.90 | 118.90 |
| 2 | 2 | 1678 | C | P-O3'-C3' | 8.31 | 129.67 | 119.70 |
| 2 | 2 | 467 | U | N1-C2-O2 | 8.28 | 128.60 | 122.80 |
| 2 | 2 | 141 | C | C5-C6-N1 | 8.28 | 125.14 | 121.00 |
| 2 | 2 | 2410 | C | C5-C6-N1 | 8.27 | 125.14 | 121.00 |
| 2 | 2 | 467 | U | N3-C2-O2 | -8.27 | 116.41 | 122.20 |
| 2 | 2 | 1929 | A | C2-N3-C4 | 8.25 | 114.73 | 110.60 |
| 2 | 2 | 1726 | U | N3-C2-O2 | -8.25 | 116.43 | 122.20 |
| 2 | 2 | 4068 | U | N1-C2-O2 | 8.24 | 128.57 | 122.80 |
| 2 | 2 | 3636 | C | N3-C2-O2 | -8.21 | 116.15 | 121.90 |
| 2 | 2 | 4498 | U | N1-C2-O2 | 8.21 | 128.55 | 122.80 |
| 2 | 2 | 4714 | C | N1-C2-O2 | 8.21 | 123.83 | 118.90 |
| 2 | 2 | 2820 | C | C6-N1-C2 | -8.21 | 117.02 | 120.30 |
| 2 | 2 | 4138 | C | C6-N1-C2 | -8.21 | 117.02 | 120.30 |
| 2 | 2 | 1966 | C | C2-N1-C1' | 8.21 | 127.83 | 118.80 |
| 2 | 2 | 4682 | U | N1-C2-O2 | 8.19 | 128.53 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 1241 | C | C2-N1-C1' | 8.18 | 127.79 | 118.80 |
| 2 | 2 | 4608 | G | N7-C8-N9 | 8.16 | 117.18 | 113.10 |
| 2 | 2 | 1402 | C | C6-N1-C2 | -8.16 | 117.04 | 120.30 |
| 2 | 2 | 322 | C | C6-N1-C2 | -8.15 | 117.04 | 120.30 |
| 2 | 2 | 2760 | G | P-O3'-C3' | 8.09 | 129.41 | 119.70 |
| 2 | 2 | 1477 | C | C6-N1-C2 | -8.06 | 117.07 | 120.30 |
| 2 | 2 | 2022 | C | N3-C2-O2 | -8.06 | 116.25 | 121.90 |
| 2 | 2 | 963 | G | N3-C4-N9 | 8.06 | 130.84 | 126.00 |
| 2 | 2 | 112 | C | C2-N1-C1' | 8.04 | 127.65 | 118.80 |
| 2 | 2 | 4505 | C | C6-N1-C2 | -8.04 | 117.08 | 120.30 |
| 8 | B | 360 | LEU | CA-CB-CG | 8.04 | 133.79 | 115.30 |
| 2 | 2 | 2351 | C | C5-C6-N1 | 8.00 | 125.00 | 121.00 |
| 2 | 2 | 4695 | C | N1-C2-O2 | 8.00 | 123.70 | 118.90 |
| 2 | 2 | 178 | C | N1-C2-O2 | 7.97 | 123.68 | 118.90 |
| 2 | 2 | 141 | C | C6-N1-C2 | -7.96 | 117.12 | 120.30 |
| 2 | 2 | 2528 | G | C4-N9-C1' | 7.96 | 136.85 | 126.50 |
| 56 | 3 | 78 | C | C5-C6-N1 | 7.96 | 124.98 | 121.00 |
| 2 | 2 | 4714 | C | C6-N1-C2 | -7.95 | 117.12 | 120.30 |
| 2 | 2 | 499 | G | C8-N9-C1' | -7.94 | 116.68 | 127.00 |
| 2 | 2 | 4923 | C | C6-N1-C2 | -7.93 | 117.13 | 120.30 |
| 56 | 3 | 72 | U | O5'-P-OP2 | -7.93 | 98.57 | 105.70 |
| 2 | 2 | 2505 | C | N1-C2-O2 | 7.91 | 123.65 | 118.90 |
| 2 | 2 | 499 | G | N3-C4-C5 | -7.90 | 124.65 | 128.60 |
| 2 | 2 | 1963 | C | N1-C2-O2 | 7.89 | 123.63 | 118.90 |
| 2 | 2 | 1671 | U | C2-N1-C1' | 7.89 | 127.17 | 117.70 |
| 2 | 2 | 5035 | U | N1-C2-O2 | 7.88 | 128.32 | 122.80 |
| 2 | 2 | 4294 | C | C6-N1-C2 | -7.88 | 117.15 | 120.30 |
| 2 | 2 | 985 | C | N1-C2-O2 | 7.87 | 123.62 | 118.90 |
| 2 | 2 | 2667 | C | N1-C2-O2 | 7.86 | 123.61 | 118.90 |
| 56 | 3 | 95 | C | N3-C2-O2 | -7.82 | 116.42 | 121.90 |
| 2 | 2 | 1607 | C | N1-C2-O2 | 7.82 | 123.59 | 118.90 |
| 2 | 2 | 1893 | C | C6-N1-C2 | -7.82 | 117.17 | 120.30 |
| 2 | 2 | 472 | C | C2-N1-C1' | 7.81 | 127.39 | 118.80 |
| 2 | 2 | 2011 | C | N1-C2-O2 | 7.81 | 123.58 | 118.90 |
| 2 | 2 | 2410 | C | N1-C2-O2 | 7.81 | 123.58 | 118.90 |
| 2 | 2 | 4319 | C | C6-N1-C2 | -7.80 | 117.18 | 120.30 |
| 2 | 2 | 1632 | A | C2-N3-C4 | 7.79 | 114.50 | 110.60 |
| 2 | 2 | 963 | G | N3-C4-C5 | -7.79 | 124.70 | 128.60 |
| 2 | 2 | 1978 | C | N1-C2-O2 | 7.79 | 123.57 | 118.90 |
| 2 | 2 | 100 | C | C6-N1-C2 | -7.79 | 117.19 | 120.30 |
| 2 | 2 | 2627 | C | C5-C6-N1 | 7.79 | 124.89 | 121.00 |
| 40 | R | 211 | LEU | CA-CB-CG | 7.78 | 133.20 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 1966 | C | N1-C2-O2 | 7.77 | 123.56 | 118.90 |
| 2 | 2 | 4228 | G | P-O3'-C3' | 7.76 | 129.02 | 119.70 |
| 2 | 2 | 2362 | U | N3-C2-O2 | -7.76 | 116.77 | 122.20 |
| 55 | O | 19 | ASP | CB-CG-OD1 | 7.75 | 125.27 | 118.30 |
| 2 | 2 | 914 | U | P-O3'-C3' | 7.74 | 128.99 | 119.70 |
| 2 | 2 | 220 | C | C2-N1-C1' | 7.72 | 127.30 | 118.80 |
| 2 | 2 | 4453 | C | C2-N1-C1' | 7.72 | 127.29 | 118.80 |
| 2 | 2 | 209 | U | N1-C2-O2 | 7.72 | 128.20 | 122.80 |
| 2 | 2 | 2528 | G | N3-C4-N9 | 7.71 | 130.63 | 126.00 |
| 2 | 2 | 3774 | A | P-O3'-C3' | 7.70 | 128.94 | 119.70 |
| 2 | 2 | 4171 | C | N1-C2-O2 | 7.70 | 123.52 | 118.90 |
| 2 | 2 | 4662 | C | C6-N1-C2 | -7.70 | 117.22 | 120.30 |
| 2 | 2 | 1276 | C | N1-C2-O2 | 7.68 | 123.51 | 118.90 |
| 2 | 2 | 1344 | C | C6-N1-C2 | -7.67 | 117.23 | 120.30 |
| 2 | 2 | 4158 | C | N1-C2-O2 | 7.67 | 123.50 | 118.90 |
| 2 | 2 | 2528 | G | N3-C4-C5 | -7.65 | 124.77 | 128.60 |
| 2 | 2 | 2351 | C | C2-N1-C1' | 7.65 | 127.22 | 118.80 |
| 5 | 8 | 54 | C | N1-C2-O2 | 7.64 | 123.48 | 118.90 |
| 2 | 2 | 195 | C | C6-N1-C2 | -7.64 | 117.25 | 120.30 |
| 2 | 2 | 282 | C | N3-C2-O2 | -7.64 | 116.55 | 121.90 |
| 2 | 2 | 2439 | G | N3-C4-N9 | 7.62 | 130.57 | 126.00 |
| 2 | 2 | 1703 | C | N1-C2-O2 | 7.61 | 123.47 | 118.90 |
| 2 | 2 | 2337 | C | N1-C2-O2 | 7.60 | 123.46 | 118.90 |
| 2 | 2 | 1081 | C | N1-C2-O2 | 7.59 | 123.46 | 118.90 |
| 2 | 2 | 4885 | U | N1-C2-O2 | 7.58 | 128.10 | 122.80 |
| 2 | 2 | 1401 | C | C2-N1-C1' | 7.57 | 127.13 | 118.80 |
| 2 | 2 | 2532 | C | C6-N1-C2 | -7.57 | 117.27 | 120.30 |
| 2 | 2 | 904 | C | N1-C2-O2 | 7.57 | 123.44 | 118.90 |
| 2 | 2 | 688 | U | N3-C2-O2 | -7.57 | 116.90 | 122.20 |
| 2 | 2 | 2486 | G | P-O3'-C3' | 7.57 | 128.78 | 119.70 |
| 2 | 2 | 4349 | C | N1-C2-O2 | 7.57 | 123.44 | 118.90 |
| 2 | 2 | 963 | G | C8-N9-C1' | -7.56 | 117.17 | 127.00 |
| 2 | 2 | 1994 | C | C6-N1-C1' | -7.56 | 111.73 | 120.80 |
| 2 | 2 | 2505 | C | C2-N1-C1' | 7.55 | 127.11 | 118.80 |
| 2 | 2 | 4275 | G | N3-C4-C5 | -7.55 | 124.82 | 128.60 |
| 50 | c | 237 | LEU | CA-CB-CG | 7.55 | 132.67 | 115.30 |
| 2 | 2 | 2262 | G | C8-N9-C1' | -7.54 | 117.19 | 127.00 |
| 2 | 2 | 2850 | A | C2-N3-C4 | 7.54 | 114.37 | 110.60 |
| 2 | 2 | 2563 | C | N1-C2-O2 | 7.53 | 123.42 | 118.90 |
| 2 | 2 | 1607 | C | N3-C2-O2 | -7.52 | 116.64 | 121.90 |
| 2 | 2 | 4206 | C | N1-C2-O2 | 7.50 | 123.40 | 118.90 |
| 5 | 8 | 64 | U | N1-C2-O2 | 7.50 | 128.05 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 47 | d | 24 | ASP | CB-CG-OD2 | 7.50 | 125.05 | 118.30 |
| 2 | 2 | 96 | U | N1-C2-O2 | 7.50 | 128.05 | 122.80 |
| 2 | 2 | 4747 | C | C6-N1-C2 | -7.50 | 117.30 | 120.30 |
| 2 | 2 | 4505 | C | C5-C6-N1 | 7.49 | 124.75 | 121.00 |
| 2 | 2 | 4775 | C | N3-C2-O2 | -7.49 | 116.66 | 121.90 |
| 2 | 2 | 4614 | G | C5-C6-O6 | 7.48 | 133.09 | 128.60 |
| 2 | 2 | 1921 | C | N1-C2-O2 | 7.48 | 123.39 | 118.90 |
| 2 | 2 | 3650 | C | C6-N1-C2 | -7.48 | 117.31 | 120.30 |
| 2 | 2 | 209 | U | N3-C2-O2 | -7.47 | 116.97 | 122.20 |
| 2 | 2 | 4505 | C | C2-N1-C1' | 7.46 | 127.00 | 118.80 |
| 2 | 2 | 115 | C | C2-N1-C1' | 7.44 | 126.99 | 118.80 |
| 2 | 2 | 5002 | U | N3-C2-O2 | -7.44 | 116.99 | 122.20 |
| 2 | 2 | 1096 | C | N1-C2-O2 | 7.43 | 123.36 | 118.90 |
| 2 | 2 | 178 | C | C5-C6-N1 | 7.43 | 124.72 | 121.00 |
| 2 | 2 | 489 | C | C6-N1-C2 | -7.43 | 117.33 | 120.30 |
| 2 | 2 | 4923 | C | C2-N1-C1' | 7.43 | 126.97 | 118.80 |
| 2 | 2 | 1720 | C | N1-C2-O2 | 7.43 | 123.36 | 118.90 |
| 2 | 2 | 472 | C | N1-C2-O2 | 7.43 | 123.36 | 118.90 |
| 2 | 2 | 1315 | C | C6-N1-C2 | -7.42 | 117.33 | 120.30 |
| 5 | 8 | 35 | C | C6-N1-C2 | -7.42 | 117.33 | 120.30 |
| 2 | 2 | 2814 | C | N1-C2-O2 | 7.40 | 123.34 | 118.90 |
| 2 | 2 | 1245 | C | C6-N1-C2 | -7.39 | 117.34 | 120.30 |
| 2 | 2 | 100 | C | C6-N1-C1' | -7.39 | 111.93 | 120.80 |
| 2 | 2 | 485 | C | C2-N1-C1' | 7.39 | 126.93 | 118.80 |
| 2 | 2 | 3905 | A | P-O3'-C3' | 7.37 | 128.55 | 119.70 |
| 2 | 2 | 753 | C | C6-N1-C2 | -7.36 | 117.36 | 120.30 |
| 2 | 2 | 112 | C | N1-C2-O2 | 7.36 | 123.31 | 118.90 |
| 2 | 2 | 365 | U | N1-C2-O2 | 7.36 | 127.95 | 122.80 |
| 2 | 2 | 1980 | U | P-O3'-C3' | 7.35 | 128.52 | 119.70 |
| 2 | 2 | 3622 | C | N1-C2-O2 | 7.34 | 123.31 | 118.90 |
| 2 | 2 | 115 | C | N1-C2-O2 | 7.34 | 123.30 | 118.90 |
| 2 | 2 | 753 | C | C6-N1-C1' | -7.34 | 112.00 | 120.80 |
| 2 | 2 | 2478 | C | N3-C2-O2 | -7.34 | 116.76 | 121.90 |
| 56 | 3 | 92 | C | C2-N1-C1' | 7.33 | 126.86 | 118.80 |
| 2 | 2 | 365 | U | N3-C2-O2 | -7.33 | 117.07 | 122.20 |
| 2 | 2 | 1726 | U | N1-C2-O2 | 7.33 | 127.93 | 122.80 |
| 2 | 2 | 4138 | C | N1-C2-O2 | 7.33 | 123.30 | 118.90 |
| 2 | 2 | 4561 | C | C6-N1-C2 | -7.32 | 117.37 | 120.30 |
| 2 | 2 | 4562 | C | N1-C2-O2 | 7.32 | 123.29 | 118.90 |
| 2 | 2 | 4426 | C | C5-C6-N1 | 7.31 | 124.66 | 121.00 |
| 2 | 2 | 4880 | C | N3-C2-O2 | -7.31 | 116.78 | 121.90 |
| 2 | 2 | 4294 | C | N1-C2-O2 | 7.31 | 123.28 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 1732 | C | C6-N1-C2 | -7.30 | 117.38 | 120.30 |
| 2 | 2 | 4133 | C | C6-N1-C2 | -7.30 | 117.38 | 120.30 |
| 2 | 2 | 3772 | U | N1-C2-O2 | 7.28 | 127.89 | 122.80 |
| 2 | 2 | 3926 | C | N1-C2-O2 | 7.28 | 123.27 | 118.90 |
| 2 | 2 | 467 | U | C2-N1-C1' | 7.27 | 126.43 | 117.70 |
| 56 | 3 | 57 | C | C6-N1-C2 | -7.26 | 117.39 | 120.30 |
| 2 | 2 | 2627 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 43 | 4 | 407 | ASP | CB-CG-OD1 | 7.26 | 124.84 | 118.30 |
| 2 | 2 | 516 | C | C2-N1-C1' | 7.25 | 126.77 | 118.80 |
| 2 | 2 | 672 | C | N1-C2-O2 | 7.24 | 123.25 | 118.90 |
| 2 | 2 | 1315 | C | C5-C6-N1 | 7.24 | 124.62 | 121.00 |
| 2 | 2 | 4162 | C | N1-C2-O2 | 7.24 | 123.25 | 118.90 |
| 2 | 2 | 1915 | C | N1-C2-O2 | 7.23 | 123.24 | 118.90 |
| 2 | 2 | 4402 | C | N1-C2-O2 | 7.22 | 123.23 | 118.90 |
| 2 | 2 | 1861 | U | N1-C2-O2 | 7.20 | 127.84 | 122.80 |
| 2 | 2 | 485 | C | N1-C2-O2 | 7.20 | 123.22 | 118.90 |
| 2 | 2 | 2033 | A | P-O3'-C3' | 7.20 | 128.34 | 119.70 |
| 2 | 2 | 3878 | C | C2-N1-C1' | 7.20 | 126.72 | 118.80 |
| 56 | 3 | 84 | U | C6-N1-C1' | -7.19 | 111.13 | 121.20 |
| 2 | 2 | 1276 | C | C6-N1-C2 | -7.19 | 117.42 | 120.30 |
| 35 | v | 87 | ASP | CB-CG-OD2 | 7.18 | 124.77 | 118.30 |
| 2 | 2 | 1402 | C | C5-C6-N1 | 7.18 | 124.59 | 121.00 |
| 2 | 2 | 1931 | C | P-O3'-C3' | 7.17 | 128.30 | 119.70 |
| 2 | 2 | 4266 | G | C2-N3-C4 | 7.16 | 115.48 | 111.90 |
| 2 | 2 | 4275 | G | N3-C4-N9 | 7.16 | 130.30 | 126.00 |
| 2 | 2 | 3774 | A | OP1-P-O3' | 7.16 | 120.95 | 105.20 |
| 2 | 2 | 1978 | C | C6-N1-C2 | -7.16 | 117.44 | 120.30 |
| 56 | 3 | 92 | C | C5-C6-N1 | 7.15 | 124.58 | 121.00 |
| 56 | 3 | 102 | U | N3-C2-O2 | -7.15 | 117.19 | 122.20 |
| 2 | 2 | 1993 | C | C6-N1-C2 | -7.14 | 117.44 | 120.30 |
| 2 | 2 | 688 | U | N1-C2-O2 | 7.13 | 127.80 | 122.80 |
| 2 | 2 | 985 | C | C2-N1-C1' | 7.13 | 126.65 | 118.80 |
| 2 | 2 | 2729 | C | C6-N1-C2 | -7.13 | 117.45 | 120.30 |
| 2 | 2 | 485 | C | C6-N1-C2 | -7.12 | 117.45 | 120.30 |
| 2 | 2 | 4148 | C | C2-N1-C1' | 7.12 | 126.63 | 118.80 |
| 2 | 2 | 4453 | C | N3-C2-O2 | -7.12 | 116.92 | 121.90 |
| 2 | 2 | 2362 | U | N1-C2-O2 | 7.11 | 127.78 | 122.80 |
| 2 | 2 | 4972 | U | N3-C2-O2 | -7.11 | 117.22 | 122.20 |
| 2 | 2 | 4712 | C | C6-N1-C2 | -7.11 | 117.46 | 120.30 |
| 2 | 2 | 1245 | C | C5-C6-N1 | 7.10 | 124.55 | 121.00 |
| 2 | 2 | 1816 | C | N1-C2-O2 | 7.09 | 123.15 | 118.90 |
| 2 | 2 | 390 | C | C5-C6-N1 | 7.09 | 124.54 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5 | 8 | 99 | U | N3-C2-O2 | -7.09 | 117.24 | 122.20 |
| 2 | 2 | 4996 | C | C6-N1-C2 | -7.09 | 117.47 | 120.30 |
| 2 | 2 | 155 | C | N1-C2-O2 | 7.08 | 123.15 | 118.90 |
| 2 | 2 | 4708 | A | C2-N3-C4 | 7.07 | 114.13 | 110.60 |
| 56 | 3 | 102 | U | N1-C2-O2 | 7.06 | 127.75 | 122.80 |
| 2 | 2 | 2290 | C | C6-N1-C2 | -7.06 | 117.48 | 120.30 |
| 2 | 2 | 4387 | C | C6-N1-C2 | -7.04 | 117.48 | 120.30 |
| 2 | 2 | 4887 | C | N3-C2-O2 | -7.04 | 116.97 | 121.90 |
| 15 | L | 102 | ASP | CB-CG-OD2 | 7.04 | 124.64 | 118.30 |
| 2 | 2 | 2281 | U | N1-C2-O2 | 7.04 | 127.73 | 122.80 |
| 2 | 2 | 4498 | U | N3-C2-O2 | -7.04 | 117.27 | 122.20 |
| 2 | 2 | 2094 | G | C4-N9-C1' | 7.03 | 135.64 | 126.50 |
| 2 | 2 | 4341 | C | N1-C2-O2 | 7.02 | 123.11 | 118.90 |
| 2 | 2 | 4710 | C | C6-N1-C2 | -7.02 | 117.49 | 120.30 |
| 2 | 2 | 4171 | C | C6-N1-C2 | -7.02 | 117.49 | 120.30 |
| 56 | 3 | 92 | C | N3-C2-O2 | -7.02 | 116.99 | 121.90 |
| 2 | 2 | 4275 | G | C8-N9-C1' | -7.01 | 117.89 | 127.00 |
| 2 | 2 | 4476 | C | C2-N1-C1' | 7.01 | 126.51 | 118.80 |
| 2 | 2 | 4112 | C | N1-C2-O2 | 7.01 | 123.11 | 118.90 |
| 2 | 2 | 472 | C | C5-C6-N1 | 7.01 | 124.50 | 121.00 |
| 2 | 2 | 2072 | C | C6-N1-C2 | -7.00 | 117.50 | 120.30 |
| 2 | 2 | 4229 | U | C6-N1-C1' | -7.00 | 111.40 | 121.20 |
| 2 | 2 | 4345 | C | C6-N1-C2 | -7.00 | 117.50 | 120.30 |
| 2 | 2 | 406 | C | P-O3'-C3' | 7.00 | 128.09 | 119.70 |
| 2 | 2 | 3637 | U | N3-C2-O2 | -7.00 | 117.30 | 122.20 |
| 2 | 2 | 4537 | C | C6-N1-C2 | -7.00 | 117.50 | 120.30 |
| 56 | 3 | 29 | C | C6-N1-C2 | -6.99 | 117.50 | 120.30 |
| 2 | 2 | 1458 | C | N3-C2-O2 | -6.99 | 117.01 | 121.90 |
| 2 | 2 | 1191 | C | N3-C2-O2 | -6.98 | 117.01 | 121.90 |
| 2 | 2 | 1096 | C | C6-N1-C2 | -6.98 | 117.51 | 120.30 |
| 2 | 2 | 1367 | C | C2-N1-C1' | 6.97 | 126.47 | 118.80 |
| 2 | 2 | 1216 | C | C5-C6-N1 | 6.96 | 124.48 | 121.00 |
| 2 | 2 | 1079 | C | N1-C2-O2 | 6.95 | 123.07 | 118.90 |
| 2 | 2 | 4284 | C | C2-N1-C1' | 6.95 | 126.45 | 118.80 |
| 2 | 2 | 2371 | U | N3-C2-O2 | -6.95 | 117.33 | 122.20 |
| 2 | 2 | 178 | C | C2-N1-C1' | 6.95 | 126.44 | 118.80 |
| 2 | 2 | 4294 | C | C5-C6-N1 | 6.95 | 124.47 | 121.00 |
| 2 | 2 | 4864 | U | C2-N1-C1' | 6.95 | 126.04 | 117.70 |
| 2 | 2 | 904 | C | N3-C2-O2 | -6.94 | 117.04 | 121.90 |
| 2 | 2 | 155 | C | N3-C2-O2 | -6.94 | 117.04 | 121.90 |
| 2 | 2 | 2892 | C | C2-N1-C1' | 6.93 | 126.42 | 118.80 |
| 56 | 3 | 95 | C | C6-N1-C1' | -6.93 | 112.48 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 4913 | G | P-O3'-C3' | 6.92 | 128.01 | 119.70 |
| 2 | 2 | 26 | C | N1-C2-O2 | 6.92 | 123.05 | 118.90 |
| 2 | 2 | 489 | C | C2-N1-C1' | 6.91 | 126.40 | 118.80 |
| 2 | 2 | 4771 | C | C6-N1-C2 | -6.91 | 117.54 | 120.30 |
| 2 | 2 | 657 | C | N1-C2-O2 | 6.91 | 123.04 | 118.90 |
| 2 | 2 | 4747 | C | C2-N1-C1' | 6.91 | 126.39 | 118.80 |
| 2 | 2 | 4231 | C | C5-C6-N1 | 6.90 | 124.45 | 121.00 |
| 2 | 2 | 1893 | C | C2-N1-C1' | 6.90 | 126.39 | 118.80 |
| 2 | 2 | 4266 | G | C8-N9-C1' | -6.89 | 118.04 | 127.00 |
| 2 | 2 | 516 | C | C5-C6-N1 | 6.89 | 124.44 | 121.00 |
| 2 | 2 | 49 | U | N3-C2-O2 | -6.88 | 117.38 | 122.20 |
| 2 | 2 | 4360 | U | N3-C2-O2 | -6.88 | 117.39 | 122.20 |
| 2 | 2 | 322 | C | C5-C6-N1 | 6.87 | 124.44 | 121.00 |
| 2 | 2 | 175 | C | C6-N1-C2 | -6.86 | 117.55 | 120.30 |
| 2 | 2 | 50 | C | N3-C2-O2 | -6.86 | 117.10 | 121.90 |
| 2 | 2 | 2653 | C | C6-N1-C2 | -6.86 | 117.56 | 120.30 |
| 2 | 2 | 112 | C | C5-C6-N1 | 6.85 | 124.42 | 121.00 |
| 56 | 3 | 57 | C | C5-C6-N1 | 6.85 | 124.42 | 121.00 |
| 2 | 2 | 5002 | U | N1-C2-O2 | 6.85 | 127.59 | 122.80 |
| 2 | 2 | 1401 | C | C6-N1-C2 | -6.84 | 117.56 | 120.30 |
| 2 | 2 | 4505 | C | N1-C2-O2 | 6.84 | 123.00 | 118.90 |
| 2 | 2 | 2533 | C | N1-C2-O2 | 6.83 | 123.00 | 118.90 |
| 2 | 2 | 3657 | U | N3-C2-O2 | -6.82 | 117.42 | 122.20 |
| 2 | 2 | 4350 | C | C5-C6-N1 | 6.82 | 124.41 | 121.00 |
| 2 | 2 | 4674 | C | C6-N1-C2 | -6.82 | 117.57 | 120.30 |
| 2 | 2 | 1216 | C | C6-N1-C1' | -6.81 | 112.62 | 120.80 |
| 2 | 2 | 4283 | G | N3-C4-N9 | 6.81 | 130.09 | 126.00 |
| 2 | 2 | 1245 | C | C2-N1-C1' | 6.81 | 126.29 | 118.80 |
| 2 | 2 | 2632 | U | N3-C2-O2 | -6.81 | 117.44 | 122.20 |
| 2 | 2 | 49 | U | N1-C2-O2 | 6.80 | 127.56 | 122.80 |
| 2 | 2 | 4508 | C | N1-C2-O2 | 6.80 | 122.98 | 118.90 |
| 2 | 2 | 985 | C | C5-C6-N1 | 6.80 | 124.40 | 121.00 |
| 2 | 2 | 1477 | C | C2-N1-C1' | 6.79 | 126.27 | 118.80 |
| 40 | R | 235 | MET | CA-CB-CG | 6.79 | 124.85 | 113.30 |
| 2 | 2 | 4423 | U | C5-C6-N1 | 6.79 | 126.09 | 122.70 |
| 2 | 2 | 1860 | U | N3-C2-O2 | -6.79 | 117.45 | 122.20 |
| 2 | 2 | 4426 | C | N1-C2-O2 | 6.79 | 122.97 | 118.90 |
| 40 | R | 211 | LEU | CB-CG-CD2 | 6.79 | 122.53 | 111.00 |
| 56 | 3 | 84 | U | C5-C4-O4 | -6.78 | 121.83 | 125.90 |
| 2 | 2 | 4880 | C | C6-N1-C2 | -6.78 | 117.59 | 120.30 |
| 2 | 2 | 282 | C | C6-N1-C2 | -6.77 | 117.59 | 120.30 |
| 2 | 2 | 4709 | U | C2-N1-C1' | 6.77 | 125.83 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 1190 | C | N1-C2-O2 | 6.76 | 122.95 | 118.90 |
| 2 | 2 | 2101 | C | C6-N1-C2 | -6.76 | 117.60 | 120.30 |
| 2 | 2 | 44 | A | C2-N3-C4 | 6.76 | 113.98 | 110.60 |
| 2 | 2 | 4887 | C | C6-N1-C2 | -6.76 | 117.60 | 120.30 |
| 2 | 2 | 4714 | C | N3-C2-O2 | -6.75 | 117.17 | 121.90 |
| 2 | 2 | 3636 | C | C5-C6-N1 | 6.75 | 124.37 | 121.00 |
| 2 | 2 | 1720 | C | C6-N1-C2 | -6.74 | 117.60 | 120.30 |
| 2 | 2 | 3892 | U | N3-C2-O2 | -6.74 | 117.48 | 122.20 |
| 2 | 2 | 4923 | C | C5-C6-N1 | 6.74 | 124.37 | 121.00 |
| 2 | 2 | 2528 | G | C8-N9-C1' | -6.73 | 118.25 | 127.00 |
| 2 | 2 | 3892 | U | N1-C2-O2 | 6.73 | 127.51 | 122.80 |
| 2 | 2 | 972 | C | N1-C2-O2 | 6.73 | 122.94 | 118.90 |
| 2 | 2 | 26 | C | C6-N1-C2 | -6.73 | 117.61 | 120.30 |
| 2 | 2 | 4627 | U | N3-C2-O2 | -6.73 | 117.49 | 122.20 |
| 2 | 2 | 4299 | U | N3-C2-O2 | -6.73 | 117.49 | 122.20 |
| 2 | 2 | 2281 | U | N3-C2-O2 | -6.72 | 117.49 | 122.20 |
| 56 | 3 | 24 | C | N1-C2-O2 | 6.72 | 122.93 | 118.90 |
| 2 | 2 | 2589 | C | C6-N1-C2 | -6.72 | 117.61 | 120.30 |
| 2 | 2 | 4120 | U | C2-N1-C1' | 6.71 | 125.76 | 117.70 |
| 2 | 2 | 4714 | C | C5-C6-N1 | 6.71 | 124.36 | 121.00 |
| 56 | 3 | 26 | C | C6-N1-C2 | -6.71 | 117.62 | 120.30 |
| 47 | d | 43 | LEU | CA-CB-CG | 6.71 | 130.72 | 115.30 |
| 2 | 2 | 2729 | C | C2-N1-C1' | 6.70 | 126.17 | 118.80 |
| 2 | 2 | 322 | C | C2-N1-C1' | 6.69 | 126.16 | 118.80 |
| 2 | 2 | 4561 | C | N1-C2-O2 | 6.69 | 122.91 | 118.90 |
| 2 | 2 | 4423 | U | C6-N1-C1' | -6.68 | 111.84 | 121.20 |
| 2 | 2 | 4522 | G | C4-N9-C1' | 6.68 | 135.18 | 126.50 |
| 2 | 2 | 1401 | C | N1-C2-O2 | 6.67 | 122.90 | 118.90 |
| 2 | 2 | 1428 | U | N3-C2-O2 | -6.67 | 117.53 | 122.20 |
| 2 | 2 | 972 | C | C6-N1-C2 | -6.67 | 117.63 | 120.30 |
| 2 | 2 | 4481 | U | N3-C2-O2 | -6.66 | 117.53 | 122.20 |
| 5 | 8 | 99 | U | N1-C2-O2 | 6.66 | 127.46 | 122.80 |
| 2 | 2 | 1963 | C | C5-C6-N1 | 6.65 | 124.33 | 121.00 |
| 5 | 8 | 54 | C | C6-N1-C2 | -6.65 | 117.64 | 120.30 |
| 2 | 2 | 1814 | C | C5-C6-N1 | 6.65 | 124.32 | 121.00 |
| 2 | 2 | 1469 | C | C6-N1-C2 | -6.64 | 117.64 | 120.30 |
| 58 | g | 118 | ASP | CB-CG-OD2 | 6.64 | 124.28 | 118.30 |
| 5 | 8 | 111 | U | C2-N1-C1' | 6.64 | 125.67 | 117.70 |
| 2 | 2 | 2615 | C | N1-C2-O2 | 6.63 | 122.88 | 118.90 |
| 56 | 3 | 51 | G | P-O3'-C3' | 6.62 | 127.65 | 119.70 |
| 2 | 2 | 3587 | C | N1-C2-O2 | 6.62 | 122.87 | 118.90 |
| 2 | 2 | 274 | C | C2-N1-C1' | 6.61 | 126.08 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 4563 | U | N3-C2-O2 | -6.61 | 117.57 | 122.20 |
| 2 | 2 | 1694 | C | C6-N1-C2 | -6.61 | 117.66 | 120.30 |
| 2 | 2 | 1856 | C | C6-N1-C2 | -6.61 | 117.66 | 120.30 |
| 2 | 2 | 3637 | U | N1-C2-O2 | 6.61 | 127.42 | 122.80 |
| 56 | 3 | 72 | U | OP1-P-OP2 | -6.61 | 109.69 | 119.60 |
| 2 | 2 | 2478 | C | C6-N1-C2 | -6.60 | 117.66 | 120.30 |
| 2 | 2 | 3882 | C | C6-N1-C2 | -6.60 | 117.66 | 120.30 |
| 2 | 2 | 2772 | C | N1-C2-O2 | 6.59 | 122.86 | 118.90 |
| 2 | 2 | 1796 | U | C2-N1-C1' | 6.59 | 125.61 | 117.70 |
| 2 | 2 | 673 | C | C6-N1-C2 | -6.58 | 117.67 | 120.30 |
| 2 | 2 | 4771 | C | N1-C2-O2 | 6.58 | 122.85 | 118.90 |
| 2 | 2 | 4972 | U | N1-C2-O2 | 6.58 | 127.40 | 122.80 |
| 2 | 2 | 1344 | C | C2-N1-C1' | 6.57 | 126.03 | 118.80 |
| 2 | 2 | 2031 | C | C6-N1-C2 | -6.57 | 117.67 | 120.30 |
| 2 | 2 | 2532 | C | C5-C6-N1 | 6.56 | 124.28 | 121.00 |
| 2 | 2 | 489 | C | C5-C6-N1 | 6.55 | 124.27 | 121.00 |
| 2 | 2 | 1812 | C | C6-N1-C2 | -6.54 | 117.68 | 120.30 |
| 2 | 2 | 2017 | A | O4'-C1'-N9 | 6.54 | 113.43 | 108.20 |
| 2 | 2 | 1250 | C | N1-C2-O2 | 6.53 | 122.82 | 118.90 |
| 31 | o | 202 | ASP | CB-CG-OD2 | 6.53 | 124.18 | 118.30 |
| 2 | 2 | 1993 | C | C5-C6-N1 | 6.52 | 124.26 | 121.00 |
| 2 | 2 | 4695 | C | N3-C2-O2 | -6.52 | 117.33 | 121.90 |
| 2 | 2 | 4627 | U | N1-C2-O2 | 6.52 | 127.37 | 122.80 |
| 2 | 2 | 1428 | U | N1-C2-O2 | 6.51 | 127.36 | 122.80 |
| 2 | 2 | 1477 | C | N1-C2-O2 | 6.51 | 122.81 | 118.90 |
| 2 | 2 | 1702 | C | C2-N1-C1' | 6.51 | 125.97 | 118.80 |
| 2 | 2 | 2856 | C | N1-C2-O2 | 6.51 | 122.81 | 118.90 |
| 2 | 2 | 3690 | U | N3-C2-O2 | -6.51 | 117.64 | 122.20 |
| 2 | 2 | 1893 | C | C5-C6-N1 | 6.51 | 124.26 | 121.00 |
| 2 | 2 | 1402 | C | C2-N1-C1' | 6.51 | 125.96 | 118.80 |
| 2 | 2 | 4319 | C | N1-C2-O2 | 6.51 | 122.81 | 118.90 |
| 20 | U | 147 | ASP | CB-CG-OD2 | 6.51 | 124.16 | 118.30 |
| 2 | 2 | 2011 | C | C6-N1-C2 | -6.50 | 117.70 | 120.30 |
| 2 | 2 | 3769 | C | N1-C2-O2 | 6.50 | 122.80 | 118.90 |
| 2 | 2 | 985 | C | N3-C2-O2 | -6.49 | 117.36 | 121.90 |
| 2 | 2 | 30 | C | C6-N1-C2 | -6.49 | 117.70 | 120.30 |
| 56 | 3 | 72 | U | P-O3'-C3' | 6.49 | 127.49 | 119.70 |
| 41 | W | 260 | LEU | CA-CB-CG | 6.49 | 130.22 | 115.30 |
| 2 | 2 | 1663 | C | C6-N1-C2 | -6.49 | 117.71 | 120.30 |
| 2 | 2 | 1367 | C | N1-C2-O2 | 6.48 | 122.79 | 118.90 |
| 2 | 2 | 1663 | C | C5-C6-N1 | 6.48 | 124.24 | 121.00 |
| 2 | 2 | 4123 | C | N3-C2-O2 | -6.48 | 117.36 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 4133 | C | C2-N1-C1' | 6.48 | 125.93 | 118.80 |
| 2 | 2 | 4880 | C | C2-N1-C1' | 6.48 | 125.92 | 118.80 |
| 2 | 2 | 1477 | C | C5-C6-N1 | 6.47 | 124.24 | 121.00 |
| 2 | 2 | 4887 | C | C2-N1-C1' | 6.47 | 125.92 | 118.80 |
| 2 | 2 | 1096 | C | C5-C6-N1 | 6.47 | 124.23 | 121.00 |
| 2 | 2 | 126 | C | C6-N1-C2 | -6.47 | 117.71 | 120.30 |
| 2 | 2 | 274 | C | C6-N1-C2 | -6.47 | 117.71 | 120.30 |
| 2 | 2 | 1808 | C | P-O3'-C3' | 6.46 | 127.46 | 119.70 |
| 2 | 2 | 1861 | U | N3-C2-O2 | -6.46 | 117.68 | 122.20 |
| 2 | 2 | 122 | U | N3-C2-O2 | -6.46 | 117.68 | 122.20 |
| 2 | 2 | 4387 | C | N1-C2-O2 | 6.46 | 122.78 | 118.90 |
| 2 | 2 | 204 | U | N3-C2-O2 | -6.46 | 117.68 | 122.20 |
| 2 | 2 | 1402 | C | N1-C2-O2 | 6.45 | 122.77 | 118.90 |
| 2 | 2 | 9 | C | C6-N1-C2 | -6.45 | 117.72 | 120.30 |
| 2 | 2 | 1938 | C | N1-C2-O2 | 6.45 | 122.77 | 118.90 |
| 2 | 2 | 2592 | U | N3-C2-O2 | -6.44 | 117.69 | 122.20 |
| 2 | 2 | 4350 | C | C2-N1-C1' | 6.44 | 125.89 | 118.80 |
| 2 | 2 | 4423 | U | C6-N1-C2 | -6.44 | 117.14 | 121.00 |
| 2 | 2 | 4288 | C | N3-C4-C5 | 6.44 | 124.47 | 121.90 |
| 2 | 2 | 1325 | C | N1-C2-O2 | 6.43 | 122.76 | 118.90 |
| 2 | 2 | 4402 | C | C6-N1-C2 | -6.43 | 117.73 | 120.30 |
| 2 | 2 | 4710 | C | C5-C6-N1 | 6.43 | 124.22 | 121.00 |
| 2 | 2 | 50 | C | C6-N1-C2 | -6.43 | 117.73 | 120.30 |
| 2 | 2 | 2892 | C | C6-N1-C2 | -6.42 | 117.73 | 120.30 |
| 2 | 2 | 4498 | U | C6-N1-C1' | -6.42 | 112.21 | 121.20 |
| 2 | 2 | 4561 | C | C2-N1-C1' | 6.42 | 125.86 | 118.80 |
| 2 | 2 | 5008 | C | N1-C2-O2 | 6.42 | 122.75 | 118.90 |
| 2 | 2 | 2011 | C | N3-C2-O2 | -6.42 | 117.41 | 121.90 |
| 2 | 2 | 1276 | C | N3-C2-O2 | -6.41 | 117.41 | 121.90 |
| 2 | 2 | 4148 | C | C5-C6-N1 | 6.41 | 124.21 | 121.00 |
| 2 | 2 | 4476 | C | N1-C2-O2 | 6.41 | 122.75 | 118.90 |
| 2 | 2 | 2667 | C | N3-C2-O2 | -6.41 | 117.42 | 121.90 |
| 2 | 2 | 2791 | C | C6-N1-C2 | -6.41 | 117.74 | 120.30 |
| 2 | 2 | 1963 | C | C2-N1-C1' | 6.40 | 125.84 | 118.80 |
| 2 | 2 | 3631 | U | N3-C2-O2 | -6.40 | 117.72 | 122.20 |
| 2 | 2 | 3848 | U | N3-C2-O2 | -6.40 | 117.72 | 122.20 |
| 2 | 2 | 2038 | U | N3-C2-O2 | -6.40 | 117.72 | 122.20 |
| 2 | 2 | 1812 | C | C5-C6-N1 | 6.39 | 124.20 | 121.00 |
| 2 | 2 | 2532 | C | C2-N1-C1' | 6.39 | 125.83 | 118.80 |
| 2 | 2 | 1097 | C | C6-N1-C2 | -6.39 | 117.74 | 120.30 |
| 2 | 2 | 2632 | U | N1-C2-O2 | 6.39 | 127.28 | 122.80 |
| 2 | 2 | 4969 | C | C6-N1-C2 | -6.39 | 117.74 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 1702 | C | N1-C2-O2 | 6.39 | 122.73 | 118.90 |
| 2 | 2 | 2867 | C | C6-N1-C2 | -6.39 | 117.75 | 120.30 |
| 2 | 2 | 4771 | C | C5-C6-N1 | 6.38 | 124.19 | 121.00 |
| 2 | 2 | 26 | C | C2-N1-C1' | 6.38 | 125.82 | 118.80 |
| 2 | 2 | 1978 | C | N3-C2-O2 | -6.37 | 117.44 | 121.90 |
| 2 | 2 | 4294 | C | C2-N1-C1' | 6.37 | 125.81 | 118.80 |
| 2 | 2 | 1994 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 2 | 2 | 2037 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 2 | 2 | 1467 | C | C6-N1-C2 | -6.36 | 117.75 | 120.30 |
| 2 | 2 | 1822 | U | N1-C2-O2 | 6.36 | 127.25 | 122.80 |
| 2 | 2 | 3866 | C | C5-C6-N1 | 6.36 | 124.18 | 121.00 |
| 2 | 2 | 489 | C | N1-C2-O2 | 6.36 | 122.72 | 118.90 |
| 2 | 2 | 1607 | C | C6-N1-C2 | -6.36 | 117.76 | 120.30 |
| 2 | 2 | 86 | U | N3-C2-O2 | -6.36 | 117.75 | 122.20 |
| 2 | 2 | 1251 | C | C6-N1-C2 | -6.36 | 117.76 | 120.30 |
| 2 | 2 | 2820 | C | C2-N1-C1' | 6.36 | 125.79 | 118.80 |
| 2 | 2 | 4747 | C | C5-C6-N1 | 6.36 | 124.18 | 121.00 |
| 2 | 2 | 100 | C | C5-C6-N1 | 6.35 | 124.18 | 121.00 |
| 2 | 2 | 4695 | C | C6-N1-C2 | -6.35 | 117.76 | 120.30 |
| 2 | 2 | 4283 | G | C4-N9-C1' | 6.35 | 134.75 | 126.50 |
| 2 | 2 | 440 | U | N3-C2-O2 | -6.35 | 117.76 | 122.20 |
| 2 | 2 | 2094 | G | N3-C4-N9 | 6.35 | 129.81 | 126.00 |
| 2 | 2 | 4387 | C | C2-N1-C1' | 6.35 | 125.78 | 118.80 |
| 2 | 2 | 4284 | C | N1-C2-O2 | 6.34 | 122.71 | 118.90 |
| 2 | 2 | 4171 | C | N3-C2-O2 | -6.34 | 117.46 | 121.90 |
| 30 | n | 5 | LEU | CA-CB-CG | 6.34 | 129.88 | 115.30 |
| 2 | 2 | 3915 | U | N3-C2-O2 | -6.34 | 117.77 | 122.20 |
| 5 | 8 | 153 | C | C6-N1-C2 | -6.33 | 117.77 | 120.30 |
| 5 | 8 | 54 | C | N3-C2-O2 | -6.32 | 117.47 | 121.90 |
| 2 | 2 | 141 | C | C6-N1-C1' | -6.32 | 113.21 | 120.80 |
| 2 | 2 | 4133 | C | C5-C6-N1 | 6.32 | 124.16 | 121.00 |
| 2 | 2 | 4299 | U | N1-C2-O2 | 6.32 | 127.22 | 122.80 |
| 56 | 3 | 3 | C | C6-N1-C2 | -6.32 | 117.77 | 120.30 |
| 2 | 2 | 712 | C | C6-N1-C2 | -6.32 | 117.77 | 120.30 |
| 2 | 2 | 4471 | U | N3-C2-O2 | -6.32 | 117.78 | 122.20 |
| 2 | 2 | 1893 | C | N1-C2-O2 | 6.31 | 122.69 | 118.90 |
| 2 | 2 | 4149 | C | C2-N1-C1' | 6.31 | 125.74 | 118.80 |
| 2 | 2 | 4262 | C | C6-N1-C2 | -6.31 | 117.78 | 120.30 |
| 2 | 2 | 1822 | U | N3-C2-O2 | -6.31 | 117.78 | 122.20 |
| 2 | 2 | 3851 | U | N3-C2-O2 | -6.31 | 117.78 | 122.20 |
| 2 | 2 | 3870 | C | C6-N1-C2 | -6.31 | 117.78 | 120.30 |
| 5 | 8 | 101 | C | C6-N1-C2 | -6.31 | 117.78 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 4923 | C | N1-C2-O2 | 6.31 | 122.68 | 118.90 |
| 2 | 2 | 2019 | C | C6-N1-C2 | -6.30 | 117.78 | 120.30 |
| 2 | 2 | 2371 | U | N1-C2-O2 | 6.30 | 127.21 | 122.80 |
| 2 | 2 | 1566 | C | C6-N1-C2 | -6.29 | 117.78 | 120.30 |
| 2 | 2 | 2337 | C | N3-C2-O2 | -6.29 | 117.50 | 121.90 |
| 2 | 2 | 3739 | C | C6-N1-C2 | -6.29 | 117.78 | 120.30 |
| 2 | 2 | 4561 | C | C5-C6-N1 | 6.29 | 124.14 | 121.00 |
| 2 | 2 | 345 | C | C6-N1-C2 | -6.29 | 117.78 | 120.30 |
| 2 | 2 | 4406 | U | C2-N1-C1' | 6.28 | 125.24 | 117.70 |
| 56 | 3 | 29 | C | C5-C6-N1 | 6.28 | 124.14 | 121.00 |
| 2 | 2 | 4133 | C | N1-C2-O2 | 6.28 | 122.67 | 118.90 |
| 2 | 2 | 322 | C | N1-C2-O2 | 6.28 | 122.67 | 118.90 |
| 2 | 2 | 3606 | U | N3-C2-O2 | -6.28 | 117.81 | 122.20 |
| 2 | 2 | 3622 | C | C6-N1-C2 | -6.28 | 117.79 | 120.30 |
| 2 | 2 | 4137 | C | N1-C2-O2 | 6.28 | 122.67 | 118.90 |
| 2 | 2 | 4406 | U | N3-C2-O2 | -6.27 | 117.81 | 122.20 |
| 2 | 2 | 4426 | C | N3-C2-O2 | -6.27 | 117.51 | 121.90 |
| 2 | 2 | 485 | C | OP1-P-O3' | 6.27 | 118.99 | 105.20 |
| 2 | 2 | 1938 | C | C2-N1-C1' | 6.26 | 125.69 | 118.80 |
| 2 | 2 | 984 | C | C6-N1-C2 | -6.26 | 117.80 | 120.30 |
| 2 | 2 | 4350 | C | N1-C2-O2 | 6.25 | 122.65 | 118.90 |
| 2 | 2 | 3878 | C | N3-C2-O2 | -6.25 | 117.53 | 121.90 |
| 2 | 2 | 1856 | C | C2-N1-C1' | 6.25 | 125.67 | 118.80 |
| 2 | 2 | 1472 | C | C2-N1-C1' | 6.24 | 125.67 | 118.80 |
| 2 | 2 | 204 | U | N1-C2-O2 | 6.24 | 127.17 | 122.80 |
| 2 | 2 | 4481 | U | N1-C2-O2 | 6.24 | 127.17 | 122.80 |
| 56 | 3 | 26 | C | N1-C2-O2 | 6.24 | 122.64 | 118.90 |
| 2 | 2 | 195 | C | C5-C6-N1 | 6.24 | 124.12 | 121.00 |
| 2 | 2 | 1732 | C | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 2 | 2 | 1325 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 2 | 2 | 1686 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 2 | 2 | 2563 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 2 | 2 | 2729 | C | C5-C6-N1 | 6.23 | 124.11 | 121.00 |
| 40 | R | 51 | MET | CA-CB-CG | 6.23 | 123.89 | 113.30 |
| 2 | 2 | 4148 | C | C6-N1-C2 | -6.22 | 117.81 | 120.30 |
| 2 | 2 | 4241 | C | C6-N1-C2 | -6.22 | 117.81 | 120.30 |
| 59 | f | 206 | LEU | CA-CB-CG | 6.22 | 129.60 | 115.30 |
| 2 | 2 | 2008 | U | C2-N1-C1' | 6.21 | 125.16 | 117.70 |
| 2 | 2 | 1796 | U | N1-C2-O2 | 6.21 | 127.15 | 122.80 |
| 2 | 2 | 1963 | C | N3-C2-O2 | -6.21 | 117.55 | 121.90 |
| 2 | 2 | 4775 | C | C6-N1-C1' | -6.21 | 113.35 | 120.80 |
| 2 | 2 | 2019 | C | N1-C2-O2 | 6.21 | 122.62 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 19 | S | 32 | ASP | CB-CG-OD1 | 6.21 | 123.89 | 118.30 |
| 2 | 2 | 2563 | C | N3-C2-O2 | -6.20 | 117.56 | 121.90 |
| 2 | 2 | 3721 | U | N3-C2-O2 | -6.20 | 117.86 | 122.20 |
| 2 | 2 | 1202 | C | C6-N1-C2 | -6.20 | 117.82 | 120.30 |
| 2 | 2 | 4429 | C | N1-C2-O2 | 6.20 | 122.62 | 118.90 |
| 2 | 2 | 4497 | U | N3-C2-O2 | -6.20 | 117.86 | 122.20 |
| 2 | 2 | 4921 | C | N1-C2-O2 | 6.20 | 122.62 | 118.90 |
| 2 | 2 | 2072 | C | C5-C6-N1 | 6.19 | 124.10 | 121.00 |
| 2 | 2 | 115 | C | N3-C2-O2 | -6.19 | 117.57 | 121.90 |
| 2 | 2 | 4775 | C | C6-N1-C2 | -6.17 | 117.83 | 120.30 |
| 2 | 2 | 4970 | C | C6-N1-C2 | -6.17 | 117.83 | 120.30 |
| 2 | 2 | 2351 | C | N1-C2-O2 | 6.16 | 122.60 | 118.90 |
| 2 | 2 | 3866 | C | C6-N1-C2 | -6.16 | 117.84 | 120.30 |
| 2 | 2 | 4502 | C | N1-C2-O2 | 6.16 | 122.60 | 118.90 |
| 2 | 2 | 2062 | C | C6-N1-C2 | -6.15 | 117.84 | 120.30 |
| 2 | 2 | 1448 | G | C4-N9-C1' | 6.15 | 134.50 | 126.50 |
| 2 | 2 | 2667 | C | C6-N1-C2 | -6.15 | 117.84 | 120.30 |
| 5 | 8 | 32 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 2 | 2 | 68 | U | N3-C2-O2 | -6.15 | 117.90 | 122.20 |
| 2 | 2 | 4112 | C | N3-C2-O2 | -6.14 | 117.60 | 121.90 |
| 2 | 2 | 4308 | C | N1-C2-O2 | 6.14 | 122.59 | 118.90 |
| 2 | 2 | 3650 | C | C5-C6-N1 | 6.14 | 124.07 | 121.00 |
| 2 | 2 | 1378 | C | C2-N1-C1' | 6.14 | 125.55 | 118.80 |
| 2 | 2 | 2892 | C | C5-C6-N1 | 6.14 | 124.07 | 121.00 |
| 2 | 2 | 1439 | C | C6-N1-C2 | -6.13 | 117.85 | 120.30 |
| 2 | 2 | 1666 | C | C6-N1-C2 | -6.13 | 117.85 | 120.30 |
| 5 | 8 | 32 | C | C6-N1-C2 | -6.13 | 117.85 | 120.30 |
| 2 | 2 | 1860 | U | N1-C2-O2 | 6.12 | 127.08 | 122.80 |
| 2 | 2 | 4682 | U | C2-N1-C1' | 6.12 | 125.04 | 117.70 |
| 2 | 2 | 274 | C | N1-C2-O2 | 6.12 | 122.57 | 118.90 |
| 2 | 2 | 672 | C | N3-C2-O2 | -6.12 | 117.62 | 121.90 |
| 2 | 2 | 1401 | C | C5-C6-N1 | 6.12 | 124.06 | 121.00 |
| 2 | 2 | 2002 | A | C2-N3-C4 | 6.12 | 113.66 | 110.60 |
| 5 | 8 | 96 | C | C6-N1-C2 | -6.12 | 117.85 | 120.30 |
| 2 | 2 | 281 | U | N3-C2-O2 | -6.11 | 117.92 | 122.20 |
| 2 | 2 | 753 | C | C5-C6-N1 | 6.11 | 124.05 | 121.00 |
| 2 | 2 | 2486 | G | OP1-P-O3' | 6.10 | 118.63 | 105.20 |
| 2 | 2 | 4231 | C | C6-N1-C1' | -6.10 | 113.48 | 120.80 |
| 5 | 8 | 111 | U | N1-C2-O2 | 6.09 | 127.07 | 122.80 |
| 2 | 2 | 4563 | U | N1-C2-O2 | 6.09 | 127.06 | 122.80 |
| 2 | 2 | 1720 | C | N3-C2-O2 | -6.09 | 117.64 | 121.90 |
| 2 | 2 | 4464 | A | C2-N3-C4 | 6.09 | 113.64 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 390 | C | C2-N1-C1' | 6.08 | 125.49 | 118.80 |
| 2 | 2 | 694 | C | N1-C2-O2 | 6.08 | 122.55 | 118.90 |
| 2 | 2 | 3926 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 2 | 2 | 1241 | C | N3-C2-O2 | -6.08 | 117.65 | 121.90 |
| 2 | 2 | 2820 | C | C5-C6-N1 | 6.07 | 124.04 | 121.00 |
| 2 | 2 | 4319 | C | C5-C6-N1 | 6.07 | 124.04 | 121.00 |
| 2 | 2 | 1429 | C | C6-N1-C2 | -6.07 | 117.87 | 120.30 |
| 2 | 2 | 1472 | C | N1-C2-O2 | 6.07 | 122.54 | 118.90 |
| 2 | 2 | 4569 | U | N3-C2-O2 | -6.07 | 117.95 | 122.20 |
| 2 | 2 | 1309 | C | C6-N1-C2 | -6.06 | 117.87 | 120.30 |
| 2 | 2 | 1577 | G | N3-C2-N2 | -6.06 | 115.66 | 119.90 |
| 2 | 2 | 1381 | U | N1-C2-O2 | 6.06 | 127.04 | 122.80 |
| 2 | 2 | 2264 | C | N1-C2-O2 | 6.06 | 122.54 | 118.90 |
| 33 | r | 310 | LEU | CA-CB-CG | 6.06 | 129.24 | 115.30 |
| 2 | 2 | 1568 | C | C6-N1-C2 | -6.06 | 117.88 | 120.30 |
| 2 | 2 | 4895 | C | N1-C2-O2 | 6.06 | 122.53 | 118.90 |
| 2 | 2 | 4147 | G | N1-C6-O6 | -6.06 | 116.27 | 119.90 |
| 2 | 2 | 1795 | A | C4-N9-C1' | 6.05 | 137.19 | 126.30 |
| 2 | 2 | 1796 | U | N3-C2-O2 | -6.05 | 117.96 | 122.20 |
| 2 | 2 | 1678 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 2 | 2 | 2362 | U | C2-N1-C1' | 6.05 | 124.96 | 117.70 |
| 2 | 2 | 1344 | C | C5-C6-N1 | 6.04 | 124.02 | 121.00 |
| 2 | 2 | 1662 | C | C6-N1-C2 | -6.04 | 117.89 | 120.30 |
| 2 | 2 | 1191 | C | N1-C2-O2 | 6.04 | 122.52 | 118.90 |
| 2 | 2 | 1203 | G | N3-C4-C5 | -6.04 | 125.58 | 128.60 |
| 2 | 2 | 4945 | G | N3-C4-N9 | 6.04 | 129.62 | 126.00 |
| 5 | 8 | 96 | C | N1-C2-O2 | 6.04 | 122.52 | 118.90 |
| 2 | 2 | 36 | U | N3-C2-O2 | -6.03 | 117.98 | 122.20 |
| 2 | 2 | 4207 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 2 | 2 | 4402 | C | N3-C2-O2 | -6.03 | 117.68 | 121.90 |
| 2 | 2 | 3606 | U | N1-C2-O2 | 6.03 | 127.02 | 122.80 |
| 2 | 2 | 4360 | U | N1-C2-O2 | 6.03 | 127.02 | 122.80 |
| 2 | 2 | 750 | U | N3-C2-O2 | -6.02 | 117.98 | 122.20 |
| 2 | 2 | 2892 | C | N1-C2-O2 | 6.02 | 122.51 | 118.90 |
| 5 | 8 | 35 | C | C5-C6-N1 | 6.01 | 124.01 | 121.00 |
| 2 | 2 | 78 | U | N3-C2-O2 | -6.01 | 117.99 | 122.20 |
| 2 | 2 | 4440 | G | N3-C4-N9 | 6.01 | 129.61 | 126.00 |
| 2 | 2 | 4261 | C | C6-N1-C2 | -6.01 | 117.90 | 120.30 |
| 2 | 2 | 4764 | A | N1-C2-N3 | -6.01 | 126.30 | 129.30 |
| 2 | 2 | 3882 | C | C2-N1-C1' | 6.01 | 125.41 | 118.80 |
| 2 | 2 | 657 | C | C6-N1-C2 | -6.01 | 117.90 | 120.30 |
| 30 | n | 105 | LEU | C-N-CA | 6.01 | 136.72 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 3851 | U | N1-C2-O2 | 6.00 | 127.00 | 122.80 |
| 9 | D | 138 | MET | CG-SD-CE | 6.00 | 109.81 | 100.20 |
| 2 | 2 | 679 | C | C6-N1-C2 | -6.00 | 117.90 | 120.30 |
| 2 | 2 | 4262 | C | C5-C6-N1 | 6.00 | 124.00 | 121.00 |
| 2 | 2 | 4895 | C | C2-N1-C1' | 6.00 | 125.40 | 118.80 |
| 2 | 2 | 1250 | C | N3-C2-O2 | -5.99 | 117.70 | 121.90 |
| 2 | 2 | 2403 | A | C2-N3-C4 | 5.99 | 113.60 | 110.60 |
| 2 | 2 | 2532 | C | N1-C2-O2 | 5.99 | 122.49 | 118.90 |
| 2 | 2 | 3690 | U | N1-C2-O2 | 5.99 | 126.99 | 122.80 |
| 1 | N | 345 | PRO | CA-N-CD | -5.99 | 103.12 | 111.50 |
| 2 | 2 | 1381 | U | N3-C2-O2 | -5.99 | 118.01 | 122.20 |
| 2 | 2 | 86 | U | N1-C2-O2 | 5.98 | 126.99 | 122.80 |
| 2 | 2 | 1472 | C | C6-N1-C2 | -5.98 | 117.91 | 120.30 |
| 2 | 2 | 4562 | C | N3-C2-O2 | -5.98 | 117.71 | 121.90 |
| 5 | 8 | 111 | U | N3-C2-O2 | -5.98 | 118.02 | 122.20 |
| 2 | 2 | 440 | U | N1-C2-O2 | 5.97 | 126.98 | 122.80 |
| 2 | 2 | 4068 | U | C2-N1-C1' | 5.97 | 124.87 | 117.70 |
| 2 | 2 | 1309 | C | C5-C6-N1 | 5.97 | 123.99 | 121.00 |
| 2 | 2 | 2094 | G | N3-C4-C5 | -5.97 | 125.61 | 128.60 |
| 2 | 2 | 988 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 2 | 2 | 988 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 2 | 2 | 1378 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 2 | 2 | 4502 | C | C2-N1-C1' | 5.96 | 125.36 | 118.80 |
| 2 | 2 | 36 | U | N1-C2-O2 | 5.96 | 126.97 | 122.80 |
| 2 | 2 | 2445 | C | C6-N1-C2 | -5.96 | 117.92 | 120.30 |
| 2 | 2 | 2094 | G | C8-N9-C1' | -5.96 | 119.26 | 127.00 |
| 2 | 2 | 259 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 2 | 2 | 2478 | C | C6-N1-C1' | -5.94 | 113.67 | 120.80 |
| 5 | 8 | 4 | C | C6-N1-C2 | -5.94 | 117.92 | 120.30 |
| 2 | 2 | 3876 | A | N3-C4-N9 | 5.94 | 132.15 | 127.40 |
| 2 | 2 | 1856 | C | N1-C2-O2 | 5.94 | 122.46 | 118.90 |
| 2 | 2 | 1592 | G | C4-N9-C1' | 5.94 | 134.22 | 126.50 |
| 2 | 2 | 4996 | C | C5-C6-N1 | 5.94 | 123.97 | 121.00 |
| 27 | h | 82 | ILE | CG1-CB-CG2 | -5.94 | 98.34 | 111.40 |
| 2 | 2 | 4555 | U | P-O3'-C3' | 5.93 | 126.81 | 119.70 |
| 2 | 2 | 3622 | C | N3-C2-O2 | -5.93 | 117.75 | 121.90 |
| 2 | 2 | 3587 | C | C6-N1-C2 | -5.93 | 117.93 | 120.30 |
| 2 | 2 | 4206 | C | N3-C2-O2 | -5.92 | 117.75 | 121.90 |
| 2 | 2 | 1671 | U | C5-C6-N1 | 5.92 | 125.66 | 122.70 |
| 2 | 2 | 2520 | C | C6-N1-C2 | -5.92 | 117.93 | 120.30 |
| 2 | 2 | 4712 | C | N1-C2-O2 | 5.91 | 122.45 | 118.90 |
| 2 | 2 | 1088 | C | C6-N1-C2 | -5.91 | 117.94 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5 | 8 | 80 | A | C2-N3-C4 | 5.91 | 113.55 | 110.60 |
| 2 | 2 | 1468 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 2 | 2 | 1245 | C | N1-C2-O2 | 5.90 | 122.44 | 118.90 |
| 2 | 2 | 1966 | C | N3-C2-O2 | -5.90 | 117.77 | 121.90 |
| 2 | 2 | 2325 | C | N3-C2-O2 | -5.90 | 117.77 | 121.90 |
| 2 | 2 | 1567 | U | N3-C2-O2 | -5.89 | 118.08 | 122.20 |
| 2 | 2 | 1991 | A | C2-N3-C4 | 5.88 | 113.54 | 110.60 |
| 2 | 2 | 30 | C | C2-N1-C1' | 5.88 | 125.27 | 118.80 |
| 2 | 2 | 4522 | G | N3-C4-C5 | -5.88 | 125.66 | 128.60 |
| 5 | 8 | 55 | U | N3-C2-O2 | -5.88 | 118.09 | 122.20 |
| 2 | 2 | 3926 | C | N3-C2-O2 | -5.87 | 117.79 | 121.90 |
| 43 | 4 | 406 | GLY | C-N-CA | 5.87 | 136.38 | 121.70 |
| 2 | 2 | 2496 | G | P-O3'-C3' | 5.87 | 126.75 | 119.70 |
| 2 | 2 | 1915 | C | N3-C2-O2 | -5.87 | 117.79 | 121.90 |
| 2 | 2 | 4349 | C | N3-C2-O2 | -5.87 | 117.79 | 121.90 |
| 13 | I | 188 | GLN | CA-CB-CG | 5.87 | 126.31 | 113.40 |
| 2 | 2 | 1996 | C | C6-N1-C2 | -5.87 | 117.95 | 120.30 |
| 2 | 2 | 2843 | U | N3-C2-O2 | -5.87 | 118.09 | 122.20 |
| 2 | 2 | 2867 | C | C2-N1-C1' | 5.86 | 125.25 | 118.80 |
| 36 | w | 425 | LEU | CB-CG-CD2 | 5.86 | 120.97 | 111.00 |
| 2 | 2 | 14 | C | C6-N1-C2 | -5.86 | 117.95 | 120.30 |
| 5 | 8 | 101 | C | C2-N1-C1' | 5.86 | 125.25 | 118.80 |
| 2 | 2 | 2528 | G | C2-N3-C4 | 5.86 | 114.83 | 111.90 |
| 2 | 2 | 4662 | C | C5-C6-N1 | 5.86 | 123.93 | 121.00 |
| 2 | 2 | 1633 | G | P-O3'-C3' | 5.86 | 126.73 | 119.70 |
| 2 | 2 | 4747 | C | N1-C2-O2 | 5.86 | 122.41 | 118.90 |
| 2 | 2 | 446 | C | C6-N1-C2 | -5.85 | 117.96 | 120.30 |
| 2 | 2 | 673 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 2 | 2 | 4112 | C | C6-N1-C2 | -5.85 | 117.96 | 120.30 |
| 2 | 2 | 4773 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 10 | E | 20 | LEU | CA-CB-CG | 5.85 | 128.75 | 115.30 |
| 2 | 2 | 2592 | U | N1-C2-O2 | 5.84 | 126.89 | 122.80 |
| 2 | 2 | 195 | C | C2-N1-C1' | 5.84 | 125.22 | 118.80 |
| 2 | 2 | 3769 | C | C5-C6-N1 | 5.84 | 123.92 | 121.00 |
| 2 | 2 | 1732 | C | N3-C2-O2 | -5.84 | 117.81 | 121.90 |
| 2 | 2 | 4771 | C | C2-N1-C1' | 5.84 | 125.22 | 118.80 |
| 2 | 2 | 1978 | C | C5-C6-N1 | 5.83 | 123.92 | 121.00 |
| 2 | 2 | 2615 | C | N3-C2-O2 | -5.83 | 117.82 | 121.90 |
| 2 | 2 | 195 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 2 | 2 | 271 | C | C5-C6-N1 | 5.83 | 123.91 | 121.00 |
| 2 | 2 | 2031 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 2 | 2 | 4522 | G | N3-C4-N9 | 5.83 | 129.50 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 4996 | C | C2-N1-C1' | 5.83 | 125.21 | 118.80 |
| 2 | 2 | 485 | C | P-O3'-C3' | 5.82 | 126.69 | 119.70 |
| 2 | 2 | 1678 | C | C2-N1-C1' | 5.82 | 125.20 | 118.80 |
| 2 | 2 | 1942 | A | C2-N3-C4 | 5.82 | 113.51 | 110.60 |
| 2 | 2 | 4913 | G | OP2-P-O3' | 5.81 | 117.99 | 105.20 |
| 2 | 2 | 4349 | C | C2-N1-C1' | 5.81 | 125.19 | 118.80 |
| 2 | 2 | 485 | C | N3-C2-O2 | -5.81 | 117.83 | 121.90 |
| 24 | a | 76 | MET | C-N-CA | 5.81 | 134.50 | 122.30 |
| 2 | 2 | 3636 | C | C2-N1-C1' | 5.80 | 125.18 | 118.80 |
| 2 | 2 | 4315 | A | N1-C2-N3 | -5.80 | 126.40 | 129.30 |
| 2 | 2 | 4653 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 2 | 2 | 30 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 2 | 2 | 2772 | C | N3-C2-O2 | -5.80 | 117.84 | 121.90 |
| 2 | 2 | 2814 | C | C2-N1-C1' | 5.80 | 125.18 | 118.80 |
| 2 | 2 | 4508 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 56 | 3 | 28 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 2 | 2 | 3858 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 2 | 2 | 1807 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 2 | 2 | 1241 | C | C6-N1-C1' | -5.79 | 113.85 | 120.80 |
| 2 | 2 | 3840 | U | N3-C2-O2 | -5.79 | 118.14 | 122.20 |
| 2 | 2 | 221 | C | C6-N1-C2 | -5.79 | 117.98 | 120.30 |
| 2 | 2 | 175 | C | N3-C2-O2 | -5.79 | 117.85 | 121.90 |
| 2 | 2 | 5002 | U | C2-N1-C1' | 5.79 | 124.65 | 117.70 |
| 5 | 8 | 4 | C | C5-C6-N1 | 5.78 | 123.89 | 121.00 |
| 2 | 2 | 2821 | U | N3-C2-O2 | -5.78 | 118.15 | 122.20 |
| 56 | 3 | 28 | C | C6-N1-C2 | -5.78 | 117.99 | 120.30 |
| 2 | 2 | 4596 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 2 | 2 | 2262 | G | C2-N3-C4 | 5.78 | 114.79 | 111.90 |
| 56 | 3 | 2 | U | N3-C2-O2 | -5.78 | 118.16 | 122.20 |
| 2 | 2 | 1901 | C | C6-N1-C2 | -5.78 | 117.99 | 120.30 |
| 2 | 2 | 4453 | C | C6-N1-C1' | -5.78 | 113.87 | 120.80 |
| 2 | 2 | 719 | C | C6-N1-C2 | -5.77 | 117.99 | 120.30 |
| 2 | 2 | 2505 | C | N3-C2-O2 | -5.77 | 117.86 | 121.90 |
| 2 | 2 | 178 | C | N3-C2-O2 | -5.77 | 117.86 | 121.90 |
| 2 | 2 | 4406 | U | N1-C2-O2 | 5.77 | 126.84 | 122.80 |
| 2 | 2 | 365 | U | C2-N1-C1' | 5.77 | 124.62 | 117.70 |
| 56 | 3 | 24 | C | C6-N1-C2 | -5.77 | 117.99 | 120.30 |
| 2 | 2 | 1978 | C | C2-N1-C1' | 5.77 | 125.14 | 118.80 |
| 56 | 3 | 29 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 2 | 2 | 2845 | A | C2-N3-C4 | 5.76 | 113.48 | 110.60 |
| 2 | 2 | 1417 | C | C6-N1-C2 | -5.76 | 118.00 | 120.30 |
| 2 | 2 | 1929 | A | C4-N9-C1' | 5.75 | 136.66 | 126.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 4088 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 5 | 8 | 54 | C | C5-C6-N1 | 5.75 | 123.87 | 121.00 |
| 2 | 2 | 1814 | C | C6-N1-C2 | -5.74 | 118.00 | 120.30 |
| 2 | 2 | 3598 | C | C6-N1-C2 | -5.74 | 118.00 | 120.30 |
| 2 | 2 | 1448 | G | N3-C4-N9 | 5.73 | 129.44 | 126.00 |
| 2 | 2 | 1795 | A | N3-C4-N9 | 5.73 | 131.98 | 127.40 |
| 2 | 2 | 1582 | U | N3-C2-O2 | -5.73 | 118.19 | 122.20 |
| 2 | 2 | 4532 | U | N3-C2-O2 | -5.73 | 118.19 | 122.20 |
| 38 | z | 33 | LEU | CA-CB-CG | 5.73 | 128.47 | 115.30 |
| 2 | 2 | 4283 | G | N3-C4-C5 | -5.72 | 125.74 | 128.60 |
| 2 | 2 | 972 | C | N3-C2-O2 | -5.72 | 117.90 | 121.90 |
| 2 | 2 | 977 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 2 | 2 | 1859 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 2 | 2 | 1251 | C | N3-C2-O2 | -5.72 | 117.90 | 121.90 |
| 2 | 2 | 1994 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 2 | 2 | 281 | U | N1-C2-O2 | 5.71 | 126.80 | 122.80 |
| 2 | 2 | 1906 | U | N3-C2-O2 | -5.71 | 118.20 | 122.20 |
| 2 | 2 | 2729 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 2 | 2 | 3905 | A | OP2-P-O3' | 5.70 | 117.75 | 105.20 |
| 2 | 2 | 4537 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 2 | 2 | 122 | U | N1-C2-O2 | 5.70 | 126.79 | 122.80 |
| 2 | 2 | 4709 | U | C5-C6-N1 | 5.70 | 125.55 | 122.70 |
| 2 | 2 | 1813 | U | C5-C4-O4 | -5.70 | 122.48 | 125.90 |
| 2 | 2 | 386 | A | C2-N3-C4 | 5.69 | 113.45 | 110.60 |
| 2 | 2 | 2337 | C | C6-N1-C2 | -5.69 | 118.02 | 120.30 |
| 2 | 2 | 2779 | C | C6-N1-C2 | -5.69 | 118.03 | 120.30 |
| 2 | 2 | 1096 | C | C2-N1-C1' | 5.69 | 125.05 | 118.80 |
| 2 | 2 | 7 | C | C5-C6-N1 | 5.68 | 123.84 | 121.00 |
| 2 | 2 | 3870 | C | C5-C6-N1 | 5.68 | 123.84 | 121.00 |
| 2 | 2 | 3848 | U | N1-C2-O2 | 5.68 | 126.78 | 122.80 |
| 2 | 2 | 689 | U | N3-C2-O2 | -5.68 | 118.22 | 122.20 |
| 2 | 2 | 1808 | C | C6-N1-C2 | -5.67 | 118.03 | 120.30 |
| 2 | 2 | 1921 | C | N3-C2-O2 | -5.67 | 117.93 | 121.90 |
| 2 | 2 | 1915 | C | C2-N1-C1' | 5.67 | 125.04 | 118.80 |
| 2 | 2 | 1577 | G | C8-N9-C4 | -5.66 | 104.13 | 106.40 |
| 2 | 2 | 4709 | U | C6-N1-C2 | -5.66 | 117.60 | 121.00 |
| 2 | 2 | 5050 | C | C6-N1-C2 | -5.66 | 118.03 | 120.30 |
| 2 | 2 | 4137 | C | N3-C2-O2 | -5.66 | 117.94 | 121.90 |
| 2 | 2 | 26 | C | C5-C6-N1 | 5.66 | 123.83 | 121.00 |
| 2 | 2 | 4275 | G | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 2 | 2 | 4207 | C | N3-C2-O2 | -5.66 | 117.94 | 121.90 |
| 2 | 2 | 1703 | C | C2-N1-C1' | 5.65 | 125.02 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 274 | C | C5-C6-N1 | 5.65 | 123.83 | 121.00 |
| 2 | 2 | 1816 | C | N3-C2-O2 | -5.65 | 117.95 | 121.90 |
| 2 | 2 | 2290 | C | C5-C6-N1 | 5.65 | 123.83 | 121.00 |
| 2 | 2 | 4341 | C | C2-N1-C1' | 5.65 | 125.01 | 118.80 |
| 2 | 2 | 390 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 2 | 2 | 112 | C | N3-C2-O2 | -5.64 | 117.95 | 121.90 |
| 2 | 2 | 4295 | U | N3-C2-O2 | -5.64 | 118.25 | 122.20 |
| 2 | 2 | 1074 | G | N3-C4-N9 | 5.64 | 129.38 | 126.00 |
| 2 | 2 | 1993 | C | C2-N1-C1' | 5.64 | 125.00 | 118.80 |
| 2 | 2 | 1079 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 2 | 2 | 3769 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 2 | 2 | 3915 | U | N1-C2-O2 | 5.64 | 126.75 | 122.80 |
| 2 | 2 | 3882 | C | C5-C6-N1 | 5.64 | 123.82 | 121.00 |
| 2 | 2 | 1310 | C | C6-N1-C2 | -5.63 | 118.05 | 120.30 |
| 2 | 2 | 4758 | U | C6-N1-C1' | -5.63 | 113.32 | 121.20 |
| 2 | 2 | 1921 | C | C2-N1-C1' | 5.63 | 124.99 | 118.80 |
| 2 | 2 | 3876 | A | N3-C4-C5 | -5.63 | 122.86 | 126.80 |
| 2 | 2 | 4689 | U | C5-C6-N1 | 5.63 | 125.51 | 122.70 |
| 2 | 2 | 4752 | U | N1-C2-O2 | 5.63 | 126.74 | 122.80 |
| 2 | 2 | 126 | C | N1-C2-O2 | 5.62 | 122.28 | 118.90 |
| 2 | 2 | 1856 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 2 | 2 | 2498 | C | C2-N1-C1' | 5.62 | 124.99 | 118.80 |
| 2 | 2 | 4148 | C | N3-C2-O2 | -5.62 | 117.97 | 121.90 |
| 2 | 2 | 1707 | C | C6-N1-C2 | -5.62 | 118.05 | 120.30 |
| 2 | 2 | 4171 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 43 | 4 | 12 | VAL | CA-CB-CG1 | 5.62 | 119.33 | 110.90 |
| 2 | 2 | 1276 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 2 | 2 | 4228 | G | OP1-P-O3' | 5.62 | 117.56 | 105.20 |
| 2 | 2 | 4880 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 2 | 2 | 2410 | C | N3-C2-O2 | -5.61 | 117.97 | 121.90 |
| 2 | 2 | 4162 | C | C2-N1-C1' | 5.61 | 124.97 | 118.80 |
| 2 | 2 | 485 | C | C5-C6-N1 | 5.61 | 123.81 | 121.00 |
| 2 | 2 | 2281 | U | C5-C6-N1 | 5.61 | 125.50 | 122.70 |
| 56 | 3 | 24 | C | N3-C2-O2 | -5.61 | 117.97 | 121.90 |
| 2 | 2 | 4752 | U | N3-C2-O2 | -5.61 | 118.27 | 122.20 |
| 2 | 2 | 1656 | U | N3-C2-O2 | -5.60 | 118.28 | 122.20 |
| 2 | 2 | 5008 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 48 | t | 56 | LEU | CA-CB-CG | 5.60 | 128.19 | 115.30 |
| 2 | 2 | 499 | G | C2-N3-C4 | 5.60 | 114.70 | 111.90 |
| 2 | 2 | 1884 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 2 | 2 | 4387 | C | C5-C6-N1 | 5.60 | 123.80 | 121.00 |
| 2 | 2 | 4562 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 1832 | C | N1-C2-O2 | 5.60 | 122.26 | 118.90 |
| 2 | 2 | 4235 | G | N3-C4-N9 | 5.59 | 129.36 | 126.00 |
| 43 | 4 | 503 | THR | C-N-CA | 5.58 | 135.66 | 121.70 |
| 56 | 3 | 73 | U | O5'-P-OP2 | -5.58 | 100.67 | 105.70 |
| 2 | 2 | 4319 | C | N3-C2-O2 | -5.58 | 117.99 | 121.90 |
| 2 | 2 | 1384 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 2 | 2 | 1467 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 2 | 2 | 266 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 2 | 2 | 2689 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 2 | 2 | 4348 | A | C2-N3-C4 | 5.57 | 113.39 | 110.60 |
| 2 | 2 | 2836 | A | C2-N3-C4 | 5.57 | 113.38 | 110.60 |
| 2 | 2 | 4370 | G | C4-N9-C1' | 5.57 | 133.74 | 126.50 |
| 2 | 2 | 201 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 2 | 2 | 1947 | U | C2-N1-C1' | 5.57 | 124.38 | 117.70 |
| 2 | 2 | 1458 | C | C6-N1-C2 | -5.56 | 118.07 | 120.30 |
| 2 | 2 | 4476 | C | N3-C2-O2 | -5.56 | 118.00 | 121.90 |
| 2 | 2 | 1308 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 56 | 3 | 2 | U | N1-C2-O2 | 5.56 | 126.69 | 122.80 |
| 2 | 2 | 2533 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 5 | 8 | 156 | U | N3-C2-O2 | -5.56 | 118.31 | 122.20 |
| 2 | 2 | 131 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 2 | 2 | 1582 | U | N1-C2-O2 | 5.56 | 126.69 | 122.80 |
| 2 | 2 | 486 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 2 | 2 | 4308 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 2 | 2 | 2508 | U | N3-C2-O2 | -5.55 | 118.31 | 122.20 |
| 2 | 2 | 2439 | G | N3-C4-C5 | -5.55 | 125.83 | 128.60 |
| 2 | 2 | 4981 | G | C4-N9-C1' | 5.55 | 133.71 | 126.50 |
| 2 | 2 | 1430 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |
| 2 | 2 | 712 | C | C5-C6-N1 | 5.54 | 123.77 | 121.00 |
| 2 | 2 | 4500 | U | C2-N1-C1' | 5.54 | 124.35 | 117.70 |
| 2 | 2 | 124 | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 56 | 3 | 3 | C | C5-C6-N1 | 5.54 | 123.77 | 121.00 |
| 29 | m | 102 | LEU | CA-CB-CG | 5.54 | 128.04 | 115.30 |
| 2 | 2 | 1795 | A | N1-C2-N3 | -5.54 | 126.53 | 129.30 |
| 2 | 2 | 988 | C | C5-C6-N1 | 5.54 | 123.77 | 121.00 |
| 2 | 2 | 2290 | C | C2-N1-C1' | 5.53 | 124.88 | 118.80 |
| 2 | 2 | 3772 | U | C2-N1-C1' | 5.53 | 124.34 | 117.70 |
| 2 | 2 | 4078 | C | C6-N1-C2 | -5.53 | 118.09 | 120.30 |
| 2 | 2 | 4700 | A | C2-N3-C4 | 5.53 | 113.36 | 110.60 |
| 2 | 2 | 4885 | U | C2-N1-C1' | 5.53 | 124.34 | 117.70 |
| 2 | 2 | 1468 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 2 | 2 | 2708 | U | N1-C2-O2 | 5.53 | 126.67 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 5 | 8 | 107 | C | C6-N1-C2 | -5.53 | 118.09 | 120.30 |
| 56 | 3 | 71 | G | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 2 | 2 | 963 | G | C2-N3-C4 | 5.53 | 114.66 | 111.90 |
| 2 | 2 | 1632 | A | N1-C2-N3 | -5.53 | 126.54 | 129.30 |
| 2 | 2 | 4639 | G | C4-N9-C1' | 5.53 | 133.68 | 126.50 |
| 43 | 4 | 238 | MET | CB-CG-SD | 5.53 | 128.98 | 112.40 |
| 2 | 2 | 100 | C | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 2 | 2 | 1097 | C | C5-C6-N1 | 5.52 | 123.76 | 121.00 |
| 2 | 2 | 2783 | A | N1-C2-N3 | -5.52 | 126.54 | 129.30 |
| 2 | 2 | 4683 | U | N3-C2-O2 | -5.52 | 118.34 | 122.20 |
| 47 | d | 23 | LEU | CA-CB-CG | 5.52 | 127.99 | 115.30 |
| 2 | 2 | 2505 | C | C6-N1-C1' | -5.51 | 114.19 | 120.80 |
| 2 | 2 | 3876 | A | C4-N9-C1' | 5.51 | 136.22 | 126.30 |
| 5 | 8 | 156 | U | N1-C2-O2 | 5.51 | 126.66 | 122.80 |
| 56 | 3 | 19 | C | C5-C6-N1 | 5.51 | 123.76 | 121.00 |
| 2 | 2 | 4313 | A | C2-N3-C4 | 5.51 | 113.36 | 110.60 |
| 2 | 2 | 4283 | G | C8-N9-C1' | -5.51 | 119.84 | 127.00 |
| 2 | 2 | 4147 | G | C5-C6-O6 | 5.51 | 131.90 | 128.60 |
| 2 | 2 | 4461 | C | C6-N1-C2 | -5.51 | 118.10 | 120.30 |
| 2 | 2 | 71 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 2 | 2 | 209 | U | C2-N1-C1' | 5.50 | 124.30 | 117.70 |
| 2 | 2 | 2568 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 2 | 2 | 1672 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 2 | 2 | 4206 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 2 | 2 | 4758 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 2 | 2 | 4370 | G | C8-N9-C4 | -5.50 | 104.20 | 106.40 |
| 2 | 2 | 984 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 2 | 2 | 1683 | U | N3-C2-O2 | -5.49 | 118.35 | 122.20 |
| 43 | 4 | 21 | LEU | CA-CB-CG | 5.49 | 127.94 | 115.30 |
| 2 | 2 | 1703 | C | N3-C2-O2 | -5.49 | 118.06 | 121.90 |
| 2 | 2 | 3932 | U | N3-C2-O2 | -5.49 | 118.36 | 122.20 |
| 24 | a | 38 | ARG | C-N-CA | 5.49 | 135.42 | 121.70 |
| 2 | 2 | 977 | C | C6-N1-C2 | -5.49 | 118.11 | 120.30 |
| 2 | 2 | 4722 | G | C4-N9-C1' | 5.49 | 133.63 | 126.50 |
| 2 | 2 | 2850 | A | C4-N9-C1' | 5.48 | 136.17 | 126.30 |
| 2 | 2 | 4429 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 2 | 2 | 1203 | G | N3-C4-N9 | 5.48 | 129.29 | 126.00 |
| 5 | 8 | 81 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 2 | 2 | 5036 | C | C2-N1-C1' | 5.48 | 124.83 | 118.80 |
| 2 | 2 | 3858 | C | N1-C2-O2 | 5.48 | 122.19 | 118.90 |
| 2 | 2 | 4345 | C | C5-C6-N1 | 5.48 | 123.74 | 121.00 |
| 2 | 2 | 4522 | G | C8-N9-C1' | -5.48 | 119.88 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 1664 | U | N3-C2-O2 | -5.47 | 118.37 | 122.20 |
| 2 | 2 | 3893 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 2 | 2 | 2372 | U | N3-C2-O2 | -5.47 | 118.37 | 122.20 |
| 2 | 2 | 4259 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 5 | 8 | 72 | A | C2-N3-C4 | 5.47 | 113.33 | 110.60 |
| 56 | 3 | 26 | C | C5-C6-N1 | 5.47 | 123.73 | 121.00 |
| 2 | 2 | 1700 | G | N3-C4-C5 | -5.46 | 125.87 | 128.60 |
| 2 | 2 | 4712 | C | C5-C6-N1 | 5.46 | 123.73 | 121.00 |
| 2 | 2 | 259 | C | C2-N1-C1' | 5.46 | 124.81 | 118.80 |
| 2 | 2 | 4471 | U | N1-C2-O2 | 5.46 | 126.62 | 122.80 |
| 2 | 2 | 4272 | G | C4-N9-C1' | 5.46 | 133.60 | 126.50 |
| 5 | 8 | 51 | U | N1-C2-O2 | 5.45 | 126.62 | 122.80 |
| 2 | 2 | 1567 | U | N1-C2-O2 | 5.45 | 126.62 | 122.80 |
| 2 | 2 | 4295 | U | N1-C2-O2 | 5.45 | 126.62 | 122.80 |
| 6 | 9 | 35 | LEU | CA-CB-CG | 5.45 | 127.84 | 115.30 |
| 2 | 2 | 458 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 2 | 2 | 4162 | C | N3-C2-O2 | -5.45 | 118.08 | 121.90 |
| 2 | 2 | 4639 | G | N3-C4-C5 | -5.45 | 125.88 | 128.60 |
| 2 | 2 | 1079 | C | C5-C6-N1 | 5.45 | 123.72 | 121.00 |
| 2 | 2 | 1505 | C | C5-C6-N1 | 5.45 | 123.72 | 121.00 |
| 2 | 2 | 4991 | U | N3-C2-O2 | -5.45 | 118.39 | 122.20 |
| 2 | 2 | 271 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 2 | 2 | 5050 | C | C2-N1-C1' | 5.45 | 124.79 | 118.80 |
| 2 | 2 | 1505 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 2 | 2 | 2417 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 2 | 2 | 3657 | U | N1-C2-O2 | 5.45 | 126.61 | 122.80 |
| 2 | 2 | 123 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 2 | 2 | 421 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 2 | 2 | 1203 | G | C2-N3-C4 | 5.44 | 114.62 | 111.90 |
| 2 | 2 | 673 | C | C5-C6-N1 | 5.44 | 123.72 | 121.00 |
| 2 | 2 | 1720 | C | C5-C6-N1 | 5.44 | 123.72 | 121.00 |
| 19 | S | 127 | VAL | CG1-CB-CG2 | -5.44 | 102.20 | 110.90 |
| 2 | 2 | 1888 | A | C2-N3-C4 | 5.43 | 113.32 | 110.60 |
| 2 | 2 | 657 | C | N3-C2-O2 | -5.43 | 118.10 | 121.90 |
| 2 | 2 | 1577 | G | C2-N3-C4 | 5.43 | 114.62 | 111.90 |
| 2 | 2 | 4569 | U | N1-C2-O2 | 5.43 | 126.60 | 122.80 |
| 56 | 3 | 67 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 2 | 2 | 3876 | A | N1-C2-N3 | -5.43 | 126.58 | 129.30 |
| 2 | 2 | 1727 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 2 | 2 | 1940 | G | O4'-C1'-N9 | 5.43 | 112.54 | 108.20 |
| 2 | 2 | 2078 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 2 | 2 | 2779 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 692 | A | N1-C2-N3 | -5.43 | 126.59 | 129.30 |
| 2 | 2 | 977 | C | C2-N1-C1' | 5.43 | 124.77 | 118.80 |
| 2 | 2 | 1096 | C | N3-C2-O2 | -5.43 | 118.10 | 121.90 |
| 2 | 2 | 972 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 2 | 2 | 1592 | G | N3-C4-C5 | -5.42 | 125.89 | 128.60 |
| 2 | 2 | 4639 | G | N3-C4-N9 | 5.42 | 129.25 | 126.00 |
| 2 | 2 | 1566 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 2 | 2 | 984 | C | C5-C6-N1 | 5.41 | 123.71 | 121.00 |
| 2 | 2 | 1566 | C | N1-C2-O2 | 5.41 | 122.15 | 118.90 |
| 2 | 2 | 1725 | U | N3-C2-O2 | -5.41 | 118.41 | 122.20 |
| 2 | 2 | 3882 | C | N1-C2-O2 | 5.41 | 122.15 | 118.90 |
| 2 | 2 | 4312 | U | N3-C2-O2 | -5.41 | 118.41 | 122.20 |
| 2 | 2 | 174 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 2 | 2 | 2779 | C | C2-N1-C1' | 5.41 | 124.75 | 118.80 |
| 2 | 2 | 2856 | C | N3-C2-O2 | -5.41 | 118.12 | 121.90 |
| 2 | 2 | 2699 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 2 | 2 | 480 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 2 | 2 | 1431 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 5 | 8 | 135 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 42 | T | 127 | GLN | CA-CB-CG | 5.40 | 125.27 | 113.40 |
| 2 | 2 | 2373 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 2 | 2 | 4981 | G | N3-C4-N9 | 5.40 | 129.24 | 126.00 |
| 2 | 2 | 282 | C | C2-N1-C1' | 5.39 | 124.73 | 118.80 |
| 2 | 2 | 4440 | G | C4-N9-C1' | 5.39 | 133.51 | 126.50 |
| 2 | 2 | 1906 | U | N1-C2-O2 | 5.39 | 126.57 | 122.80 |
| 2 | 2 | 2497 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 2 | 2 | 4694 | G | N3-C4-C5 | -5.39 | 125.91 | 128.60 |
| 56 | 3 | 26 | C | N3-C2-O2 | -5.39 | 118.13 | 121.90 |
| 2 | 2 | 4497 | U | N1-C2-O2 | 5.39 | 126.57 | 122.80 |
| 2 | 2 | 4887 | C | C5-C6-N1 | 5.39 | 123.69 | 121.00 |
| 2 | 2 | 472 | C | N3-C2-O2 | -5.38 | 118.13 | 121.90 |
| 2 | 2 | 1847 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 37 | y | 125 | LEU | CA-CB-CG | 5.38 | 127.68 | 115.30 |
| 2 | 2 | 259 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 2 | 2 | 4456 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 2 | 2 | 2498 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 52 | K | 97 | MET | CA-CB-CG | 5.37 | 122.44 | 113.30 |
| 2 | 2 | 1662 | C | C5-C6-N1 | 5.37 | 123.69 | 121.00 |
| 48 | t | 130 | LEU | CA-CB-CG | 5.37 | 127.65 | 115.30 |
| 2 | 2 | 2439 | G | C6-C5-N7 | -5.37 | 127.18 | 130.40 |
| 2 | 2 | 1344 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 2 | 2 | 1861 | U | C2-N1-C1' | 5.37 | 124.14 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | 2 | 653 | U | N1-C2-O2 | 5.36 | 126.56 | 122.80 |
| 2 | 2 | 2290 | C | N1-C2-O2 | 5.36 | 122.11 | 118.90 |
| 2 | 2 | 4662 | C | N1-C2-O2 | 5.36 | 122.11 | 118.90 |
| 2 | 2 | 1938 | C | N3-C2-O2 | -5.36 | 118.15 | 121.90 |
| 2 | 2 | 2077 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 2 | 2 | 228 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 2 | 2 | 4700 | A | N1-C2-N3 | -5.35 | 126.62 | 129.30 |
| 2 | 2 | 332 | C | N1-C2-O2 | 5.35 | 122.11 | 118.90 |
| 55 | O | 13 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |
| 2 | 2 | 1448 | G | C8-N9-C1' | -5.35 | 120.05 | 127.00 |
| 2 | 2 | 2101 | C | C6-N1-C1' | 5.35 | 127.22 | 120.80 |
| 2 | 2 | 4713 | G | N3-C4-C5 | -5.35 | 125.93 | 128.60 |
| 2 | 2 | 1656 | U | N1-C2-O2 | 5.35 | 126.54 | 122.80 |
| 2 | 2 | 5008 | C | N3-C2-O2 | -5.35 | 118.16 | 121.90 |
| 2 | 2 | 1540 | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 2 | 2 | 2589 | C | C5-C6-N1 | 5.34 | 123.67 | 121.00 |
| 2 | 2 | 3878 | C | C6-N1-C1' | -5.34 | 114.39 | 120.80 |
| 2 | 2 | 4370 | G | N3-C4-C5 | -5.34 | 125.93 | 128.60 |
| 2 | 2 | 406 | C | C2'-C3'-O3' | 5.34 | 122.24 | 113.70 |
| 2 | 2 | 3901 | A | C2-N3-C4 | 5.34 | 113.27 | 110.60 |
| 2 | 2 | 4708 | A | N1-C2-N3 | -5.34 | 126.63 | 129.30 |
| 56 | 3 | 84 | U | N1-C2-O2 | 5.34 | 126.54 | 122.80 |
| 2 | 2 | 2821 | U | N1-C2-O2 | 5.34 | 126.54 | 122.80 |
| 2 | 2 | 4310 | A | N1-C2-N3 | -5.34 | 126.63 | 129.30 |
| 5 | 8 | 99 | U | C2-N1-C1' | 5.33 | 124.09 | 117.70 |
| 2 | 2 | 914 | U | C5-C4-O4 | -5.33 | 122.70 | 125.90 |
| 2 | 2 | 2886 | U | N3-C2-O2 | -5.33 | 118.47 | 122.20 |
| 2 | 2 | 1478 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 2 | 2 | 1535 | C | N1-C2-O2 | 5.33 | 122.09 | 118.90 |
| 2 | 2 | 4699 | U | OP1-P-O3' | 5.32 | 116.91 | 105.20 |
| 2 | 2 | 1700 | G | N3-C4-N9 | 5.32 | 129.19 | 126.00 |
| 2 | 2 | 2791 | C | C2-N1-C1' | 5.32 | 124.65 | 118.80 |
| 2 | 2 | 694 | C | C6-N1-C2 | -5.31 | 118.17 | 120.30 |
| 2 | 2 | 2593 | C | C6-N1-C2 | -5.31 | 118.17 | 120.30 |
| 2 | 2 | 2814 | C | N3-C2-O2 | -5.31 | 118.18 | 121.90 |
| 2 | 2 | 486 | C | OP1-P-OP2 | -5.31 | 111.63 | 119.60 |
| 2 | 2 | 3835 | C | C6-N1-C2 | -5.31 | 118.18 | 120.30 |
| 2 | 2 | 4294 | C | N3-C2-O2 | -5.31 | 118.18 | 121.90 |
| 5 | 8 | 101 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 2 | 2 | 115 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 2 | 2 | 4286 | C | C5-C6-N1 | 5.30 | 123.65 | 121.00 |
| 2 | 2 | 662 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 1190 | C | N3-C2-O2 | -5.30 | 118.19 | 121.90 |
| 2 | 2 | 1538 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 2 | 2 | 4662 | C | N3-C2-O2 | -5.30 | 118.19 | 121.90 |
| 2 | 2 | 4653 | C | C5-C6-N1 | 5.30 | 123.65 | 121.00 |
| 2 | 2 | 4918 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 51 | 1 | 139 | MET | CA-CB-CG | 5.30 | 122.31 | 113.30 |
| 2 | 2 | 1472 | C | C5-C6-N1 | 5.30 | 123.65 | 121.00 |
| 2 | 2 | 2508 | U | N1-C2-O2 | 5.30 | 126.51 | 122.80 |
| 2 | 2 | 4068 | U | C6-N1-C2 | -5.30 | 117.82 | 121.00 |
| 5 | 8 | 82 | A | C2-N3-C4 | 5.29 | 113.25 | 110.60 |
| 2 | 2 | 1325 | C | N3-C2-O2 | -5.29 | 118.20 | 121.90 |
| 2 | 2 | 4711 | C | C6-N1-C2 | -5.29 | 118.18 | 120.30 |
| 2 | 2 | 2403 | A | N1-C2-N3 | -5.29 | 126.66 | 129.30 |
| 2 | 2 | 4714 | C | C2-N1-C1' | 5.29 | 124.62 | 118.80 |
| 2 | 2 | 750 | U | N1-C2-O2 | 5.29 | 126.50 | 122.80 |
| 2 | 2 | 1439 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 2 | 2 | 1727 | U | N1-C2-O2 | 5.28 | 126.50 | 122.80 |
| 2 | 2 | 3631 | U | N1-C2-O2 | 5.28 | 126.50 | 122.80 |
| 30 | n | 83 | MET | CA-CB-CG | 5.28 | 122.27 | 113.30 |
| 56 | 3 | 94 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 2 | 2 | 657 | C | C5-C6-N1 | 5.28 | 123.64 | 121.00 |
| 2 | 2 | 125 | C | C6-N1-C2 | -5.27 | 118.19 | 120.30 |
| 2 | 2 | 26 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 2 | 2 | 1241 | C | C5-C6-N1 | 5.27 | 123.64 | 121.00 |
| 2 | 2 | 3587 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 2 | 2 | 5050 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 6 | 9 | 99 | GLN | CA-CB-CG | 5.27 | 125.00 | 113.40 |
| 2 | 2 | 1436 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |
| 2 | 2 | 1592 | G | N3-C4-N9 | 5.27 | 129.16 | 126.00 |
| 2 | 2 | 4299 | U | C2-N1-C1' | 5.27 | 124.02 | 117.70 |
| 1 | N | 59 | LEU | CA-CB-CG | 5.27 | 127.41 | 115.30 |
| 2 | 2 | 1687 | U | N3-C2-O2 | -5.27 | 118.51 | 122.20 |
| 2 | 2 | 988 | C | C2-N1-C1' | 5.27 | 124.59 | 118.80 |
| 2 | 2 | 1367 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 2 | 2 | 486 | C | C5-C6-N1 | 5.26 | 123.63 | 121.00 |
| 2 | 2 | 1074 | G | C4-N9-C1' | 5.26 | 133.34 | 126.50 |
| 2 | 2 | 2802 | C | C6-N1-C2 | -5.26 | 118.19 | 120.30 |
| 2 | 2 | 2478 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 2 | 2 | 3739 | C | C5-C6-N1 | 5.26 | 123.63 | 121.00 |
| 2 | 2 | 163 | A | N1-C2-N3 | -5.26 | 126.67 | 129.30 |
| 56 | 3 | 4 | U | N3-C2-O2 | -5.26 | 118.52 | 122.20 |
| 2 | 2 | 2019 | C | C5-C6-N1 | 5.26 | 123.63 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 2684 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 2 | 2 | 5036 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 2 | 2 | 2465 | C | C5-C6-N1 | 5.25 | 123.63 | 121.00 |
| 2 | 2 | 2867 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 2 | 2 | 1628 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 2 | 2 | 1996 | C | C5-C6-N1 | 5.25 | 123.63 | 121.00 |
| 2 | 2 | 2367 | A | N1-C2-N3 | -5.25 | 126.67 | 129.30 |
| 2 | 2 | 2533 | C | N3-C2-O2 | -5.25 | 118.22 | 121.90 |
| 2 | 2 | 294 | G | C4-N9-C1' | 5.25 | 133.32 | 126.50 |
| 2 | 2 | 2038 | U | N1-C2-O2 | 5.25 | 126.47 | 122.80 |
| 5 | 8 | 52 | A | N1-C2-N3 | -5.24 | 126.68 | 129.30 |
| 2 | 2 | 4469 | U | N3-C2-O2 | -5.24 | 118.53 | 122.20 |
| 2 | 2 | 4440 | G | N3-C4-C5 | -5.24 | 125.98 | 128.60 |
| 2 | 2 | 4614 | G | N1-C6-O6 | -5.24 | 116.76 | 119.90 |
| 2 | 2 | 2264 | C | C6-N1-C2 | -5.24 | 118.21 | 120.30 |
| 2 | 2 | 2791 | C | C5-C6-N1 | 5.24 | 123.62 | 121.00 |
| 2 | 2 | 4674 | C | C5-C6-N1 | 5.24 | 123.62 | 121.00 |
| 2 | 2 | 5030 | U | C5-C6-N1 | 5.24 | 125.32 | 122.70 |
| 2 | 2 | 78 | U | N1-C2-O2 | 5.23 | 126.46 | 122.80 |
| 5 | 8 | 28 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 56 | 3 | 14 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 2 | 2 | 3685 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 2 | 2 | 2833 | A | C2-N3-C4 | 5.22 | 113.21 | 110.60 |
| 2 | 2 | 4532 | U | N1-C2-O2 | 5.22 | 126.45 | 122.80 |
| 2 | 2 | 4628 | U | N3-C2-O2 | -5.22 | 118.54 | 122.20 |
| 2 | 2 | 3622 | C | C5-C6-N1 | 5.22 | 123.61 | 121.00 |
| 5 | 8 | 141 | C | C5-C6-N1 | 5.22 | 123.61 | 121.00 |
| 2 | 2 | 1467 | C | C2-N1-C1' | 5.22 | 124.54 | 118.80 |
| 2 | 2 | 4261 | C | C5-C6-N1 | 5.21 | 123.61 | 121.00 |
| 2 | 2 | 131 | C | C5-C6-N1 | 5.21 | 123.61 | 121.00 |
| 45 | k | 90 | MET | CG-SD-CE | 5.21 | 108.54 | 100.20 |
| 2 | 2 | 1993 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 2 | 2 | 4508 | C | N3-C2-O2 | -5.21 | 118.25 | 121.90 |
| 56 | 3 | 19 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 2 | 2 | 2022 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 5 | 8 | 141 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 2 | 2 | 4508 | C | C5-C6-N1 | 5.21 | 123.60 | 121.00 |
| 2 | 2 | 5010 | U | N3-C2-O2 | -5.21 | 118.56 | 122.20 |
| 5 | 8 | 19 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 2 | 2 | 1894 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 2 | 2 | 4308 | C | N3-C2-O2 | -5.20 | 118.26 | 121.90 |
| 2 | 2 | 4683 | U | N1-C2-O2 | 5.20 | 126.44 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 683 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 2 | 2 | 5048 | A | N1-C2-N3 | -5.20 | 126.70 | 129.30 |
| 2 | 2 | 2625 | U | N3-C2-O2 | -5.20 | 118.56 | 122.20 |
| 2 | 2 | 345 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 2 | 2 | 446 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 2 | 2 | 1325 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 5 | 8 | 26 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 45 | k | 90 | MET | CB-CG-SD | 5.20 | 128.00 | 112.40 |
| 2 | 2 | 1469 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 5 | 8 | 55 | U | N1-C2-O2 | 5.20 | 126.44 | 122.80 |
| 5 | 8 | 128 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 40 | R | 288 | LEU | CA-CB-CG | 5.20 | 127.25 | 115.30 |
| 2 | 2 | 2025 | A | N1-C2-N3 | -5.19 | 126.70 | 129.30 |
| 2 | 2 | 4758 | U | C5-C6-N1 | 5.19 | 125.30 | 122.70 |
| 2 | 2 | 1572 | U | N3-C2-O2 | -5.19 | 118.57 | 122.20 |
| 2 | 2 | 2008 | U | N3-C2-O2 | -5.19 | 118.57 | 122.20 |
| 2 | 2 | 4682 | U | C6-N1-C2 | -5.19 | 117.89 | 121.00 |
| 2 | 2 | 30 | C | C5-C6-N1 | 5.19 | 123.59 | 121.00 |
| 2 | 2 | 1340 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |
| 41 | W | 330 | LEU | CA-CB-CG | 5.19 | 127.23 | 115.30 |
| 2 | 2 | 4319 | C | C2-N1-C1' | 5.18 | 124.50 | 118.80 |
| 2 | 2 | 974 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 2 | 2 | 2867 | C | C5-C6-N1 | 5.18 | 123.59 | 121.00 |
| 5 | 8 | 73 | U | N3-C2-O2 | -5.18 | 118.57 | 122.20 |
| 2 | 2 | 201 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 2 | 2 | 436 | C | C6-N1-C2 | -5.18 | 118.23 | 120.30 |
| 2 | 2 | 259 | C | C5-C6-N1 | 5.18 | 123.59 | 121.00 |
| 2 | 2 | 2018 | C | C6-N1-C2 | -5.18 | 118.23 | 120.30 |
| 2 | 2 | 2726 | G | N3-C4-C5 | -5.18 | 126.01 | 128.60 |
| 2 | 2 | 1585 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 2 | 2 | 4267 | G | C2-N3-C4 | 5.17 | 114.49 | 111.90 |
| 2 | 2 | 2497 | C | C2-N1-C1' | 5.17 | 124.49 | 118.80 |
| 2 | 2 | 77 | U | C2-N1-C1' | 5.17 | 123.91 | 117.70 |
| 2 | 2 | 2539 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 2 | 2 | 4267 | G | N3-C4-C5 | -5.17 | 126.02 | 128.60 |
| 2 | 2 | 4284 | C | C2-N3-C4 | 5.17 | 122.48 | 119.90 |
| 2 | 2 | 365 | U | C5-C6-N1 | 5.17 | 125.28 | 122.70 |
| 2 | 2 | 4149 | C | C5-C6-N1 | 5.17 | 123.58 | 121.00 |
| 2 | 2 | 1294 | A | C2-N3-C4 | 5.17 | 113.18 | 110.60 |
| 2 | 2 | 4120 | U | N1-C2-O2 | 5.17 | 126.42 | 122.80 |
| 19 | S | 39 | ASP | CB-CG-OD1 | 5.17 | 122.95 | 118.30 |
| 2 | 2 | 1694 | C | C2-N1-C1' | 5.16 | 124.48 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 35 | v | 7 | ASP | CB-CG-OD1 | 5.16 | 122.95 | 118.30 |
| 2 | 2 | 141 | C | N3-C2-O2 | -5.16 | 118.29 | 121.90 |
| 2 | 2 | 4775 | C | C5-C6-N1 | 5.16 | 123.58 | 121.00 |
| 2 | 2 | 300 | A | N1-C2-N3 | -5.16 | 126.72 | 129.30 |
| 2 | 2 | 3926 | C | C5-C6-N1 | 5.16 | 123.58 | 121.00 |
| 2 | 2 | 4442 | U | N3-C2-O2 | -5.16 | 118.59 | 122.20 |
| 2 | 2 | 5035 | U | C6-N1-C2 | -5.16 | 117.91 | 121.00 |
| 2 | 2 | 694 | C | N3-C2-O2 | -5.16 | 118.29 | 121.90 |
| 2 | 2 | 2031 | C | C5-C6-N1 | 5.16 | 123.58 | 121.00 |
| 2 | 2 | 2281 | U | C2-N1-C1' | 5.15 | 123.89 | 117.70 |
| 5 | 8 | 153 | C | C5-C6-N1 | 5.15 | 123.58 | 121.00 |
| 2 | 2 | 1795 | A | N3-C4-C5 | -5.14 | 123.20 | 126.80 |
| 2 | 2 | 2615 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 2 | 2 | 4695 | C | C5-C6-N1 | 5.14 | 123.57 | 121.00 |
| 56 | 3 | 14 | C | C5-C6-N1 | 5.14 | 123.57 | 121.00 |
| 2 | 2 | 2603 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 2 | 2 | 2325 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 2 | 2 | 1807 | C | C5-C6-N1 | 5.14 | 123.57 | 121.00 |
| 2 | 2 | 4093 | G | C4-N9-C1' | 5.14 | 133.18 | 126.50 |
| 2 | 2 | 4286 | C | C6-N1-C2 | -5.14 | 118.25 | 120.30 |
| 2 | 2 | 4886 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 2 | 2 | 1418 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 2 | 2 | 979 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 2 | 2 | 1847 | C | C5-C6-N1 | 5.13 | 123.57 | 121.00 |
| 2 | 2 | 3668 | C | C2-N1-C1' | 5.13 | 124.45 | 118.80 |
| 2 | 2 | 4272 | G | N3-C4-C5 | -5.13 | 126.03 | 128.60 |
| 2 | 2 | 1686 | C | C5-C6-N1 | 5.13 | 123.57 | 121.00 |
| 2 | 2 | 1812 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 2 | 2 | 2011 | C | C5-C6-N1 | 5.13 | 123.56 | 121.00 |
| 2 | 2 | 2683 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 2 | 2 | 7 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 2 | 2 | 4241 | C | C5-C6-N1 | 5.12 | 123.56 | 121.00 |
| 2 | 2 | 4687 | A | C2-N3-C4 | 5.12 | 113.16 | 110.60 |
| 5 | 8 | 32 | C | N3-C2-O2 | -5.12 | 118.31 | 121.90 |
| 2 | 2 | 914 | U | OP2-P-O3' | 5.12 | 116.46 | 105.20 |
| 2 | 2 | 2031 | C | C2-N1-C1' | 5.12 | 124.43 | 118.80 |
| 2 | 2 | 2872 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 39 | C | 115 | LEU | CA-CB-CG | 5.12 | 127.07 | 115.30 |
| 50 | c | 244 | LYS | CB-CA-C | 5.12 | 120.64 | 110.40 |
| 43 | 4 | 41 | HIS | C-N-CA | 5.12 | 134.49 | 121.70 |
| 34 | u | 54 | ALA | CB-CA-C | 5.12 | 117.77 | 110.10 |
| 2 | 2 | 385 | A | N1-C2-N3 | -5.11 | 126.74 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | 2 | 657 | C | C2-N1-C1' | 5.11 | 124.42 | 118.80 |
| 2 | 2 | 3694 | U | N1-C2-O2 | 5.11 | 126.38 | 122.80 |
| 2 | 2 | 3694 | U | N3-C2-O2 | -5.11 | 118.62 | 122.20 |
| 2 | 2 | 1340 | C | C5-C6-N1 | 5.11 | 123.56 | 121.00 |
| 2 | 2 | 2792 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 2 | 2 | 2899 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 2 | 2 | 4442 | U | N1-C2-O2 | 5.11 | 126.37 | 122.80 |
| 2 | 2 | 653 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 2 | 2 | 909 | A | N1-C2-N3 | -5.10 | 126.75 | 129.30 |
| 56 | 3 | 28 | C | C5-C6-N1 | 5.10 | 123.55 | 121.00 |
| 2 | 2 | 1929 | A | N3-C4-N9 | 5.10 | 131.48 | 127.40 |
| 2 | 2 | 5036 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 2 | 2 | 68 | U | N1-C2-O2 | 5.10 | 126.37 | 122.80 |
| 2 | 2 | 2059 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 2 | 2 | 3834 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 2 | 2 | 221 | C | C5-C6-N1 | 5.10 | 123.55 | 121.00 |
| 2 | 2 | 1508 | A | N1-C2-N3 | -5.10 | 126.75 | 129.30 |
| 2 | 2 | 1572 | U | N1-C2-O2 | 5.10 | 126.37 | 122.80 |
| 21 | V | 190 | ASP | CB-CG-OD2 | 5.10 | 122.89 | 118.30 |
| 2 | 2 | 486 | C | O5'-P-OP2 | -5.09 | 101.11 | 105.70 |
| 2 | 2 | 1525 | A | C2-N3-C4 | 5.09 | 113.15 | 110.60 |
| 2 | 2 | 4535 | A | N1-C2-N3 | -5.09 | 126.75 | 129.30 |
| 2 | 2 | 1333 | A | N1-C2-N3 | -5.09 | 126.75 | 129.30 |
| 2 | 2 | 1373 | A | N1-C2-N3 | -5.09 | 126.75 | 129.30 |
| 2 | 2 | 1637 | A | N1-C2-N3 | -5.09 | 126.75 | 129.30 |
| 50 | c | 190 | LEU | CA-CB-CG | 5.09 | 127.01 | 115.30 |
| 2 | 2 | 367 | C | C6-N1-C2 | -5.09 | 118.26 | 120.30 |
| 2 | 2 | 1700 | G | C4-N9-C1' | 5.09 | 133.12 | 126.50 |
| 2 | 2 | 4229 | U | C5-C6-N1 | 5.09 | 125.24 | 122.70 |
| 56 | 3 | 51 | G | C2'-C3'-O3' | 5.09 | 121.84 | 113.70 |
| 57 | q | 27 | LEU | CA-CB-CG | 5.09 | 127.00 | 115.30 |
| 2 | 2 | 110 | C | C6-N1-C2 | -5.09 | 118.27 | 120.30 |
| 2 | 2 | 3650 | C | C2-N1-C1' | 5.09 | 124.39 | 118.80 |
| 2 | 2 | 4970 | C | C2-N1-C1' | 5.08 | 124.39 | 118.80 |
| 2 | 2 | 343 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 2 | 2 | 1602 | U | N3-C2-O2 | -5.08 | 118.64 | 122.20 |
| 2 | 2 | 3721 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 2 | 2 | 4996 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 2 | 2 | 1334 | A | N1-C2-N3 | -5.08 | 126.76 | 129.30 |
| 2 | 2 | 1554 | A | N1-C2-N3 | -5.08 | 126.76 | 129.30 |
| 2 | 2 | 4267 | G | C8-N9-C4 | -5.08 | 104.37 | 106.40 |
| 2 | 2 | 4994 | G | N3-C4-N9 | 5.08 | 129.05 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 40 | R | 109 | LEU | CA-CB-CG | 5.08 | 126.99 | 115.30 |
| 2 | 2 | 736 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 2 | 2 | 1086 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 2 | 2 | 3912 | U | N3-C2-O2 | -5.08 | 118.64 | 122.20 |
| 2 | 2 | 2856 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 21 | V | 100 | ASP | CB-CG-OD1 | 5.08 | 122.87 | 118.30 |
| 2 | 2 | 1577 | G | N1-C6-O6 | -5.08 | 116.86 | 119.90 |
| 1 | N | 320 | LEU | CB-CG-CD2 | 5.07 | 119.62 | 111.00 |
| 2 | 2 | 35 | U | C2-N1-C1' | 5.07 | 123.79 | 117.70 |
| 2 | 2 | 703 | G | C4-N9-C1' | 5.07 | 133.09 | 126.50 |
| 2 | 2 | 1816 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 2 | 2 | 2678 | A | N1-C2-N3 | -5.07 | 126.76 | 129.30 |
| 2 | 2 | 220 | C | C2-N3-C4 | 5.07 | 122.44 | 119.90 |
| 2 | 2 | 1655 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 2 | 2 | 4628 | U | N1-C2-O2 | 5.07 | 126.35 | 122.80 |
| 2 | 2 | 4864 | U | C5-C6-N1 | 5.07 | 125.23 | 122.70 |
| 36 | w | 130 | LEU | CA-CB-CG | 5.07 | 126.95 | 115.30 |
| 2 | 2 | 2603 | C | C5-C6-N1 | 5.07 | 123.53 | 121.00 |
| 2 | 2 | 4436 | U | C2-N1-C1' | 5.07 | 123.78 | 117.70 |
| 41 | W | 361 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |
| 2 | 2 | 1632 | A | C4-N9-C1' | 5.06 | 135.41 | 126.30 |
| 56 | 3 | 78 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 2 | 2 | 499 | G | C6-C5-N7 | -5.06 | 127.36 | 130.40 |
| 2 | 2 | 1671 | U | C6-N1-C2 | -5.06 | 117.96 | 121.00 |
| 2 | 2 | 2410 | C | C6-N1-C1' | -5.06 | 114.73 | 120.80 |
| 2 | 2 | 4429 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 2 | 2 | 2062 | C | N1-C2-O2 | 5.06 | 121.93 | 118.90 |
| 2 | 2 | 1203 | G | C4-N9-C1' | 5.05 | 133.07 | 126.50 |
| 2 | 2 | 3606 | U | C2-N1-C1' | 5.05 | 123.76 | 117.70 |
| 56 | 3 | 17 | C | C6-N1-C2 | -5.05 | 118.28 | 120.30 |
| 2 | 2 | 1093 | C | C6-N1-C2 | -5.05 | 118.28 | 120.30 |
| 2 | 2 | 4425 | G | C4-N9-C1' | 5.05 | 133.07 | 126.50 |
| 59 | f | 202 | LEU | C-N-CA | 5.05 | 134.33 | 121.70 |
| 2 | 2 | 1874 | A | N1-C2-N3 | -5.05 | 126.78 | 129.30 |
| 5 | 8 | 41 | A | N1-C2-N3 | -5.05 | 126.78 | 129.30 |
| 56 | 3 | 71 | G | OP1-P-O3' | 5.05 | 116.31 | 105.20 |
| 2 | 2 | 2689 | C | C5-C6-N1 | 5.05 | 123.52 | 121.00 |
| 2 | 2 | 4969 | C | C5-C6-N1 | 5.05 | 123.52 | 121.00 |
| 2 | 2 | 201 | C | C2-N1-C1' | 5.04 | 124.35 | 118.80 |
| 2 | 2 | 2544 | G | C4-N9-C1' | 5.04 | 133.06 | 126.50 |
| 2 | 2 | 2667 | C | C5-C6-N1 | 5.04 | 123.52 | 121.00 |
| 2 | 2 | 1813 | U | C5-C6-N1 | 5.04 | 125.22 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 4864 | U | C6-N1-C2 | -5.04 | 117.97 | 121.00 |
| 2 | 2 | 1860 | U | C2-N1-C1' | 5.04 | 123.75 | 117.70 |
| 2 | 2 | 2708 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 5 | 8 | 9 | A | N1-C2-N3 | -5.04 | 126.78 | 129.30 |
| 10 | E | 81 | LEU | CA-CB-CG | 5.04 | 126.90 | 115.30 |
| 36 | w | 169 | MET | CG-SD-CE | 5.04 | 108.26 | 100.20 |
| 5 | 8 | 43 | A | C2-N3-C4 | 5.04 | 113.12 | 110.60 |
| 2 | 2 | 2304 | U | N1-C2-O2 | 5.04 | 126.33 | 122.80 |
| 41 | W | 374 | LEU | CA-CB-CG | 5.04 | 126.88 | 115.30 |
| 2 | 2 | 4612 | C | N1-C2-O2 | 5.04 | 121.92 | 118.90 |
| 2 | 2 | 4619 | U | N3-C2-O2 | -5.04 | 118.68 | 122.20 |
| 56 | 3 | 45 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 2 | 2 | 126 | C | C5-C6-N1 | 5.03 | 123.52 | 121.00 |
| 2 | 2 | 2616 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 2 | 2 | 4981 | G | N3-C4-C5 | -5.03 | 126.08 | 128.60 |
| 5 | 8 | 51 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 2 | 2 | 1694 | C | C5-C6-N1 | 5.03 | 123.52 | 121.00 |
| 11 | G | 131 | LYS | C-N-CA | 5.03 | 134.28 | 121.70 |
| 14 | J | 229 | LEU | CA-CB-CG | 5.03 | 126.87 | 115.30 |
| 2 | 2 | 4123 | C | C2-N1-C1' | 5.03 | 124.33 | 118.80 |
| 59 | f | 298 | CYS | CA-CB-SG | 5.03 | 123.05 | 114.00 |
| 2 | 2 | 2611 | A | N1-C2-N3 | -5.03 | 126.79 | 129.30 |
| 2 | 2 | 3623 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 2 | 2 | 1795 | A | C8-N9-C1' | -5.03 | 118.65 | 127.70 |
| 2 | 2 | 2749 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 2 | 2 | 4371 | G | N3-C4-N9 | 5.03 | 129.01 | 126.00 |
| 2 | 2 | 1682 | A | N1-C2-N3 | -5.02 | 126.79 | 129.30 |
| 2 | 2 | 1891 | A | N1-C2-N3 | -5.02 | 126.79 | 129.30 |
| 2 | 2 | 4341 | C | N3-C2-O2 | -5.02 | 118.38 | 121.90 |
| 2 | 2 | 4464 | A | N1-C2-N3 | -5.02 | 126.79 | 129.30 |
| 1 | N | 98 | MET | CB-CG-SD | 5.02 | 127.46 | 112.40 |
| 2 | 2 | 2653 | C | C5-C6-N1 | 5.02 | 123.51 | 121.00 |
| 2 | 2 | 4945 | G | C4-N9-C1' | 5.02 | 133.03 | 126.50 |
| 56 | 3 | 77 | A | N1-C2-N3 | -5.02 | 126.79 | 129.30 |
| 2 | 2 | 51 | A | N1-C2-N3 | -5.02 | 126.79 | 129.30 |
| 2 | 2 | 162 | A | N1-C2-N3 | -5.02 | 126.79 | 129.30 |
| 2 | 2 | 2071 | A | C2-N3-C4 | 5.02 | 113.11 | 110.60 |
| 2 | 2 | 4088 | C | C5-C6-N1 | 5.02 | 123.51 | 121.00 |
| 2 | 2 | 148 | C | C6-N1-C2 | -5.01 | 118.29 | 120.30 |
| 2 | 2 | 378 | A | N1-C2-N3 | -5.01 | 126.79 | 129.30 |
| 2 | 2 | 4469 | U | N1-C2-O2 | 5.01 | 126.31 | 122.80 |
| 2 | 2 | 2304 | U | C2-N1-C1' | 5.01 | 123.72 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 4970 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 2 | 2 | 3847 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 2 | 2 | 4402 | C | C5-C6-N1 | 5.01 | 123.51 | 121.00 |
| 2 | 2 | 125 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 2 | 2 | 1293 | G | N3-C4-C5 | -5.01 | 126.09 | 128.60 |
| 2 | 2 | 4123 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 2 | 2 | 4642 | U | N3-C2-O2 | -5.01 | 118.69 | 122.20 |
| 2 | 2 | 4758 | U | C6-N1-C2 | -5.01 | 117.99 | 121.00 |
| 2 | 2 | 447 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 2 | 2 | 2362 | U | C6-N1-C2 | -5.01 | 118.00 | 121.00 |
| 2 | 2 | 4317 | A | N1-C2-N3 | -5.01 | 126.80 | 129.30 |
| 5 | 8 | 32 | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 2 | 2 | 1439 | C | C5-C6-N1 | 5.00 | 123.50 | 121.00 |
| 2 | 2 | 4325 | A | N1-C2-N3 | -5.00 | 126.80 | 129.30 |
| 2 | 2 | 4691 | A | N1-C2-N3 | -5.00 | 126.80 | 129.30 |
| 5 | 8 | 51 | U | C2-N1-C1' | 5.00 | 123.70 | 117.70 |
| 2 | 2 | 408 | A | N1-C2-N3 | -5.00 | 126.80 | 129.30 |
| 2 | 2 | 1889 | U | N3-C2-O2 | -5.00 | 118.70 | 122.20 |
| 2 | 2 | 4243 | C | C6-N1-C2 | -5.00 | 118.30 | 120.30 |
| 2 | 2 | 4381 | A | N1-C2-N3 | -5.00 | 126.80 | 129.30 |
| 51 | 1 | 21 | VAL | CA-CB-CG2 | 5.00 | 118.40 | 110.90 |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 51 | 1 | 200 | GLU | Peptide |
| 43 | 4 | 294 | LYS | Peptide |
| 43 | 4 | 503 | THR | Peptide |
| 7 | A | 107 | ARG | Sidechain |
| 8 | B | 241 | PRO | Peptide |
| 11 | G | 162 | ASP | Peptide |
| 11 | G | 189 | ARG | Sidechain |
| 42 | T | 53 | PRO | Peptide |
| 44 | Y | 131 | ARG | Peptide |
| 59 | f | 204 | ARG | Peptide |
| 30 | n | 106 | TYR | Peptide |
| 33 | r | 254 | PHE | Peptide |
| 48 | t | 142 | SER | Peptide |
| 34 | u | 54 | ALA | Peptide |

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1 | N | 324/687 (47%) | 309 (95%) | 15 (5%) | 0 | 100 | 100 |
| 3 | 6 | 242/245 (99%) | 227 (94%) | 15 (6%) | 0 | 100 | 100 |
| 4 | 7 | 133/163 (82%) | 128 (96%) | 5 (4%) | 0 | 100 | 100 |
| 6 | 9 | 82/134 (61%) | 71 (87%) | 11 (13%) | 0 | 100 | 100 |
| 7 | A | 41/159 (26%) | 39 (95%) | 2 (5%) | 0 | 100 | 100 |
| 8 | B | 401/403 (100%) | 382 (95%) | 18 (4%) | 1 (0%) | 47 | 79 |
| 9 | D | 356/427 (83%) | 334 (94%) | 22 (6%) | 0 | 100 | 100 |
| 10 | E | 96/115 (84%) | 91 (95%) | 5 (5%) | 0 | 100 | 100 |
| 11 | G | 239/266 (90%) | 225 (94%) | 14 (6%) | 0 | 100 | 100 |
| 12 | H | 120/123 (98%) | 117 (98%) | 3 (2%) | 0 | 100 | 100 |
| 13 | I | 188/192 (98%) | 179 (95%) | 9 (5%) | 0 | 100 | 100 |
| 14 | J | 213/260 (82%) | 207 (97%) | 6 (3%) | 0 | 100 | 100 |
| 15 | L | 108/148 (73%) | 101 (94%) | 7 (6%) | 0 | 100 | 100 |
| 16 | M | 84/97 (87%) | 80 (95%) | 4 (5%) | 0 | 100 | 100 |
| 17 | P | 48/51 (94%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 18 | Q | 208/211 (99%) | 200 (96%) | 8 (4%) | 0 | 100 | 100 |
| 19 | S | 133/215 (62%) | 127 (96%) | 6 (4%) | 0 | 100 | 100 |
| 20 | U | 201/204 (98%) | 191 (95%) | 10 (5%) | 0 | 100 | 100 |
| 21 | V | 199/203 (98%) | 192 (96%) | 7 (4%) | 0 | 100 | 100 |
| 22 | X | 89/92 (97%) | 85 (96%) | 4 (4%) | 0 | 100 | 100 |
| 23 | Z | 149/188 (79%) | 147 (99%) | 2 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 24 | a | 146/196 (74%) | 142 (97%) | 4 (3%) | 0 | 100 | 100 |
| 25 | b | 174/176 (99%) | 170 (98%) | 4 (2%) | 0 | 100 | 100 |
| 26 | e | 129/140 (92%) | 118 (92%) | 11 (8%) | 0 | 100 | 100 |
| 27 | h | 132/145 (91%) | 126 (96%) | 6 (4%) | 0 | 100 | 100 |
| 28 | l | 123/137 (90%) | 115 (94%) | 8 (6%) | 0 | 100 | 100 |
| 29 | m | 246/257 (96%) | 221 (90%) | 25 (10%) | 0 | 100 | 100 |
| 30 | n | 107/110 (97%) | 102 (95%) | 5 (5%) | 0 | 100 | 100 |
| 31 | o | 231/288 (80%) | 220 (95%) | 11 (5%) | 0 | 100 | 100 |
| 32 | p | 224/248 (90%) | 216 (96%) | 8 (4%) | 0 | 100 | 100 |
| 33 | r | 80/360 (22%) | 77 (96%) | 3 (4%) | 0 | 100 | 100 |
| 34 | u | 63/549 (12%) | 58 (92%) | 4 (6%) | 1 (2%) | 9 | 43 |
| 35 | v | 215/239 (90%) | 206 (96%) | 9 (4%) | 0 | 100 | 100 |
| 36 | w | 427/731 (58%) | 406 (95%) | 19 (4%) | 2 (0%) | 29 | 67 |
| 37 | y | 163/165 (99%) | 155 (95%) | 8 (5%) | 0 | 100 | 100 |
| 38 | z | 63/129 (49%) | 60 (95%) | 3 (5%) | 0 | 100 | 100 |
| 39 | C | 163/178 (92%) | 145 (89%) | 18 (11%) | 0 | 100 | 100 |
| 40 | R | 291/297 (98%) | 273 (94%) | 17 (6%) | 1 (0%) | 41 | 74 |
| 41 | W | 386/485 (80%) | 365 (95%) | 21 (5%) | 0 | 100 | 100 |
| 42 | T | 120/160 (75%) | 112 (93%) | 8 (7%) | 0 | 100 | 100 |
| 43 | 4 | 607/634 (96%) | 555 (91%) | 47 (8%) | 5 (1%) | 19 | 58 |
| 44 | Y | 165/184 (90%) | 158 (96%) | 7 (4%) | 0 | 100 | 100 |
| 45 | k | 127/135 (94%) | 120 (94%) | 7 (6%) | 0 | 100 | 100 |
| 46 | j | 109/125 (87%) | 103 (94%) | 6 (6%) | 0 | 100 | 100 |
| 47 | d | 102/128 (80%) | 95 (93%) | 7 (7%) | 0 | 100 | 100 |
| 48 | t | 109/293 (37%) | 105 (96%) | 4 (4%) | 0 | 100 | 100 |
| 50 | c | 237/490 (48%) | 231 (98%) | 6 (2%) | 0 | 100 | 100 |
| 51 | l | 224/255 (88%) | 216 (96%) | 7 (3%) | 1 (0%) | 34 | 69 |
| 52 | K | 100/105 (95%) | 96 (96%) | 4 (4%) | 0 | 100 | 100 |
| 53 | F | 111/117 (95%) | 109 (98%) | 2 (2%) | 0 | 100 | 100 |
| 54 | i | 133/136 (98%) | 126 (95%) | 7 (5%) | 0 | 100 | 100 |
| 55 | O | 67/70 (96%) | 61 (91%) | 6 (9%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|----------|----------|-------------|-----|
| 57 | q | 398/588 (68%) | 382 (96%) | 16 (4%) | 0 | 100 | 100 |
| 58 | g | 143/156 (92%) | 135 (94%) | 8 (6%) | 0 | 100 | 100 |
| 59 | f | 254/478 (53%) | 236 (93%) | 17 (7%) | 1 (0%) | 34 | 69 |
| All | All | 10023/13467 (74%) | 9493 (95%) | 518 (5%) | 12 (0%) | 54 | 83 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | u | 55 | PRO |
| 51 | 1 | 24 | ASN |
| 59 | f | 203 | ASP |
| 40 | R | 270 | LYS |
| 43 | 4 | 88 | ASP |
| 36 | w | 132 | VAL |
| 43 | 4 | 230 | LEU |
| 43 | 4 | 407 | ASP |
| 36 | w | 323 | LYS |
| 43 | 4 | 427 | ASP |
| 43 | 4 | 366 | THR |
| 8 | B | 5 | LYS |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | N | 308/629 (49%) | 308 (100%) | 0 | 100 | 100 |
| 3 | 6 | 212/213 (100%) | 212 (100%) | 0 | 100 | 100 |
| 4 | 7 | 126/149 (85%) | 126 (100%) | 0 | 100 | 100 |
| 6 | 9 | 74/114 (65%) | 74 (100%) | 0 | 100 | 100 |
| 7 | A | 34/126 (27%) | 34 (100%) | 0 | 100 | 100 |
| 8 | B | 349/349 (100%) | 349 (100%) | 0 | 100 | 100 |
| 9 | D | 298/348 (86%) | 298 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 10 | E | 83/97 (86%) | 82 (99%) | 1 (1%) | 71 | 88 |
| 11 | G | 203/223 (91%) | 203 (100%) | 0 | 100 | 100 |
| 12 | H | 109/110 (99%) | 108 (99%) | 1 (1%) | 78 | 91 |
| 13 | I | 169/171 (99%) | 169 (100%) | 0 | 100 | 100 |
| 14 | J | 191/228 (84%) | 191 (100%) | 0 | 100 | 100 |
| 15 | L | 94/121 (78%) | 94 (100%) | 0 | 100 | 100 |
| 16 | M | 73/80 (91%) | 73 (100%) | 0 | 100 | 100 |
| 17 | P | 47/48 (98%) | 47 (100%) | 0 | 100 | 100 |
| 18 | Q | 176/177 (99%) | 175 (99%) | 1 (1%) | 86 | 94 |
| 19 | S | 115/161 (71%) | 115 (100%) | 0 | 100 | 100 |
| 20 | U | 171/172 (99%) | 171 (100%) | 0 | 100 | 100 |
| 21 | V | 173/174 (99%) | 172 (99%) | 1 (1%) | 86 | 94 |
| 22 | X | 74/75 (99%) | 74 (100%) | 0 | 100 | 100 |
| 23 | Z | 136/165 (82%) | 136 (100%) | 0 | 100 | 100 |
| 24 | a | 133/175 (76%) | 133 (100%) | 0 | 100 | 100 |
| 25 | b | 157/157 (100%) | 157 (100%) | 0 | 100 | 100 |
| 26 | e | 101/107 (94%) | 101 (100%) | 0 | 100 | 100 |
| 27 | h | 124/135 (92%) | 124 (100%) | 0 | 100 | 100 |
| 28 | l | 109/121 (90%) | 109 (100%) | 0 | 100 | 100 |
| 29 | m | 190/199 (96%) | 190 (100%) | 0 | 100 | 100 |
| 30 | n | 88/89 (99%) | 88 (100%) | 0 | 100 | 100 |
| 31 | o | 208/252 (82%) | 207 (100%) | 1 (0%) | 88 | 95 |
| 32 | p | 195/215 (91%) | 195 (100%) | 0 | 100 | 100 |
| 33 | r | 76/312 (24%) | 76 (100%) | 0 | 100 | 100 |
| 34 | u | 61/485 (13%) | 61 (100%) | 0 | 100 | 100 |
| 35 | v | 194/214 (91%) | 194 (100%) | 0 | 100 | 100 |
| 36 | w | 385/654 (59%) | 385 (100%) | 0 | 100 | 100 |
| 37 | y | 137/137 (100%) | 137 (100%) | 0 | 100 | 100 |
| 38 | z | 61/115 (53%) | 61 (100%) | 0 | 100 | 100 |
| 39 | C | 138/149 (93%) | 138 (100%) | 0 | 100 | 100 |
| 40 | R | 246/250 (98%) | 246 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 41 | W | 322/404 (80%) | 321 (100%) | 1 (0%) | 92 | 96 |
| 42 | T | 109/140 (78%) | 109 (100%) | 0 | 100 | 100 |
| 43 | 4 | 554/574 (96%) | 553 (100%) | 1 (0%) | 93 | 98 |
| 44 | Y | 147/163 (90%) | 146 (99%) | 1 (1%) | 84 | 94 |
| 45 | k | 115/121 (95%) | 115 (100%) | 0 | 100 | 100 |
| 46 | j | 101/110 (92%) | 101 (100%) | 0 | 100 | 100 |
| 47 | d | 94/115 (82%) | 94 (100%) | 0 | 100 | 100 |
| 48 | t | 103/274 (38%) | 101 (98%) | 2 (2%) | 57 | 81 |
| 50 | c | 222/437 (51%) | 222 (100%) | 0 | 100 | 100 |
| 51 | l | 206/228 (90%) | 205 (100%) | 1 (0%) | 88 | 95 |
| 52 | K | 86/89 (97%) | 86 (100%) | 0 | 100 | 100 |
| 53 | F | 97/100 (97%) | 97 (100%) | 0 | 100 | 100 |
| 54 | i | 117/118 (99%) | 116 (99%) | 1 (1%) | 78 | 91 |
| 55 | O | 64/65 (98%) | 64 (100%) | 0 | 100 | 100 |
| 57 | q | 359/509 (70%) | 358 (100%) | 1 (0%) | 92 | 96 |
| 58 | g | 126/133 (95%) | 126 (100%) | 0 | 100 | 100 |
| 59 | f | 222/402 (55%) | 221 (100%) | 1 (0%) | 88 | 95 |
| All | All | 8862/11678 (76%) | 8848 (100%) | 14 (0%) | 93 | 98 |

All (14) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | E | 106 | ARG |
| 12 | H | 101 | ASN |
| 18 | Q | 103 | ARG |
| 21 | V | 117 | ARG |
| 31 | o | 56 | ARG |
| 41 | W | 470 | ARG |
| 43 | 4 | 385 | ARG |
| 44 | Y | 97 | ASN |
| 48 | t | 50 | ARG |
| 48 | t | 148 | ARG |
| 51 | l | 246 | ARG |
| 54 | i | 108 | ARG |
| 57 | q | 111 | LYS |
| 59 | f | 362 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 149 | ASN |
| 1 | N | 158 | ASN |
| 1 | N | 379 | ASN |
| 13 | I | 8 | GLN |
| 19 | S | 20 | HIS |
| 33 | r | 256 | GLN |
| 35 | v | 186 | GLN |
| 57 | q | 422 | HIS |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2 | 2 | 3441/5054 (68%) | 817 (23%) | 21 (0%) |
| 49 | x | 0/160 | - | - |
| 5 | 8 | 155/156 (99%) | 29 (18%) | 0 |
| 56 | 3 | 113/120 (94%) | 23 (20%) | 2 (1%) |
| All | All | 3709/5490 (67%) | 869 (23%) | 23 (0%) |

All (869) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 2 | 25 | A |
| 2 | 2 | 39 | A |
| 2 | 2 | 42 | A |
| 2 | 2 | 44 | A |
| 2 | 2 | 48 | G |
| 2 | 2 | 56 | A |
| 2 | 2 | 59 | A |
| 2 | 2 | 64 | A |
| 2 | 2 | 65 | A |
| 2 | 2 | 69 | A |
| 2 | 2 | 72 | C |
| 2 | 2 | 73 | A |
| 2 | 2 | 76 | A |
| 2 | 2 | 84 | A |
| 2 | 2 | 91 | G |
| 2 | 2 | 98 | A |
| 2 | 2 | 108 | A |
| 2 | 2 | 109 | G |
| 2 | 2 | 110 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 112 | C |
| 2 | 2 | 119 | G |
| 2 | 2 | 120 | A |
| 2 | 2 | 122 | U |
| 2 | 2 | 131 | C |
| 2 | 2 | 132 | G |
| 2 | 2 | 134 | G |
| 2 | 2 | 135 | G |
| 2 | 2 | 137 | G |
| 2 | 2 | 144 | G |
| 2 | 2 | 152 | U |
| 2 | 2 | 159 | C |
| 2 | 2 | 169 | G |
| 2 | 2 | 170 | C |
| 2 | 2 | 172 | C |
| 2 | 2 | 175 | C |
| 2 | 2 | 183 | C |
| 2 | 2 | 185 | C |
| 2 | 2 | 188 | G |
| 2 | 2 | 197 | A |
| 2 | 2 | 200 | U |
| 2 | 2 | 209 | U |
| 2 | 2 | 217 | C |
| 2 | 2 | 218 | A |
| 2 | 2 | 234 | G |
| 2 | 2 | 254 | G |
| 2 | 2 | 256 | G |
| 2 | 2 | 262 | G |
| 2 | 2 | 265 | C |
| 2 | 2 | 266 | C |
| 2 | 2 | 279 | A |
| 2 | 2 | 280 | G |
| 2 | 2 | 297 | U |
| 2 | 2 | 306 | A |
| 2 | 2 | 315 | G |
| 2 | 2 | 316 | U |
| 2 | 2 | 340 | C |
| 2 | 2 | 345 | C |
| 2 | 2 | 349 | A |
| 2 | 2 | 363 | A |
| 2 | 2 | 373 | OMG |
| 2 | 2 | 387 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 398 | A2M |
| 2 | 2 | 407 | A |
| 2 | 2 | 409 | G |
| 2 | 2 | 410 | A |
| 2 | 2 | 412 | G |
| 2 | 2 | 432 | U |
| 2 | 2 | 433 | A |
| 2 | 2 | 449 | C |
| 2 | 2 | 450 | G |
| 2 | 2 | 452 | A |
| 2 | 2 | 453 | G |
| 2 | 2 | 454 | U |
| 2 | 2 | 465 | G |
| 2 | 2 | 467 | U |
| 2 | 2 | 483 | G |
| 2 | 2 | 484 | U |
| 2 | 2 | 485 | C |
| 2 | 2 | 486 | C |
| 2 | 2 | 489 | C |
| 2 | 2 | 491 | G |
| 2 | 2 | 493 | G |
| 2 | 2 | 495 | C |
| 2 | 2 | 496 | G |
| 2 | 2 | 497 | G |
| 2 | 2 | 499 | G |
| 2 | 2 | 500 | G |
| 2 | 2 | 501 | C |
| 2 | 2 | 502 | C |
| 2 | 2 | 503 | C |
| 2 | 2 | 504 | G |
| 2 | 2 | 505 | G |
| 2 | 2 | 509 | A |
| 2 | 2 | 510 | U |
| 2 | 2 | 511 | C |
| 2 | 2 | 513 | U |
| 2 | 2 | 514 | U |
| 2 | 2 | 515 | C |
| 2 | 2 | 516 | C |
| 2 | 2 | 518 | G |
| 2 | 2 | 519 | C |
| 2 | 2 | 653 | U |
| 2 | 2 | 654 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 657 | C |
| 2 | 2 | 659 | G |
| 2 | 2 | 666 | G |
| 2 | 2 | 667 | A |
| 2 | 2 | 668 | C |
| 2 | 2 | 673 | C |
| 2 | 2 | 685 | C |
| 2 | 2 | 686 | A |
| 2 | 2 | 692 | A |
| 2 | 2 | 696 | C |
| 2 | 2 | 703 | G |
| 2 | 2 | 704 | C |
| 2 | 2 | 731 | G |
| 2 | 2 | 738 | C |
| 2 | 2 | 739 | G |
| 2 | 2 | 740 | G |
| 2 | 2 | 742 | G |
| 2 | 2 | 746 | A |
| 2 | 2 | 759 | G |
| 2 | 2 | 904 | C |
| 2 | 2 | 905 | C |
| 2 | 2 | 906 | C |
| 2 | 2 | 913 | U |
| 2 | 2 | 914 | U |
| 2 | 2 | 915 | A |
| 2 | 2 | 916 | C |
| 2 | 2 | 917 | A |
| 2 | 2 | 918 | G |
| 2 | 2 | 924 | C |
| 2 | 2 | 925 | C |
| 2 | 2 | 926 | G |
| 2 | 2 | 932 | A |
| 2 | 2 | 933 | G |
| 2 | 2 | 936 | C |
| 2 | 2 | 941 | C |
| 2 | 2 | 943 | A |
| 2 | 2 | 944 | A |
| 2 | 2 | 945 | U |
| 2 | 2 | 956 | A |
| 2 | 2 | 959 | G |
| 2 | 2 | 960 | A |
| 2 | 2 | 961 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 962 | C |
| 2 | 2 | 965 | G |
| 2 | 2 | 966 | A |
| 2 | 2 | 967 | C |
| 2 | 2 | 968 | C |
| 2 | 2 | 969 | C |
| 2 | 2 | 970 | G |
| 2 | 2 | 977 | C |
| 2 | 2 | 982 | U |
| 2 | 2 | 984 | C |
| 2 | 2 | 989 | U |
| 2 | 2 | 990 | C |
| 2 | 2 | 991 | C |
| 2 | 2 | 992 | C |
| 2 | 2 | 993 | G |
| 2 | 2 | 994 | G |
| 2 | 2 | 995 | C |
| 2 | 2 | 1048 | G |
| 2 | 2 | 1049 | C |
| 2 | 2 | 1051 | G |
| 2 | 2 | 1066 | G |
| 2 | 2 | 1067 | G |
| 2 | 2 | 1068 | G |
| 2 | 2 | 1070 | G |
| 2 | 2 | 1072 | C |
| 2 | 2 | 1082 | C |
| 2 | 2 | 1170 | G |
| 2 | 2 | 1173 | G |
| 2 | 2 | 1177 | U |
| 2 | 2 | 1178 | G |
| 2 | 2 | 1179 | U |
| 2 | 2 | 1180 | C |
| 2 | 2 | 1181 | C |
| 2 | 2 | 1182 | C |
| 2 | 2 | 1183 | C |
| 2 | 2 | 1184 | A |
| 2 | 2 | 1185 | G |
| 2 | 2 | 1187 | G |
| 2 | 2 | 1189 | G |
| 2 | 2 | 1194 | G |
| 2 | 2 | 1195 | G |
| 2 | 2 | 1198 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 1200 | G |
| 2 | 2 | 1202 | C |
| 2 | 2 | 1203 | G |
| 2 | 2 | 1211 | G |
| 2 | 2 | 1215 | C |
| 2 | 2 | 1216 | C |
| 2 | 2 | 1219 | G |
| 2 | 2 | 1222 | A |
| 2 | 2 | 1241 | C |
| 2 | 2 | 1243 | C |
| 2 | 2 | 1245 | C |
| 2 | 2 | 1252 | C |
| 2 | 2 | 1253 | G |
| 2 | 2 | 1255 | A |
| 2 | 2 | 1256 | G |
| 2 | 2 | 1260 | G |
| 2 | 2 | 1265 | G |
| 2 | 2 | 1266 | G |
| 2 | 2 | 1269 | G |
| 2 | 2 | 1271 | G |
| 2 | 2 | 1272 | C |
| 2 | 2 | 1275 | G |
| 2 | 2 | 1280 | C |
| 2 | 2 | 1283 | G |
| 2 | 2 | 1284 | G |
| 2 | 2 | 1287 | G |
| 2 | 2 | 1294 | A |
| 2 | 2 | 1296 | G |
| 2 | 2 | 1301 | C |
| 2 | 2 | 1302 | U |
| 2 | 2 | 1303 | A |
| 2 | 2 | 1314 | C |
| 2 | 2 | 1315 | C |
| 2 | 2 | 1323 | A |
| 2 | 2 | 1337 | A |
| 2 | 2 | 1354 | A |
| 2 | 2 | 1358 | G |
| 2 | 2 | 1359 | G |
| 2 | 2 | 1365 | C |
| 2 | 2 | 1366 | G |
| 2 | 2 | 1367 | C |
| 2 | 2 | 1370 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 1377 | G |
| 2 | 2 | 1378 | C |
| 2 | 2 | 1379 | C |
| 2 | 2 | 1381 | U |
| 2 | 2 | 1387 | A |
| 2 | 2 | 1394 | G |
| 2 | 2 | 1398 | A |
| 2 | 2 | 1399 | G |
| 2 | 2 | 1402 | C |
| 2 | 2 | 1404 | G |
| 2 | 2 | 1405 | C |
| 2 | 2 | 1407 | C |
| 2 | 2 | 1408 | G |
| 2 | 2 | 1409 | C |
| 2 | 2 | 1410 | U |
| 2 | 2 | 1412 | G |
| 2 | 2 | 1420 | A |
| 2 | 2 | 1439 | C |
| 2 | 2 | 1442 | C |
| 2 | 2 | 1444 | G |
| 2 | 2 | 1446 | C |
| 2 | 2 | 1448 | G |
| 2 | 2 | 1449 | C |
| 2 | 2 | 1465 | G |
| 2 | 2 | 1472 | C |
| 2 | 2 | 1482 | G |
| 2 | 2 | 1483 | C |
| 2 | 2 | 1486 | C |
| 2 | 2 | 1497 | A |
| 2 | 2 | 1498 | G |
| 2 | 2 | 1503 | A |
| 2 | 2 | 1518 | A |
| 2 | 2 | 1525 | A |
| 2 | 2 | 1534 | A2M |
| 2 | 2 | 1547 | A |
| 2 | 2 | 1564 | A |
| 2 | 2 | 1566 | C |
| 2 | 2 | 1578 | U |
| 2 | 2 | 1592 | G |
| 2 | 2 | 1595 | G |
| 2 | 2 | 1596 | U |
| 2 | 2 | 1612 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 1613 | A |
| 2 | 2 | 1624 | G |
| 2 | 2 | 1625 | OMG |
| 2 | 2 | 1626 | G |
| 2 | 2 | 1631 | A |
| 2 | 2 | 1633 | G |
| 2 | 2 | 1634 | A |
| 2 | 2 | 1638 | A |
| 2 | 2 | 1641 | G |
| 2 | 2 | 1649 | U |
| 2 | 2 | 1650 | A |
| 2 | 2 | 1654 | G |
| 2 | 2 | 1661 | C |
| 2 | 2 | 1671 | U |
| 2 | 2 | 1672 | U |
| 2 | 2 | 1673 | U |
| 2 | 2 | 1674 | C |
| 2 | 2 | 1675 | C |
| 2 | 2 | 1676 | C |
| 2 | 2 | 1677 | U |
| 2 | 2 | 1679 | A |
| 2 | 2 | 1680 | G |
| 2 | 2 | 1681 | G |
| 2 | 2 | 1691 | G |
| 2 | 2 | 1697 | G |
| 2 | 2 | 1699 | A |
| 2 | 2 | 1700 | G |
| 2 | 2 | 1701 | A |
| 2 | 2 | 1703 | C |
| 2 | 2 | 1704 | C |
| 2 | 2 | 1705 | G |
| 2 | 2 | 1715 | C |
| 2 | 2 | 1717 | C |
| 2 | 2 | 1718 | C |
| 2 | 2 | 1719 | A |
| 2 | 2 | 1724 | G |
| 2 | 2 | 1731 | C |
| 2 | 2 | 1732 | C |
| 2 | 2 | 1796 | U |
| 2 | 2 | 1797 | G |
| 2 | 2 | 1803 | G |
| 2 | 2 | 1804 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 1806 | G |
| 2 | 2 | 1809 | C |
| 2 | 2 | 1810 | G |
| 2 | 2 | 1815 | G |
| 2 | 2 | 1816 | C |
| 2 | 2 | 1821 | G |
| 2 | 2 | 1822 | U |
| 2 | 2 | 1832 | C |
| 2 | 2 | 1834 | U |
| 2 | 2 | 1836 | G |
| 2 | 2 | 1837 | A |
| 2 | 2 | 1842 | G |
| 2 | 2 | 1854 | G |
| 2 | 2 | 1855 | G |
| 2 | 2 | 1856 | C |
| 2 | 2 | 1861 | U |
| 2 | 2 | 1862 | U |
| 2 | 2 | 1865 | G |
| 2 | 2 | 1869 | G |
| 2 | 2 | 1870 | C |
| 2 | 2 | 1871 | A2M |
| 2 | 2 | 1882 | U |
| 2 | 2 | 1883 | OMG |
| 2 | 2 | 1888 | A |
| 2 | 2 | 1897 | A |
| 2 | 2 | 1916 | G |
| 2 | 2 | 1918 | U |
| 2 | 2 | 1919 | G |
| 2 | 2 | 1920 | C |
| 2 | 2 | 1921 | C |
| 2 | 2 | 1922 | G |
| 2 | 2 | 1931 | C |
| 2 | 2 | 1932 | A |
| 2 | 2 | 1935 | C |
| 2 | 2 | 1939 | A |
| 2 | 2 | 1940 | G |
| 2 | 2 | 1942 | A |
| 2 | 2 | 1943 | A |
| 2 | 2 | 1944 | A |
| 2 | 2 | 1948 | G |
| 2 | 2 | 1956 | A |
| 2 | 2 | 1959 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 1960 | A |
| 2 | 2 | 1966 | C |
| 2 | 2 | 1972 | G |
| 2 | 2 | 1974 | U |
| 2 | 2 | 1979 | A |
| 2 | 2 | 1980 | U |
| 2 | 2 | 1981 | G |
| 2 | 2 | 1984 | A |
| 2 | 2 | 1985 | G |
| 2 | 2 | 1990 | A |
| 2 | 2 | 1997 | U |
| 2 | 2 | 2001 | G |
| 2 | 2 | 2002 | A |
| 2 | 2 | 2003 | G |
| 2 | 2 | 2004 | U |
| 2 | 2 | 2010 | A |
| 2 | 2 | 2011 | C |
| 2 | 2 | 2017 | A |
| 2 | 2 | 2018 | C |
| 2 | 2 | 2025 | A |
| 2 | 2 | 2026 | A |
| 2 | 2 | 2033 | A |
| 2 | 2 | 2034 | G |
| 2 | 2 | 2040 | A |
| 2 | 2 | 2044 | U |
| 2 | 2 | 2046 | G |
| 2 | 2 | 2048 | U |
| 2 | 2 | 2055 | G |
| 2 | 2 | 2056 | G |
| 2 | 2 | 2069 | A |
| 2 | 2 | 2084 | C |
| 2 | 2 | 2085 | G |
| 2 | 2 | 2092 | G |
| 2 | 2 | 2093 | A |
| 2 | 2 | 2095 | A |
| 2 | 2 | 2096 | G |
| 2 | 2 | 2098 | G |
| 2 | 2 | 2101 | C |
| 2 | 2 | 2102 | G |
| 2 | 2 | 2104 | G |
| 2 | 2 | 2105 | A |
| 2 | 2 | 2110 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 2111 | G |
| 2 | 2 | 2112 | G |
| 2 | 2 | 2113 | C |
| 2 | 2 | 2252 | G |
| 2 | 2 | 2253 | A |
| 2 | 2 | 2255 | C |
| 2 | 2 | 2256 | C |
| 2 | 2 | 2258 | C |
| 2 | 2 | 2259 | G |
| 2 | 2 | 2260 | C |
| 2 | 2 | 2263 | A |
| 2 | 2 | 2268 | A |
| 2 | 2 | 2289 | C |
| 2 | 2 | 2300 | A |
| 2 | 2 | 2301 | G |
| 2 | 2 | 2306 | G |
| 2 | 2 | 2313 | A |
| 2 | 2 | 2331 | G |
| 2 | 2 | 2333 | G |
| 2 | 2 | 2348 | G |
| 2 | 2 | 2351 | C |
| 2 | 2 | 2360 | A |
| 2 | 2 | 2364 | OMG |
| 2 | 2 | 2395 | A |
| 2 | 2 | 2410 | C |
| 2 | 2 | 2416 | G |
| 2 | 2 | 2417 | A |
| 2 | 2 | 2418 | A |
| 2 | 2 | 2422 | OMC |
| 2 | 2 | 2424 | OMG |
| 2 | 2 | 2425 | U |
| 2 | 2 | 2439 | G |
| 2 | 2 | 2441 | C |
| 2 | 2 | 2450 | G |
| 2 | 2 | 2465 | C |
| 2 | 2 | 2471 | G |
| 2 | 2 | 2474 | G |
| 2 | 2 | 2475 | G |
| 2 | 2 | 2476 | G |
| 2 | 2 | 2477 | A |
| 2 | 2 | 2478 | C |
| 2 | 2 | 2484 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 2486 | G |
| 2 | 2 | 2487 | G |
| 2 | 2 | 2488 | C |
| 2 | 2 | 2489 | C |
| 2 | 2 | 2490 | U |
| 2 | 2 | 2497 | C |
| 2 | 2 | 2507 | A |
| 2 | 2 | 2511 | A |
| 2 | 2 | 2512 | A |
| 2 | 2 | 2513 | A |
| 2 | 2 | 2518 | G |
| 2 | 2 | 2519 | U |
| 2 | 2 | 2529 | A |
| 2 | 2 | 2543 | A |
| 2 | 2 | 2544 | G |
| 2 | 2 | 2545 | U |
| 2 | 2 | 2546 | G |
| 2 | 2 | 2547 | G |
| 2 | 2 | 2554 | U |
| 2 | 2 | 2555 | G |
| 2 | 2 | 2559 | G |
| 2 | 2 | 2560 | C |
| 2 | 2 | 2566 | G |
| 2 | 2 | 2567 | G |
| 2 | 2 | 2583 | C |
| 2 | 2 | 2587 | A |
| 2 | 2 | 2589 | C |
| 2 | 2 | 2601 | A |
| 2 | 2 | 2618 | G |
| 2 | 2 | 2627 | C |
| 2 | 2 | 2638 | G |
| 2 | 2 | 2653 | C |
| 2 | 2 | 2661 | U |
| 2 | 2 | 2662 | G |
| 2 | 2 | 2669 | C |
| 2 | 2 | 2670 | C |
| 2 | 2 | 2675 | G |
| 2 | 2 | 2687 | U |
| 2 | 2 | 2694 | G |
| 2 | 2 | 2695 | A |
| 2 | 2 | 2696 | A |
| 2 | 2 | 2707 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 2708 | U |
| 2 | 2 | 2709 | C |
| 2 | 2 | 2710 | C |
| 2 | 2 | 2711 | G |
| 2 | 2 | 2719 | C |
| 2 | 2 | 2721 | G |
| 2 | 2 | 2723 | U |
| 2 | 2 | 2724 | G |
| 2 | 2 | 2725 | A |
| 2 | 2 | 2726 | G |
| 2 | 2 | 2739 | C |
| 2 | 2 | 2742 | G |
| 2 | 2 | 2743 | A |
| 2 | 2 | 2753 | G |
| 2 | 2 | 2758 | G |
| 2 | 2 | 2761 | U |
| 2 | 2 | 2763 | U |
| 2 | 2 | 2769 | U |
| 2 | 2 | 2770 | C |
| 2 | 2 | 2772 | C |
| 2 | 2 | 2787 | A |
| 2 | 2 | 2788 | U |
| 2 | 2 | 2790 | U |
| 2 | 2 | 2799 | G |
| 2 | 2 | 2814 | C |
| 2 | 2 | 2815 | A |
| 2 | 2 | 2826 | U |
| 2 | 2 | 2827 | G |
| 2 | 2 | 2842 | G |
| 2 | 2 | 2855 | G |
| 2 | 2 | 2875 | C |
| 2 | 2 | 2901 | G |
| 2 | 2 | 2902 | G |
| 2 | 2 | 2904 | U |
| 2 | 2 | 2905 | C |
| 2 | 2 | 2906 | G |
| 2 | 2 | 2908 | U |
| 2 | 2 | 2909 | C |
| 2 | 2 | 3585 | G |
| 2 | 2 | 3588 | C |
| 2 | 2 | 3591 | C |
| 2 | 2 | 3594 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 3595 | U |
| 2 | 2 | 3596 | A |
| 2 | 2 | 3597 | G |
| 2 | 2 | 3606 | U |
| 2 | 2 | 3615 | G |
| 2 | 2 | 3616 | U |
| 2 | 2 | 3626 | G |
| 2 | 2 | 3635 | A |
| 2 | 2 | 3644 | U |
| 2 | 2 | 3662 | A |
| 2 | 2 | 3663 | A |
| 2 | 2 | 3672 | G |
| 2 | 2 | 3673 | C |
| 2 | 2 | 3679 | U |
| 2 | 2 | 3680 | U |
| 2 | 2 | 3682 | A |
| 2 | 2 | 3691 | G |
| 2 | 2 | 3696 | C |
| 2 | 2 | 3702 | A |
| 2 | 2 | 3710 | G |
| 2 | 2 | 3711 | A |
| 2 | 2 | 3712 | A |
| 2 | 2 | 3713 | U |
| 2 | 2 | 3714 | G |
| 2 | 2 | 3722 | G |
| 2 | 2 | 3729 | U |
| 2 | 2 | 3735 | G |
| 2 | 2 | 3736 | A |
| 2 | 2 | 3748 | A |
| 2 | 2 | 3750 | G |
| 2 | 2 | 3753 | G |
| 2 | 2 | 3771 | C |
| 2 | 2 | 3772 | U |
| 2 | 2 | 3773 | U |
| 2 | 2 | 3775 | A |
| 2 | 2 | 3776 | G |
| 2 | 2 | 3833 | C |
| 2 | 2 | 3838 | U |
| 2 | 2 | 3839 | G |
| 2 | 2 | 3840 | U |
| 2 | 2 | 3867 | A2M |
| 2 | 2 | 3875 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 3876 | A |
| 2 | 2 | 3877 | A |
| 2 | 2 | 3879 | G |
| 2 | 2 | 3881 | G |
| 2 | 2 | 3898 | G |
| 2 | 2 | 3903 | A |
| 2 | 2 | 3904 | G |
| 2 | 2 | 3905 | A |
| 2 | 2 | 3906 | A |
| 2 | 2 | 3914 | U |
| 2 | 2 | 3915 | U |
| 2 | 2 | 3924 | C |
| 2 | 2 | 3938 | G |
| 2 | 2 | 4076 | G |
| 2 | 2 | 4084 | G |
| 2 | 2 | 4085 | A |
| 2 | 2 | 4095 | G |
| 2 | 2 | 4097 | G |
| 2 | 2 | 4099 | G |
| 2 | 2 | 4100 | C |
| 2 | 2 | 4101 | C |
| 2 | 2 | 4102 | C |
| 2 | 2 | 4103 | C |
| 2 | 2 | 4104 | G |
| 2 | 2 | 4105 | A |
| 2 | 2 | 4107 | G |
| 2 | 2 | 4108 | G |
| 2 | 2 | 4111 | U |
| 2 | 2 | 4112 | C |
| 2 | 2 | 4114 | C |
| 2 | 2 | 4115 | G |
| 2 | 2 | 4116 | C |
| 2 | 2 | 4117 | U |
| 2 | 2 | 4119 | C |
| 2 | 2 | 4121 | G |
| 2 | 2 | 4127 | A |
| 2 | 2 | 4133 | C |
| 2 | 2 | 4139 | G |
| 2 | 2 | 4140 | C |
| 2 | 2 | 4141 | G |
| 2 | 2 | 4142 | C |
| 2 | 2 | 4143 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 4144 | C |
| 2 | 2 | 4146 | G |
| 2 | 2 | 4147 | G |
| 2 | 2 | 4149 | C |
| 2 | 2 | 4157 | A |
| 2 | 2 | 4158 | C |
| 2 | 2 | 4162 | C |
| 2 | 2 | 4163 | U |
| 2 | 2 | 4170 | A |
| 2 | 2 | 4183 | G |
| 2 | 2 | 4184 | G |
| 2 | 2 | 4207 | C |
| 2 | 2 | 4211 | C |
| 2 | 2 | 4223 | C |
| 2 | 2 | 4226 | G |
| 2 | 2 | 4228 | G |
| 2 | 2 | 4229 | U |
| 2 | 2 | 4230 | C |
| 2 | 2 | 4231 | C |
| 2 | 2 | 4233 | A |
| 2 | 2 | 4234 | A |
| 2 | 2 | 4235 | G |
| 2 | 2 | 4236 | G |
| 2 | 2 | 4242 | U |
| 2 | 2 | 4251 | A |
| 2 | 2 | 4254 | G |
| 2 | 2 | 4255 | A |
| 2 | 2 | 4258 | C |
| 2 | 2 | 4265 | U |
| 2 | 2 | 4266 | G |
| 2 | 2 | 4267 | G |
| 2 | 2 | 4268 | A |
| 2 | 2 | 4271 | A |
| 2 | 2 | 4273 | A |
| 2 | 2 | 4274 | A |
| 2 | 2 | 4275 | G |
| 2 | 2 | 4278 | C |
| 2 | 2 | 4279 | A |
| 2 | 2 | 4280 | A |
| 2 | 2 | 4281 | A |
| 2 | 2 | 4286 | C |
| 2 | 2 | 4288 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 4290 | U |
| 2 | 2 | 4291 | G |
| 2 | 2 | 4292 | A |
| 2 | 2 | 4297 | G |
| 2 | 2 | 4302 | U |
| 2 | 2 | 4313 | A |
| 2 | 2 | 4315 | A |
| 2 | 2 | 4319 | C |
| 2 | 2 | 4321 | U |
| 2 | 2 | 4323 | A |
| 2 | 2 | 4329 | G |
| 2 | 2 | 4330 | G |
| 2 | 2 | 4332 | C |
| 2 | 2 | 4340 | U |
| 2 | 2 | 4341 | C |
| 2 | 2 | 4342 | C |
| 2 | 2 | 4343 | U |
| 2 | 2 | 4347 | G |
| 2 | 2 | 4348 | A |
| 2 | 2 | 4349 | C |
| 2 | 2 | 4350 | C |
| 2 | 2 | 4368 | G |
| 2 | 2 | 4370 | G |
| 2 | 2 | 4371 | G |
| 2 | 2 | 4372 | U |
| 2 | 2 | 4387 | C |
| 2 | 2 | 4395 | U |
| 2 | 2 | 4396 | A |
| 2 | 2 | 4401 | G |
| 2 | 2 | 4413 | C |
| 2 | 2 | 4414 | A |
| 2 | 2 | 4416 | G |
| 2 | 2 | 4417 | C |
| 2 | 2 | 4418 | G |
| 2 | 2 | 4419 | U |
| 2 | 2 | 4420 | U |
| 2 | 2 | 4421 | C |
| 2 | 2 | 4422 | A |
| 2 | 2 | 4423 | U |
| 2 | 2 | 4424 | A |
| 2 | 2 | 4425 | G |
| 2 | 2 | 4426 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 4427 | G |
| 2 | 2 | 4428 | A |
| 2 | 2 | 4433 | G |
| 2 | 2 | 4436 | U |
| 2 | 2 | 4437 | U |
| 2 | 2 | 4438 | U |
| 2 | 2 | 4440 | G |
| 2 | 2 | 4441 | A |
| 2 | 2 | 4446 | U |
| 2 | 2 | 4447 | C |
| 2 | 2 | 4449 | A |
| 2 | 2 | 4450 | U |
| 2 | 2 | 4451 | G |
| 2 | 2 | 4452 | U |
| 2 | 2 | 4453 | C |
| 2 | 2 | 4464 | A |
| 2 | 2 | 4466 | C |
| 2 | 2 | 4475 | G |
| 2 | 2 | 4476 | C |
| 2 | 2 | 4484 | A |
| 2 | 2 | 4498 | U |
| 2 | 2 | 4499 | G |
| 2 | 2 | 4500 | U |
| 2 | 2 | 4502 | C |
| 2 | 2 | 4503 | A |
| 2 | 2 | 4512 | U |
| 2 | 2 | 4513 | A |
| 2 | 2 | 4518 | A |
| 2 | 2 | 4519 | C |
| 2 | 2 | 4524 | G |
| 2 | 2 | 4530 | UR3 |
| 2 | 2 | 4543 | G |
| 2 | 2 | 4545 | G |
| 2 | 2 | 4548 | A |
| 2 | 2 | 4550 | 7MG |
| 2 | 2 | 4555 | U |
| 2 | 2 | 4556 | U |
| 2 | 2 | 4557 | U |
| 2 | 2 | 4558 | U |
| 2 | 2 | 4560 | C |
| 2 | 2 | 4567 | G |
| 2 | 2 | 4584 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 4589 | A |
| 2 | 2 | 4590 | A |
| 2 | 2 | 4599 | A |
| 2 | 2 | 4600 | G |
| 2 | 2 | 4601 | U |
| 2 | 2 | 4607 | A |
| 2 | 2 | 4608 | G |
| 2 | 2 | 4635 | A |
| 2 | 2 | 4636 | U |
| 2 | 2 | 4637 | OMG |
| 2 | 2 | 4656 | A |
| 2 | 2 | 4670 | C |
| 2 | 2 | 4678 | G |
| 2 | 2 | 4684 | A |
| 2 | 2 | 4694 | G |
| 2 | 2 | 4695 | C |
| 2 | 2 | 4708 | A |
| 2 | 2 | 4709 | U |
| 2 | 2 | 4719 | G |
| 2 | 2 | 4730 | C |
| 2 | 2 | 4731 | G |
| 2 | 2 | 4732 | G |
| 2 | 2 | 4733 | C |
| 2 | 2 | 4734 | A |
| 2 | 2 | 4740 | G |
| 2 | 2 | 4741 | C |
| 2 | 2 | 4742 | G |
| 2 | 2 | 4745 | G |
| 2 | 2 | 4751 | G |
| 2 | 2 | 4754 | G |
| 2 | 2 | 4757 | C |
| 2 | 2 | 4759 | C |
| 2 | 2 | 4761 | G |
| 2 | 2 | 4765 | G |
| 2 | 2 | 4771 | C |
| 2 | 2 | 4773 | C |
| 2 | 2 | 4776 | G |
| 2 | 2 | 4870 | OMG |
| 2 | 2 | 4871 | C |
| 2 | 2 | 4872 | 2MG |
| 2 | 2 | 4875 | G |
| 2 | 2 | 4877 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | 2 | 4882 | U |
| 2 | 2 | 4883 | C |
| 2 | 2 | 4889 | G |
| 2 | 2 | 4893 | A |
| 2 | 2 | 4895 | C |
| 2 | 2 | 4896 | G |
| 2 | 2 | 4899 | G |
| 2 | 2 | 4900 | C |
| 2 | 2 | 4901 | G |
| 2 | 2 | 4910 | G |
| 2 | 2 | 4912 | G |
| 2 | 2 | 4914 | C |
| 2 | 2 | 4916 | G |
| 2 | 2 | 4927 | G |
| 2 | 2 | 4928 | C |
| 2 | 2 | 4938 | A |
| 2 | 2 | 4940 | C |
| 2 | 2 | 4941 | G |
| 2 | 2 | 4943 | A |
| 2 | 2 | 4949 | G |
| 2 | 2 | 4976 | U |
| 2 | 2 | 4988 | U |
| 2 | 2 | 4989 | U |
| 2 | 2 | 4991 | U |
| 2 | 2 | 5013 | C |
| 2 | 2 | 5014 | A |
| 2 | 2 | 5017 | G |
| 2 | 2 | 5022 | U |
| 2 | 2 | 5025 | C |
| 2 | 2 | 5026 | U |
| 2 | 2 | 5027 | C |
| 2 | 2 | 5028 | G |
| 2 | 2 | 5030 | U |
| 2 | 2 | 5031 | G |
| 2 | 2 | 5034 | A |
| 2 | 2 | 5041 | G |
| 2 | 2 | 5047 | C |
| 2 | 2 | 5050 | C |
| 2 | 2 | 5054 | C |
| 2 | 2 | 5058 | A |
| 2 | 2 | 5062 | G |
| 2 | 2 | 5069 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | 8 | 25 | G |
| 5 | 8 | 34 | U |
| 5 | 8 | 35 | C |
| 5 | 8 | 39 | G |
| 5 | 8 | 48 | A |
| 5 | 8 | 52 | A |
| 5 | 8 | 59 | A |
| 5 | 8 | 62 | A |
| 5 | 8 | 63 | U |
| 5 | 8 | 80 | A |
| 5 | 8 | 82 | A |
| 5 | 8 | 84 | A |
| 5 | 8 | 85 | U |
| 5 | 8 | 103 | A |
| 5 | 8 | 104 | A |
| 5 | 8 | 105 | C |
| 5 | 8 | 108 | A |
| 5 | 8 | 110 | U |
| 5 | 8 | 114 | G |
| 5 | 8 | 123 | U |
| 5 | 8 | 124 | U |
| 5 | 8 | 125 | C |
| 5 | 8 | 126 | C |
| 5 | 8 | 127 | U |
| 5 | 8 | 128 | C |
| 5 | 8 | 147 | G |
| 5 | 8 | 150 | C |
| 5 | 8 | 151 | G |
| 5 | 8 | 156 | U |
| 56 | 3 | 7 | G |
| 56 | 3 | 11 | A |
| 56 | 3 | 22 | A |
| 56 | 3 | 29 | C |
| 56 | 3 | 41 | G |
| 56 | 3 | 48 | G |
| 56 | 3 | 49 | A |
| 56 | 3 | 51 | G |
| 56 | 3 | 52 | C |
| 56 | 3 | 53 | U |
| 56 | 3 | 54 | A |
| 56 | 3 | 63 | C |
| 56 | 3 | 64 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56 | 3 | 72 | U |
| 56 | 3 | 73 | U |
| 56 | 3 | 74 | A |
| 56 | 3 | 75 | G |
| 56 | 3 | 83 | A |
| 56 | 3 | 84 | U |
| 56 | 3 | 85 | G |
| 56 | 3 | 86 | G |
| 56 | 3 | 100 | A |
| 56 | 3 | 110 | G |

All (23) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | 2 | 406 | C |
| 2 | 2 | 914 | U |
| 2 | 2 | 1184 | A |
| 2 | 2 | 1633 | G |
| 2 | 2 | 1678 | C |
| 2 | 2 | 1808 | C |
| 2 | 2 | 1931 | C |
| 2 | 2 | 1980 | U |
| 2 | 2 | 2033 | A |
| 2 | 2 | 2486 | G |
| 2 | 2 | 2487 | G |
| 2 | 2 | 2496 | G |
| 2 | 2 | 2760 | G |
| 2 | 2 | 3701 | OMC |
| 2 | 2 | 3774 | A |
| 2 | 2 | 3875 | G |
| 2 | 2 | 3905 | A |
| 2 | 2 | 4228 | G |
| 2 | 2 | 4555 | U |
| 2 | 2 | 4636 | U |
| 2 | 2 | 4913 | G |
| 56 | 3 | 51 | G |
| 56 | 3 | 72 | U |

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

67 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$ |
| 2 | B9B | 2 | 237 | 2 | 21,28,29 | 1.99 | 3 (14%) | 23,40,43 | 6.42 | 5 (21%) |
| 2 | 5MU | 2 | 4083 | 2 | 19,22,23 | 7.22 | 8 (42%) | 28,32,35 | 3.37 | 10 (35%) |
| 2 | B8T | 2 | 4671 | 2 | 19,22,23 | 3.61 | 8 (42%) | 26,31,34 | 0.93 | 1 (3%) |
| 2 | A2M | 2 | 4571 | 2 | 18,25,26 | 3.57 | 8 (44%) | 18,36,39 | 3.40 | 4 (22%) |
| 2 | B8W | 2 | 4472 | 2 | 18,26,27 | 2.08 | 2 (11%) | 21,38,41 | 2.41 | 7 (33%) |
| 2 | B8K | 2 | 4690 | 2 | 24,28,29 | 3.30 | 12 (50%) | 30,42,45 | 2.67 | 11 (36%) |
| 2 | OMG | 2 | 1522 | 2 | 18,26,27 | 2.86 | 8 (44%) | 19,38,41 | 1.49 | 4 (21%) |
| 2 | OMC | 2 | 3701 | 2 | 19,22,23 | 3.01 | 8 (42%) | 26,31,34 | 0.74 | 0 |
| 2 | E7G | 2 | 2297 | 2 | 24,27,28 | 4.04 | 11 (45%) | 30,40,43 | 2.12 | 9 (30%) |
| 2 | A2M | 2 | 3723 | 2 | 18,25,26 | 3.57 | 8 (44%) | 18,36,39 | 3.42 | 4 (22%) |
| 2 | B8K | 2 | 3897 | 2 | 24,28,29 | 3.44 | 11 (45%) | 30,42,45 | 2.53 | 11 (36%) |
| 2 | OMG | 2 | 2773 | 2 | 18,26,27 | 2.90 | 8 (44%) | 19,38,41 | 1.46 | 4 (21%) |
| 2 | B8T | 2 | 4483 | 2 | 19,22,23 | 3.66 | 8 (42%) | 26,31,34 | 1.37 | 6 (23%) |
| 2 | OMG | 2 | 2364 | 2 | 18,26,27 | 2.84 | 8 (44%) | 19,38,41 | 1.49 | 5 (26%) |
| 2 | 2MG | 2 | 1517 | 2 | 18,26,27 | 2.73 | 6 (33%) | 16,38,41 | 1.49 | 3 (18%) |
| 2 | 7MG | 2 | 4550 | 2 | 22,26,27 | 3.85 | 10 (45%) | 29,39,42 | 1.98 | 7 (24%) |
| 2 | OMG | 2 | 1316 | 2 | 18,26,27 | 2.88 | 8 (44%) | 19,38,41 | 1.52 | 5 (26%) |
| 2 | OMG | 2 | 2050 | 2 | 18,26,27 | 2.83 | 8 (44%) | 19,38,41 | 1.48 | 5 (26%) |
| 2 | OMG | 2 | 4623 | 2 | 18,26,27 | 2.88 | 8 (44%) | 19,38,41 | 1.57 | 5 (26%) |
| 2 | A2M | 2 | 1326 | 2 | 18,25,26 | 3.60 | 8 (44%) | 18,36,39 | 3.39 | 4 (22%) |
| 2 | P4U | 2 | 1348 | 2 | 21,24,25 | 3.61 | 8 (38%) | 27,33,36 | 1.06 | 2 (7%) |
| 2 | OMG | 2 | 4637 | 2 | 18,26,27 | 2.85 | 8 (44%) | 19,38,41 | 1.55 | 5 (26%) |
| 2 | A2M | 2 | 2363 | 2 | 18,25,26 | 3.59 | 8 (44%) | 18,36,39 | 3.43 | 4 (22%) |
| 2 | B8W | 2 | 4185 | 2 | 18,26,27 | 2.14 | 2 (11%) | 21,38,41 | 2.48 | 7 (33%) |
| 2 | 2MG | 2 | 729 | 2 | 18,26,27 | 2.69 | 6 (33%) | 16,38,41 | 1.38 | 3 (18%) |
| 2 | UR3 | 2 | 4530 | 2 | 19,22,23 | 2.89 | 6 (31%) | 26,32,35 | 1.26 | 2 (7%) |
| 2 | I4U | 2 | 1659 | 2 | 21,24,25 | 3.56 | 9 (42%) | 27,34,37 | 1.11 | 2 (7%) |
| 2 | B8Q | 2 | 1456 | 2 | 17,22,23 | 2.96 | 5 (29%) | 22,32,35 | 2.21 | 6 (27%) |
| 2 | 7MG | 2 | 2522 | 2 | 22,26,27 | 3.76 | 10 (45%) | 29,39,42 | 1.97 | 10 (34%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | OMC | 2 | 3887 | 2 | 19,22,23 | 3.05 | 8 (42%) | 26,31,34 | 1.01 | 1 (3%) |
| 2 | OMG | 2 | 4870 | 2 | 18,26,27 | 2.90 | 8 (44%) | 19,38,41 | 1.49 | 4 (21%) |
| 2 | P7G | 2 | 3880 | 2 | 24,28,29 | 4.19 | 11 (45%) | 27,41,44 | 1.37 | 2 (7%) |
| 2 | OMC | 2 | 3909 | 2 | 19,22,23 | 3.13 | 8 (42%) | 26,31,34 | 1.85 | 7 (26%) |
| 2 | B9B | 2 | 2754 | 2 | 21,28,29 | 2.03 | 3 (14%) | 23,40,43 | 6.50 | 5 (21%) |
| 2 | A2M | 2 | 1871 | 2 | 18,25,26 | 3.57 | 9 (50%) | 18,36,39 | 3.47 | 3 (16%) |
| 2 | OMC | 2 | 2365 | 2 | 19,22,23 | 2.99 | 8 (42%) | 26,31,34 | 0.74 | 0 |
| 2 | 7MG | 2 | 1605 | 2 | 22,26,27 | 3.87 | 10 (45%) | 29,39,42 | 2.00 | 8 (27%) |
| 2 | OMC | 2 | 2422 | 2,44 | 19,22,23 | 3.03 | 8 (42%) | 26,31,34 | 1.00 | 2 (7%) |
| 2 | A2M | 2 | 3718 | 2 | 18,25,26 | 3.60 | 8 (44%) | 18,36,39 | 3.37 | 4 (22%) |
| 2 | A2M | 2 | 3867 | 2 | 18,25,26 | 3.61 | 8 (44%) | 18,36,39 | 3.42 | 4 (22%) |
| 2 | B8W | 2 | 4529 | 2 | 18,26,27 | 2.13 | 2 (11%) | 21,38,41 | 2.53 | 8 (38%) |
| 2 | M7A | 2 | 4564 | 2 | 20,25,26 | 2.02 | 3 (15%) | 28,37,40 | 3.91 | 7 (25%) |
| 2 | OMG | 2 | 1883 | 2 | 18,26,27 | 2.91 | 8 (44%) | 19,38,41 | 1.54 | 4 (21%) |
| 2 | OMC | 2 | 2861 | 2 | 19,22,23 | 3.04 | 8 (42%) | 26,31,34 | 1.10 | 3 (11%) |
| 2 | A2M | 2 | 1534 | 2 | 18,25,26 | 3.58 | 8 (44%) | 18,36,39 | 3.48 | 3 (16%) |
| 2 | 2MG | 2 | 4872 | 2 | 18,26,27 | 2.67 | 6 (33%) | 16,38,41 | 1.61 | 4 (25%) |
| 2 | OMC | 2 | 4536 | 2 | 19,22,23 | 3.04 | 8 (42%) | 26,31,34 | 1.12 | 3 (11%) |
| 2 | B9B | 2 | 1574 | 2 | 21,28,29 | 2.00 | 3 (14%) | 23,40,43 | 6.40 | 5 (21%) |
| 2 | A2M | 2 | 1524 | 2 | 18,25,26 | 3.61 | 8 (44%) | 18,36,39 | 3.42 | 4 (22%) |
| 2 | OMU | 2 | 4620 | 2 | 19,22,23 | 2.97 | 8 (42%) | 26,31,34 | 1.74 | 5 (19%) |
| 2 | A2M | 2 | 4523 | 2 | 18,25,26 | 3.56 | 8 (44%) | 18,36,39 | 3.43 | 4 (22%) |
| 2 | A2M | 2 | 3825 | 2 | 18,25,26 | 3.59 | 8 (44%) | 18,36,39 | 3.43 | 4 (22%) |
| 2 | P7G | 2 | 1909 | 2 | 24,28,29 | 4.09 | 11 (45%) | 27,41,44 | 1.55 | 3 (11%) |
| 2 | OMC | 2 | 3869 | 2 | 19,22,23 | 3.02 | 8 (42%) | 26,31,34 | 0.90 | 1 (3%) |
| 2 | OMG | 2 | 4494 | 2 | 18,26,27 | 2.89 | 8 (44%) | 19,38,41 | 1.46 | 4 (21%) |
| 2 | 2MG | 2 | 978 | 2 | 18,26,27 | 2.74 | 6 (33%) | 16,38,41 | 1.41 | 3 (18%) |
| 2 | OMC | 2 | 2804 | 2 | 19,22,23 | 2.98 | 8 (42%) | 26,31,34 | 0.76 | 0 |
| 2 | UR3 | 2 | 4597 | 2 | 19,22,23 | 2.82 | 6 (31%) | 26,32,35 | 1.88 | 3 (11%) |
| 2 | OMG | 2 | 2424 | 2 | 18,26,27 | 2.91 | 8 (44%) | 19,38,41 | 1.48 | 4 (21%) |
| 2 | B9H | 2 | 2786 | 2 | 20,25,26 | 3.24 | 3 (15%) | 22,35,38 | 1.95 | 5 (22%) |
| 5 | OMU | 8 | 14 | 5,2 | 19,22,23 | 2.96 | 8 (42%) | 26,31,34 | 1.79 | 6 (23%) |
| 2 | A2M | 2 | 398 | 2 | 18,25,26 | 3.61 | 8 (44%) | 18,36,39 | 3.41 | 3 (16%) |
| 2 | A2M | 2 | 2401 | 2 | 18,25,26 | 3.60 | 8 (44%) | 18,36,39 | 3.39 | 3 (16%) |
| 2 | BGH | 2 | 3899 | 2 | 25,29,30 | 4.60 | 17 (68%) | 31,43,46 | 2.58 | 11 (35%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | OMG | 2 | 1625 | 2 | 18,26,27 | 2.92 | 8 (44%) | 19,38,41 | 1.46 | 4 (21%) |
| 2 | B8W | 2 | 2380 | 2 | 18,26,27 | 2.10 | 2 (11%) | 21,38,41 | 2.47 | 7 (33%) |
| 2 | OMG | 2 | 373 | 2 | 18,26,27 | 2.88 | 8 (44%) | 19,38,41 | 1.61 | 5 (26%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | B9B | 2 | 237 | 2 | - | 6/7/29/30 | 0/3/3/3 |
| 2 | 5MU | 2 | 4083 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | B8T | 2 | 4671 | 2 | - | 0/7/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 4571 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | B8W | 2 | 4472 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | B8K | 2 | 4690 | 2 | - | 0/11/41/42 | 0/3/3/3 |
| 2 | OMG | 2 | 1522 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 3701 | 2 | - | 2/9/27/28 | 0/2/2/2 |
| 2 | E7G | 2 | 2297 | 2 | - | 1/9/39/40 | 0/3/3/3 |
| 2 | A2M | 2 | 3723 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | B8K | 2 | 3897 | 2 | - | 3/11/41/42 | 0/3/3/3 |
| 2 | OMG | 2 | 2773 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | B8T | 2 | 4483 | 2 | - | 0/7/27/28 | 0/2/2/2 |
| 2 | OMG | 2 | 2364 | 2 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | 2MG | 2 | 1517 | 2 | - | 1/5/27/28 | 0/3/3/3 |
| 2 | 7MG | 2 | 4550 | 2 | - | 2/7/37/38 | 0/3/3/3 |
| 2 | OMG | 2 | 1316 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 2050 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 4623 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | A2M | 2 | 1326 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | P4U | 2 | 1348 | 2 | - | 1/10/29/30 | 0/2/2/2 |
| 2 | OMG | 2 | 4637 | 2 | - | 4/5/27/28 | 0/3/3/3 |
| 2 | A2M | 2 | 2363 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | B8W | 2 | 4185 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | 2MG | 2 | 729 | 2 | - | 1/5/27/28 | 0/3/3/3 |
| 2 | UR3 | 2 | 4530 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | I4U | 2 | 1659 | 2 | - | 1/9/29/30 | 0/2/2/2 |
| 2 | B8Q | 2 | 1456 | 2 | - | 0/7/42/43 | 0/2/2/2 |
| 2 | 7MG | 2 | 2522 | 2 | - | 0/7/37/38 | 0/3/3/3 |
| 2 | OMC | 2 | 3887 | 2 | - | 1/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | OMG | 2 | 4870 | 2 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | P7G | 2 | 3880 | 2 | - | 2/10/40/41 | 0/3/3/3 |
| 2 | OMC | 2 | 3909 | 2 | - | 2/9/27/28 | 0/2/2/2 |
| 2 | B9B | 2 | 2754 | 2 | - | 4/7/29/30 | 0/3/3/3 |
| 2 | A2M | 2 | 1871 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 2365 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | 7MG | 2 | 1605 | 2 | - | 0/7/37/38 | 0/3/3/3 |
| 2 | OMC | 2 | 2422 | 2,44 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 3718 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | A2M | 2 | 3867 | 2 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | B8W | 2 | 4529 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | M7A | 2 | 4564 | 2 | - | 0/7/37/38 | 0/3/3/3 |
| 2 | OMG | 2 | 1883 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 2861 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 1534 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | 2MG | 2 | 4872 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 4536 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | B9B | 2 | 1574 | 2 | - | 3/7/29/30 | 0/3/3/3 |
| 2 | A2M | 2 | 1524 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMU | 2 | 4620 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 4523 | 2 | - | 1/5/27/28 | 0/3/3/3 |
| 2 | A2M | 2 | 3825 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | P7G | 2 | 1909 | 2 | - | 3/10/40/41 | 0/3/3/3 |
| 2 | OMC | 2 | 3869 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | OMG | 2 | 4494 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | 2MG | 2 | 978 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | OMC | 2 | 2804 | 2 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | UR3 | 2 | 4597 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | OMG | 2 | 2424 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | B9H | 2 | 2786 | 2 | - | 1/12/47/48 | 0/2/2/2 |
| 5 | OMU | 8 | 14 | 5,2 | - | 1/9/27/28 | 0/2/2/2 |
| 2 | A2M | 2 | 398 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | A2M | 2 | 2401 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | BGH | 2 | 3899 | 2 | - | 1/13/43/44 | 0/3/3/3 |
| 2 | OMG | 2 | 1625 | 2 | - | 3/5/27/28 | 0/3/3/3 |
| 2 | B8W | 2 | 2380 | 2 | - | 2/5/27/28 | 0/3/3/3 |
| 2 | OMG | 2 | 373 | 2 | - | 1/5/27/28 | 0/3/3/3 |

All (505) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 2 | 2 | 4083 | 5MU | C4-C5 | 20.78 | 1.79 | 1.44 |
| 2 | 2 | 4083 | 5MU | C6-N1 | 16.00 | 1.65 | 1.38 |
| 2 | 2 | 4083 | 5MU | C6-C5 | -11.45 | 1.15 | 1.34 |
| 2 | 2 | 4083 | 5MU | C4-N3 | -11.05 | 1.18 | 1.38 |
| 2 | 2 | 1659 | I4U | C4-N3 | 10.65 | 1.45 | 1.31 |
| 2 | 2 | 1348 | P4U | C4-N3 | 10.59 | 1.45 | 1.31 |
| 2 | 2 | 2786 | B9H | C2-N3 | 9.82 | 1.49 | 1.37 |
| 2 | 2 | 2297 | E7G | C5-N7 | 9.67 | 1.46 | 1.35 |
| 2 | 2 | 3880 | P7G | C5-N7 | 9.64 | 1.46 | 1.35 |
| 2 | 2 | 3880 | P7G | C8-N9 | 9.43 | 1.51 | 1.46 |
| 2 | 2 | 1909 | P7G | C5-N7 | 9.38 | 1.46 | 1.35 |
| 2 | 2 | 1909 | P7G | C8-N9 | 9.28 | 1.51 | 1.46 |
| 2 | 2 | 3897 | B8K | C8-N9 | 9.27 | 1.51 | 1.46 |
| 2 | 2 | 1605 | 7MG | C8-N9 | 9.11 | 1.51 | 1.46 |
| 2 | 2 | 2297 | E7G | C8-N9 | 9.07 | 1.51 | 1.46 |
| 2 | 2 | 4550 | 7MG | C8-N9 | 9.03 | 1.51 | 1.46 |
| 2 | 2 | 3899 | BGH | O4'-C1' | 8.98 | 1.63 | 1.42 |
| 2 | 2 | 1871 | A2M | C3'-C4' | -8.89 | 1.30 | 1.53 |
| 2 | 2 | 1524 | A2M | C3'-C4' | -8.86 | 1.30 | 1.53 |
| 2 | 2 | 3825 | A2M | C3'-C4' | -8.81 | 1.30 | 1.53 |
| 2 | 2 | 1326 | A2M | C3'-C4' | -8.81 | 1.30 | 1.53 |
| 2 | 2 | 3723 | A2M | C3'-C4' | -8.81 | 1.30 | 1.53 |
| 2 | 2 | 398 | A2M | C3'-C4' | -8.78 | 1.30 | 1.53 |
| 2 | 2 | 1605 | 7MG | C5-N7 | 8.77 | 1.45 | 1.35 |
| 2 | 2 | 2363 | A2M | C3'-C4' | -8.76 | 1.30 | 1.53 |
| 2 | 2 | 2401 | A2M | C3'-C4' | -8.75 | 1.30 | 1.53 |
| 2 | 2 | 3899 | BGH | C2'-C1' | -8.75 | 1.30 | 1.53 |
| 2 | 2 | 1534 | A2M | C3'-C4' | -8.75 | 1.30 | 1.53 |
| 2 | 2 | 2522 | 7MG | C5-N7 | 8.73 | 1.45 | 1.35 |
| 2 | 2 | 3718 | A2M | C3'-C4' | -8.72 | 1.30 | 1.53 |
| 2 | 2 | 4571 | A2M | C3'-C4' | -8.72 | 1.30 | 1.53 |
| 2 | 2 | 4550 | 7MG | C5-N7 | 8.70 | 1.45 | 1.35 |
| 2 | 2 | 3867 | A2M | C3'-C4' | -8.70 | 1.30 | 1.53 |
| 2 | 2 | 4523 | A2M | C3'-C4' | -8.63 | 1.30 | 1.53 |
| 2 | 2 | 2522 | 7MG | C8-N9 | 8.57 | 1.50 | 1.46 |
| 2 | 2 | 4690 | B8K | C8-N9 | 8.38 | 1.50 | 1.46 |
| 2 | 2 | 1456 | B8Q | C6-C5 | 8.37 | 1.52 | 1.33 |
| 2 | 2 | 3899 | BGH | C8-N9 | 8.36 | 1.50 | 1.46 |
| 2 | 2 | 4185 | B8W | C2-N2 | 8.05 | 1.50 | 1.33 |
| 2 | 2 | 4529 | B8W | C2-N2 | 8.02 | 1.49 | 1.33 |
| 2 | 2 | 2380 | B8W | C2-N2 | 7.95 | 1.49 | 1.33 |
| 2 | 2 | 4472 | B8W | C2-N2 | 7.84 | 1.49 | 1.33 |
| 2 | 2 | 398 | A2M | O4'-C4' | 7.74 | 1.62 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | 2 | 3718 | A2M | O4'-C4' | 7.73 | 1.62 | 1.45 |
| 2 | 2 | 1871 | A2M | O4'-C4' | 7.69 | 1.62 | 1.45 |
| 2 | 2 | 2401 | A2M | O4'-C4' | 7.66 | 1.62 | 1.45 |
| 2 | 2 | 2363 | A2M | O4'-C4' | 7.65 | 1.62 | 1.45 |
| 2 | 2 | 3825 | A2M | O4'-C4' | 7.64 | 1.62 | 1.45 |
| 2 | 2 | 1534 | A2M | O4'-C4' | 7.63 | 1.62 | 1.45 |
| 2 | 2 | 1326 | A2M | O4'-C4' | 7.61 | 1.62 | 1.45 |
| 2 | 2 | 3867 | A2M | O4'-C1' | -7.58 | 1.30 | 1.41 |
| 2 | 2 | 4523 | A2M | O4'-C4' | 7.58 | 1.61 | 1.45 |
| 2 | 2 | 4571 | A2M | O4'-C4' | 7.52 | 1.61 | 1.45 |
| 2 | 2 | 3723 | A2M | O4'-C4' | 7.51 | 1.61 | 1.45 |
| 2 | 2 | 4483 | B8T | C2-N3 | 7.50 | 1.51 | 1.36 |
| 2 | 2 | 3899 | BGH | O4'-C4' | -7.48 | 1.28 | 1.45 |
| 2 | 2 | 1524 | A2M | O4'-C4' | 7.47 | 1.61 | 1.45 |
| 2 | 2 | 3867 | A2M | O4'-C4' | 7.42 | 1.61 | 1.45 |
| 2 | 2 | 4671 | B8T | C2-N3 | 7.27 | 1.51 | 1.36 |
| 2 | 2 | 1326 | A2M | O4'-C1' | -7.17 | 1.31 | 1.41 |
| 2 | 2 | 1524 | A2M | O4'-C1' | -7.16 | 1.31 | 1.41 |
| 2 | 2 | 398 | A2M | O4'-C1' | -7.15 | 1.31 | 1.41 |
| 2 | 2 | 4671 | B8T | C4-N3 | 7.10 | 1.45 | 1.32 |
| 2 | 2 | 3718 | A2M | O4'-C1' | -7.08 | 1.31 | 1.41 |
| 2 | 2 | 2786 | B9H | C2-N1 | 7.07 | 1.48 | 1.38 |
| 2 | 2 | 2401 | A2M | O4'-C1' | -7.05 | 1.31 | 1.41 |
| 2 | 2 | 4483 | B8T | C4-N3 | 7.04 | 1.45 | 1.32 |
| 5 | 8 | 14 | OMU | C2-N1 | 7.04 | 1.49 | 1.38 |
| 2 | 2 | 4523 | A2M | O4'-C1' | -7.02 | 1.31 | 1.41 |
| 2 | 2 | 4571 | A2M | O4'-C1' | -7.02 | 1.31 | 1.41 |
| 2 | 2 | 2363 | A2M | O4'-C1' | -7.01 | 1.31 | 1.41 |
| 2 | 2 | 3723 | A2M | O4'-C1' | -7.01 | 1.31 | 1.41 |
| 2 | 2 | 3825 | A2M | O4'-C1' | -7.00 | 1.31 | 1.41 |
| 2 | 2 | 2786 | B9H | C6-C5 | 6.99 | 1.49 | 1.33 |
| 2 | 2 | 1534 | A2M | O4'-C1' | -6.98 | 1.31 | 1.41 |
| 2 | 2 | 4620 | OMU | C2-N1 | 6.94 | 1.49 | 1.38 |
| 2 | 2 | 4671 | B8T | C6-C5 | 6.92 | 1.51 | 1.35 |
| 2 | 2 | 978 | 2MG | C2-N2 | 6.86 | 1.48 | 1.33 |
| 2 | 2 | 1517 | 2MG | C2-N2 | 6.84 | 1.48 | 1.33 |
| 2 | 2 | 4530 | UR3 | C6-C5 | 6.84 | 1.51 | 1.35 |
| 2 | 2 | 4530 | UR3 | C2-N1 | 6.82 | 1.48 | 1.38 |
| 2 | 2 | 4483 | B8T | C6-C5 | 6.82 | 1.50 | 1.35 |
| 2 | 2 | 4597 | UR3 | C6-C5 | 6.81 | 1.50 | 1.35 |
| 2 | 2 | 1871 | A2M | O4'-C1' | -6.70 | 1.31 | 1.41 |
| 2 | 2 | 1456 | B8Q | C2-N3 | 6.66 | 1.46 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | 2 | 4690 | B8K | C2-N3 | 6.66 | 1.49 | 1.33 |
| 2 | 2 | 729 | 2MG | C2-N2 | 6.65 | 1.48 | 1.33 |
| 2 | 2 | 3897 | B8K | C2-N3 | 6.62 | 1.49 | 1.33 |
| 2 | 2 | 4620 | OMU | C2-N3 | 6.60 | 1.49 | 1.38 |
| 5 | 8 | 14 | OMU | C2-N3 | 6.58 | 1.49 | 1.38 |
| 2 | 2 | 3909 | OMC | C6-C5 | 6.55 | 1.50 | 1.35 |
| 2 | 2 | 2297 | E7G | C8-N7 | 6.54 | 1.52 | 1.45 |
| 2 | 2 | 4872 | 2MG | C2-N2 | 6.53 | 1.47 | 1.33 |
| 2 | 2 | 3880 | P7G | C8-N7 | 6.43 | 1.51 | 1.45 |
| 2 | 2 | 1909 | P7G | C4-N9 | 6.43 | 1.44 | 1.35 |
| 2 | 2 | 3869 | OMC | C2-N3 | 6.42 | 1.49 | 1.36 |
| 2 | 2 | 4536 | OMC | C2-N3 | 6.42 | 1.49 | 1.36 |
| 2 | 2 | 3880 | P7G | C4-N9 | 6.39 | 1.44 | 1.35 |
| 2 | 2 | 2754 | B9B | O6-C6 | 6.38 | 1.40 | 1.35 |
| 2 | 2 | 3899 | BGH | C4-N9 | 6.37 | 1.45 | 1.37 |
| 2 | 2 | 3887 | OMC | C2-N3 | 6.37 | 1.49 | 1.36 |
| 2 | 2 | 2422 | OMC | C2-N3 | 6.35 | 1.49 | 1.36 |
| 2 | 2 | 3880 | P7G | C4-N3 | 6.35 | 1.48 | 1.37 |
| 2 | 2 | 4483 | B8T | C4-N4 | 6.34 | 1.48 | 1.35 |
| 2 | 2 | 2861 | OMC | C2-N3 | 6.34 | 1.49 | 1.36 |
| 2 | 2 | 2424 | OMG | C2-N3 | 6.34 | 1.48 | 1.33 |
| 2 | 2 | 2365 | OMC | C2-N3 | 6.32 | 1.49 | 1.36 |
| 2 | 2 | 4671 | B8T | C4-N4 | 6.31 | 1.48 | 1.35 |
| 2 | 2 | 4597 | UR3 | C2-N3 | 6.30 | 1.51 | 1.39 |
| 2 | 2 | 1909 | P7G | C4-N3 | 6.30 | 1.48 | 1.37 |
| 2 | 2 | 3701 | OMC | C2-N3 | 6.30 | 1.49 | 1.36 |
| 2 | 2 | 1625 | OMG | C2-N3 | 6.26 | 1.48 | 1.33 |
| 2 | 2 | 1659 | I4U | C2-N3 | 6.25 | 1.49 | 1.36 |
| 2 | 2 | 1883 | OMG | C2-N3 | 6.24 | 1.48 | 1.33 |
| 2 | 2 | 4494 | OMG | C2-N3 | 6.24 | 1.48 | 1.33 |
| 2 | 2 | 2804 | OMC | C2-N3 | 6.23 | 1.49 | 1.36 |
| 2 | 2 | 1348 | P4U | C2-N3 | 6.22 | 1.49 | 1.36 |
| 2 | 2 | 1574 | B9B | O6-C6 | 6.20 | 1.40 | 1.35 |
| 2 | 2 | 2773 | OMG | C2-N3 | 6.17 | 1.48 | 1.33 |
| 2 | 2 | 4870 | OMG | C2-N3 | 6.17 | 1.48 | 1.33 |
| 2 | 2 | 1348 | P4U | C6-C5 | 6.14 | 1.49 | 1.35 |
| 2 | 2 | 1659 | I4U | C6-C5 | 6.11 | 1.49 | 1.35 |
| 2 | 2 | 1883 | OMG | C2-N2 | 6.07 | 1.48 | 1.34 |
| 2 | 2 | 2424 | OMG | C2-N2 | 6.07 | 1.48 | 1.34 |
| 2 | 2 | 4870 | OMG | C2-N2 | 6.06 | 1.48 | 1.34 |
| 2 | 2 | 237 | B9B | O6-C6 | 6.06 | 1.40 | 1.35 |
| 2 | 2 | 373 | OMG | C2-N3 | 6.05 | 1.47 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | 2 | 1316 | OMG | C2-N3 | 6.05 | 1.47 | 1.33 |
| 2 | 2 | 3701 | OMC | C6-C5 | 6.05 | 1.49 | 1.35 |
| 2 | 2 | 1522 | OMG | C2-N2 | 6.04 | 1.48 | 1.34 |
| 2 | 2 | 1522 | OMG | C2-N3 | 6.04 | 1.47 | 1.33 |
| 2 | 2 | 4597 | UR3 | C2-N1 | 6.03 | 1.47 | 1.38 |
| 2 | 2 | 2773 | OMG | C2-N2 | 6.03 | 1.48 | 1.34 |
| 2 | 2 | 1625 | OMG | C2-N2 | 6.02 | 1.48 | 1.34 |
| 2 | 2 | 373 | OMG | C2-N2 | 6.02 | 1.48 | 1.34 |
| 2 | 2 | 4494 | OMG | C2-N2 | 6.00 | 1.48 | 1.34 |
| 2 | 2 | 3887 | OMC | C6-C5 | 6.00 | 1.49 | 1.35 |
| 2 | 2 | 2365 | OMC | C6-C5 | 6.00 | 1.49 | 1.35 |
| 2 | 2 | 2364 | OMG | C2-N3 | 5.99 | 1.47 | 1.33 |
| 2 | 2 | 4623 | OMG | C2-N2 | 5.97 | 1.48 | 1.34 |
| 2 | 2 | 2861 | OMC | C6-C5 | 5.97 | 1.48 | 1.35 |
| 2 | 2 | 2422 | OMC | C6-C5 | 5.96 | 1.48 | 1.35 |
| 2 | 2 | 4536 | OMC | C6-C5 | 5.95 | 1.48 | 1.35 |
| 2 | 2 | 1316 | OMG | C2-N2 | 5.95 | 1.48 | 1.34 |
| 2 | 2 | 3880 | P7G | C2-N2 | 5.93 | 1.48 | 1.34 |
| 2 | 2 | 4623 | OMG | C2-N3 | 5.93 | 1.47 | 1.33 |
| 2 | 2 | 1909 | P7G | C2-N2 | 5.93 | 1.48 | 1.34 |
| 2 | 2 | 2050 | OMG | C2-N3 | 5.92 | 1.47 | 1.33 |
| 2 | 2 | 2050 | OMG | C2-N2 | 5.92 | 1.48 | 1.34 |
| 2 | 2 | 4637 | OMG | C2-N2 | 5.92 | 1.48 | 1.34 |
| 2 | 2 | 2804 | OMC | C6-C5 | 5.91 | 1.48 | 1.35 |
| 2 | 2 | 4637 | OMG | C2-N3 | 5.90 | 1.47 | 1.33 |
| 2 | 2 | 3869 | OMC | C6-C5 | 5.89 | 1.48 | 1.35 |
| 2 | 2 | 2364 | OMG | C2-N2 | 5.88 | 1.48 | 1.34 |
| 2 | 2 | 4564 | M7A | C4-N9 | 5.86 | 1.49 | 1.38 |
| 2 | 2 | 4550 | 7MG | C2-N3 | 5.82 | 1.47 | 1.33 |
| 2 | 2 | 3897 | B8K | C4-N9 | 5.81 | 1.44 | 1.37 |
| 2 | 2 | 3899 | BGH | C4-N3 | 5.79 | 1.48 | 1.34 |
| 2 | 2 | 1605 | 7MG | C2-N3 | 5.77 | 1.47 | 1.33 |
| 2 | 2 | 3899 | BGH | C2-N3 | 5.74 | 1.47 | 1.33 |
| 2 | 2 | 4530 | UR3 | C2-N3 | 5.74 | 1.50 | 1.39 |
| 2 | 2 | 2297 | E7G | C4-N9 | 5.73 | 1.44 | 1.37 |
| 2 | 2 | 237 | B9B | C2-N2 | 5.73 | 1.45 | 1.33 |
| 2 | 2 | 2754 | B9B | C2-N2 | 5.73 | 1.45 | 1.33 |
| 2 | 2 | 3909 | OMC | C2-N3 | 5.70 | 1.47 | 1.36 |
| 2 | 2 | 2297 | E7G | C4-N3 | 5.68 | 1.47 | 1.34 |
| 2 | 2 | 2522 | 7MG | C2-N3 | 5.67 | 1.46 | 1.33 |
| 2 | 2 | 1909 | P7G | C8-N7 | 5.67 | 1.51 | 1.45 |
| 2 | 2 | 2297 | E7G | C2-N3 | 5.66 | 1.46 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | 2 | 1574 | B9B | C2-N2 | 5.62 | 1.45 | 1.33 |
| 2 | 2 | 4550 | 7MG | C4-N3 | 5.61 | 1.47 | 1.34 |
| 2 | 2 | 1605 | 7MG | C4-N3 | 5.57 | 1.47 | 1.34 |
| 2 | 2 | 3909 | OMC | C2-N1 | 5.56 | 1.52 | 1.40 |
| 2 | 2 | 4620 | OMU | C6-C5 | 5.54 | 1.47 | 1.35 |
| 2 | 2 | 4550 | 7MG | C4-N9 | 5.52 | 1.44 | 1.37 |
| 2 | 2 | 1605 | 7MG | C4-N9 | 5.48 | 1.44 | 1.37 |
| 2 | 2 | 2522 | 7MG | C4-N3 | 5.48 | 1.47 | 1.34 |
| 2 | 2 | 3909 | OMC | C4-N4 | 5.44 | 1.46 | 1.33 |
| 2 | 2 | 729 | 2MG | C4-N3 | 5.42 | 1.50 | 1.37 |
| 2 | 2 | 4690 | B8K | C4-N9 | 5.34 | 1.43 | 1.37 |
| 2 | 2 | 3880 | P7G | C2-N1 | 5.33 | 1.46 | 1.33 |
| 5 | 8 | 14 | OMU | C6-C5 | 5.30 | 1.47 | 1.35 |
| 2 | 2 | 978 | 2MG | C4-N3 | 5.27 | 1.50 | 1.37 |
| 2 | 2 | 1517 | 2MG | C4-N3 | 5.25 | 1.50 | 1.37 |
| 2 | 2 | 1909 | P7G | C2-N1 | 5.24 | 1.45 | 1.33 |
| 2 | 2 | 2522 | 7MG | C4-N9 | 5.24 | 1.43 | 1.37 |
| 2 | 2 | 3701 | OMC | C4-N3 | 5.16 | 1.44 | 1.34 |
| 2 | 2 | 2297 | E7G | C2-N2 | 5.16 | 1.46 | 1.34 |
| 2 | 2 | 4536 | OMC | C4-N3 | 5.14 | 1.44 | 1.34 |
| 2 | 2 | 4483 | B8T | C2-N1 | 5.13 | 1.51 | 1.40 |
| 2 | 2 | 3869 | OMC | C4-N3 | 5.12 | 1.44 | 1.34 |
| 2 | 2 | 3887 | OMC | C4-N3 | 5.12 | 1.44 | 1.34 |
| 2 | 2 | 2365 | OMC | C4-N3 | 5.11 | 1.44 | 1.34 |
| 2 | 2 | 2804 | OMC | C4-N3 | 5.10 | 1.44 | 1.34 |
| 2 | 2 | 2861 | OMC | C2-N1 | 5.08 | 1.51 | 1.40 |
| 2 | 2 | 2422 | OMC | C4-N3 | 5.06 | 1.44 | 1.34 |
| 2 | 2 | 2861 | OMC | C4-N3 | 5.06 | 1.44 | 1.34 |
| 2 | 2 | 3887 | OMC | C2-N1 | 4.98 | 1.50 | 1.40 |
| 2 | 2 | 4536 | OMC | C2-N1 | 4.97 | 1.50 | 1.40 |
| 2 | 2 | 3701 | OMC | C4-N4 | 4.89 | 1.45 | 1.33 |
| 2 | 2 | 2861 | OMC | C4-N4 | 4.89 | 1.45 | 1.33 |
| 2 | 2 | 3887 | OMC | C4-N4 | 4.88 | 1.45 | 1.33 |
| 2 | 2 | 2422 | OMC | C2-N1 | 4.88 | 1.50 | 1.40 |
| 2 | 2 | 3899 | BGH | C2-N2 | 4.87 | 1.45 | 1.34 |
| 2 | 2 | 2422 | OMC | C4-N4 | 4.87 | 1.45 | 1.33 |
| 2 | 2 | 4536 | OMC | C4-N4 | 4.87 | 1.45 | 1.33 |
| 2 | 2 | 1625 | OMG | C4-N3 | 4.85 | 1.49 | 1.37 |
| 2 | 2 | 2804 | OMC | C4-N4 | 4.84 | 1.45 | 1.33 |
| 2 | 2 | 2424 | OMG | C4-N3 | 4.84 | 1.49 | 1.37 |
| 2 | 2 | 2365 | OMC | C4-N4 | 4.84 | 1.45 | 1.33 |
| 2 | 2 | 4870 | OMG | C4-N3 | 4.84 | 1.49 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | 2 | 3869 | OMC | C4-N4 | 4.83 | 1.45 | 1.33 |
| 2 | 2 | 1883 | OMG | C4-N3 | 4.83 | 1.49 | 1.37 |
| 2 | 2 | 4872 | 2MG | C4-N3 | 4.81 | 1.49 | 1.37 |
| 2 | 2 | 4494 | OMG | C4-N3 | 4.80 | 1.49 | 1.37 |
| 2 | 2 | 1605 | 7MG | C2-N2 | 4.79 | 1.45 | 1.34 |
| 2 | 2 | 2522 | 7MG | C2-N2 | 4.77 | 1.45 | 1.34 |
| 2 | 2 | 3869 | OMC | C2-N1 | 4.76 | 1.50 | 1.40 |
| 2 | 2 | 2773 | OMG | C4-N3 | 4.76 | 1.48 | 1.37 |
| 2 | 2 | 4550 | 7MG | C2-N2 | 4.76 | 1.45 | 1.34 |
| 2 | 2 | 1456 | B8Q | C2-N1 | 4.73 | 1.45 | 1.38 |
| 2 | 2 | 4623 | OMG | C6-N1 | 4.72 | 1.44 | 1.37 |
| 2 | 2 | 1316 | OMG | C4-N3 | 4.71 | 1.48 | 1.37 |
| 2 | 2 | 1348 | P4U | O4-C4 | 4.71 | 1.40 | 1.35 |
| 2 | 2 | 1522 | OMG | C4-N3 | 4.67 | 1.48 | 1.37 |
| 2 | 2 | 2364 | OMG | C4-N3 | 4.66 | 1.48 | 1.37 |
| 2 | 2 | 1316 | OMG | C6-N1 | 4.66 | 1.44 | 1.37 |
| 2 | 2 | 373 | OMG | C4-N3 | 4.65 | 1.48 | 1.37 |
| 2 | 2 | 4637 | OMG | C6-N1 | 4.64 | 1.44 | 1.37 |
| 2 | 2 | 2364 | OMG | C6-N1 | 4.63 | 1.44 | 1.37 |
| 2 | 2 | 1883 | OMG | C6-N1 | 4.62 | 1.44 | 1.37 |
| 2 | 2 | 4671 | B8T | C2-N1 | 4.61 | 1.50 | 1.40 |
| 2 | 2 | 2773 | OMG | C6-N1 | 4.61 | 1.44 | 1.37 |
| 2 | 2 | 2050 | OMG | C4-N3 | 4.59 | 1.48 | 1.37 |
| 2 | 2 | 3909 | OMC | C4-N3 | 4.58 | 1.43 | 1.34 |
| 2 | 2 | 1659 | I4U | C5-C4 | 4.58 | 1.49 | 1.43 |
| 2 | 2 | 373 | OMG | C6-N1 | 4.57 | 1.44 | 1.37 |
| 2 | 2 | 4623 | OMG | C4-N3 | 4.56 | 1.48 | 1.37 |
| 2 | 2 | 4637 | OMG | C4-N3 | 4.55 | 1.48 | 1.37 |
| 2 | 2 | 3899 | BGH | C5-N7 | 4.55 | 1.47 | 1.39 |
| 2 | 2 | 1625 | OMG | C6-N1 | 4.53 | 1.44 | 1.37 |
| 2 | 2 | 2804 | OMC | C2-N1 | 4.52 | 1.49 | 1.40 |
| 2 | 2 | 4494 | OMG | C6-N1 | 4.52 | 1.44 | 1.37 |
| 2 | 2 | 1522 | OMG | C6-N1 | 4.51 | 1.44 | 1.37 |
| 2 | 2 | 4083 | 5MU | C2-N3 | 4.49 | 1.46 | 1.38 |
| 2 | 2 | 4870 | OMG | C6-N1 | 4.49 | 1.44 | 1.37 |
| 2 | 2 | 2050 | OMG | C6-N1 | 4.48 | 1.44 | 1.37 |
| 2 | 2 | 2424 | OMG | C6-N1 | 4.47 | 1.44 | 1.37 |
| 2 | 2 | 1348 | P4U | C5-C4 | 4.47 | 1.48 | 1.43 |
| 2 | 2 | 4690 | B8K | C4-N3 | 4.45 | 1.44 | 1.34 |
| 2 | 2 | 1348 | P4U | C2-N1 | 4.45 | 1.49 | 1.40 |
| 2 | 2 | 3701 | OMC | C2-N1 | 4.42 | 1.49 | 1.40 |
| 2 | 2 | 3897 | B8K | C4-N3 | 4.41 | 1.44 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2 | 2 | 1659 | I4U | C2-N1 | 4.40 | 1.49 | 1.40 |
| 2 | 2 | 2365 | OMC | C2-N1 | 4.36 | 1.49 | 1.40 |
| 2 | 2 | 4564 | M7A | C6-N6 | 4.36 | 1.45 | 1.34 |
| 2 | 2 | 3897 | B8K | C5-C6 | 4.33 | 1.54 | 1.43 |
| 2 | 2 | 3899 | BGH | C5-C6 | 4.31 | 1.54 | 1.43 |
| 2 | 2 | 978 | 2MG | C2-N1 | 4.30 | 1.43 | 1.36 |
| 2 | 2 | 3897 | B8K | C5-N7 | 4.29 | 1.47 | 1.39 |
| 2 | 2 | 4872 | 2MG | C2-N1 | 4.29 | 1.43 | 1.36 |
| 2 | 2 | 1517 | 2MG | C2-N1 | 4.27 | 1.43 | 1.36 |
| 2 | 2 | 729 | 2MG | C2-N1 | 4.15 | 1.43 | 1.36 |
| 2 | 2 | 4690 | B8K | C5-N7 | 4.10 | 1.46 | 1.39 |
| 5 | 8 | 14 | OMU | C4-N3 | 4.02 | 1.45 | 1.38 |
| 2 | 2 | 4872 | 2MG | C6-N1 | 3.94 | 1.43 | 1.37 |
| 2 | 2 | 4671 | B8T | C5-C4 | 3.93 | 1.49 | 1.40 |
| 2 | 2 | 4620 | OMU | C4-N3 | 3.93 | 1.45 | 1.38 |
| 2 | 2 | 4564 | M7A | C5-N7 | 3.90 | 1.48 | 1.39 |
| 2 | 2 | 4690 | B8K | C5-C6 | 3.90 | 1.53 | 1.43 |
| 2 | 2 | 1605 | 7MG | C5-C6 | 3.88 | 1.53 | 1.43 |
| 2 | 2 | 4550 | 7MG | C5-C6 | 3.86 | 1.53 | 1.43 |
| 2 | 2 | 1517 | 2MG | C6-N1 | 3.81 | 1.43 | 1.37 |
| 2 | 2 | 2297 | E7G | C5-C6 | 3.81 | 1.53 | 1.43 |
| 2 | 2 | 3880 | P7G | C2-N3 | 3.81 | 1.47 | 1.37 |
| 2 | 2 | 978 | 2MG | C6-N1 | 3.80 | 1.43 | 1.37 |
| 2 | 2 | 1909 | P7G | C2-N3 | 3.79 | 1.47 | 1.37 |
| 2 | 2 | 3880 | P7G | C6-N1 | 3.77 | 1.44 | 1.38 |
| 2 | 2 | 3899 | BGH | O2'-C2' | 3.71 | 1.52 | 1.42 |
| 2 | 2 | 1605 | 7MG | C2-N1 | 3.67 | 1.46 | 1.37 |
| 2 | 2 | 4483 | B8T | C5-C4 | 3.63 | 1.48 | 1.40 |
| 2 | 2 | 3909 | OMC | C6-N1 | 3.62 | 1.46 | 1.38 |
| 2 | 2 | 3897 | B8K | C6-N1 | 3.62 | 1.45 | 1.38 |
| 2 | 2 | 4690 | B8K | C6-N1 | 3.62 | 1.45 | 1.38 |
| 2 | 2 | 4872 | 2MG | C5-C6 | 3.61 | 1.54 | 1.47 |
| 2 | 2 | 2522 | 7MG | C5-C6 | 3.61 | 1.52 | 1.43 |
| 2 | 2 | 4550 | 7MG | C2-N1 | 3.61 | 1.46 | 1.37 |
| 2 | 2 | 3899 | BGH | C71-N7 | 3.58 | 1.47 | 1.39 |
| 2 | 2 | 2297 | E7G | C2-N1 | 3.57 | 1.46 | 1.37 |
| 2 | 2 | 3897 | B8K | C2-N2 | 3.56 | 1.42 | 1.34 |
| 2 | 2 | 729 | 2MG | C6-N1 | 3.56 | 1.43 | 1.37 |
| 2 | 2 | 2522 | 7MG | C2-N1 | 3.54 | 1.46 | 1.37 |
| 2 | 2 | 978 | 2MG | C5-C6 | 3.53 | 1.54 | 1.47 |
| 2 | 2 | 1909 | P7G | C6-N1 | 3.53 | 1.44 | 1.38 |
| 2 | 2 | 4690 | B8K | C71-N7 | 3.51 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2 | 2 | 729 | 2MG | C5-C6 | 3.50 | 1.54 | 1.47 |
| 2 | 2 | 4690 | B8K | C2-N2 | 3.50 | 1.42 | 1.34 |
| 2 | 2 | 3897 | B8K | C71-N7 | 3.49 | 1.47 | 1.39 |
| 2 | 2 | 1517 | 2MG | C5-C6 | 3.48 | 1.54 | 1.47 |
| 2 | 2 | 4530 | UR3 | C6-N1 | 3.46 | 1.46 | 1.38 |
| 2 | 2 | 4483 | B8T | C6-N1 | 3.44 | 1.46 | 1.38 |
| 2 | 2 | 3869 | OMC | C6-N1 | 3.39 | 1.46 | 1.38 |
| 2 | 2 | 1348 | P4U | C6-N1 | 3.39 | 1.46 | 1.38 |
| 2 | 2 | 4083 | 5MU | C2-N1 | 3.37 | 1.43 | 1.38 |
| 2 | 2 | 2773 | OMG | C5-C6 | 3.35 | 1.54 | 1.47 |
| 2 | 2 | 3899 | BGH | C6-N1 | 3.34 | 1.45 | 1.38 |
| 2 | 2 | 1909 | P7G | C5-C4 | 3.34 | 1.44 | 1.37 |
| 2 | 2 | 2522 | 7MG | C6-N1 | 3.33 | 1.45 | 1.38 |
| 2 | 2 | 3897 | B8K | C2-N1 | 3.33 | 1.45 | 1.37 |
| 2 | 2 | 3887 | OMC | C6-N1 | 3.33 | 1.46 | 1.38 |
| 2 | 2 | 1605 | 7MG | C6-N1 | 3.32 | 1.45 | 1.38 |
| 2 | 2 | 4550 | 7MG | C6-N1 | 3.32 | 1.45 | 1.38 |
| 2 | 2 | 4690 | B8K | C2-N1 | 3.31 | 1.45 | 1.37 |
| 2 | 2 | 1659 | I4U | C6-N1 | 3.28 | 1.45 | 1.38 |
| 2 | 2 | 1316 | OMG | C5-C6 | 3.27 | 1.54 | 1.47 |
| 2 | 2 | 2297 | E7G | C6-N1 | 3.27 | 1.44 | 1.38 |
| 2 | 2 | 2050 | OMG | C5-C6 | 3.27 | 1.54 | 1.47 |
| 2 | 2 | 3880 | P7G | C5-C4 | 3.27 | 1.43 | 1.37 |
| 2 | 2 | 2422 | OMC | C6-N1 | 3.27 | 1.45 | 1.38 |
| 2 | 2 | 4536 | OMC | C6-N1 | 3.27 | 1.45 | 1.38 |
| 2 | 2 | 3899 | BGH | C2-N1 | 3.27 | 1.45 | 1.37 |
| 2 | 2 | 1625 | OMG | C5-C6 | 3.26 | 1.54 | 1.47 |
| 2 | 2 | 4623 | OMG | C5-C6 | 3.26 | 1.54 | 1.47 |
| 2 | 2 | 2365 | OMC | C6-N1 | 3.25 | 1.45 | 1.38 |
| 2 | 2 | 2861 | OMC | C6-N1 | 3.24 | 1.45 | 1.38 |
| 2 | 2 | 4671 | B8T | C6-N1 | 3.22 | 1.45 | 1.38 |
| 2 | 2 | 4637 | OMG | C5-C6 | 3.22 | 1.53 | 1.47 |
| 2 | 2 | 4597 | UR3 | C6-N1 | 3.20 | 1.45 | 1.38 |
| 2 | 2 | 1909 | P7G | O6-C6 | -3.19 | 1.18 | 1.23 |
| 2 | 2 | 4870 | OMG | C5-C6 | 3.19 | 1.53 | 1.47 |
| 2 | 2 | 1522 | OMG | C5-C6 | 3.19 | 1.53 | 1.47 |
| 2 | 2 | 4494 | OMG | C5-C6 | 3.17 | 1.53 | 1.47 |
| 2 | 2 | 4523 | A2M | C6-N6 | 3.17 | 1.45 | 1.34 |
| 2 | 2 | 3825 | A2M | C6-N6 | 3.17 | 1.45 | 1.34 |
| 2 | 2 | 2424 | OMG | C5-C6 | 3.16 | 1.53 | 1.47 |
| 2 | 2 | 1524 | A2M | C6-N6 | 3.16 | 1.45 | 1.34 |
| 2 | 2 | 1871 | A2M | C6-N6 | 3.16 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | 2 | 2364 | OMG | C5-C6 | 3.15 | 1.53 | 1.47 |
| 2 | 2 | 3701 | OMC | C6-N1 | 3.15 | 1.45 | 1.38 |
| 2 | 2 | 373 | OMG | C5-C6 | 3.15 | 1.53 | 1.47 |
| 2 | 2 | 3718 | A2M | C6-N6 | 3.15 | 1.45 | 1.34 |
| 2 | 2 | 1326 | A2M | C6-N6 | 3.14 | 1.45 | 1.34 |
| 2 | 2 | 3723 | A2M | C6-N6 | 3.14 | 1.45 | 1.34 |
| 2 | 2 | 4571 | A2M | C6-N6 | 3.14 | 1.45 | 1.34 |
| 2 | 2 | 2401 | A2M | C6-N6 | 3.14 | 1.45 | 1.34 |
| 2 | 2 | 2363 | A2M | C6-N6 | 3.13 | 1.45 | 1.34 |
| 2 | 2 | 3867 | A2M | C6-N6 | 3.12 | 1.45 | 1.34 |
| 2 | 2 | 398 | A2M | C6-N6 | 3.11 | 1.45 | 1.34 |
| 2 | 2 | 1534 | A2M | C6-N6 | 3.10 | 1.45 | 1.34 |
| 2 | 2 | 2804 | OMC | C6-N1 | 3.07 | 1.45 | 1.38 |
| 2 | 2 | 3880 | P7G | O6-C6 | -3.06 | 1.18 | 1.23 |
| 2 | 2 | 1883 | OMG | C5-C6 | 2.97 | 1.53 | 1.47 |
| 5 | 8 | 14 | OMU | O4-C4 | -2.96 | 1.18 | 1.24 |
| 2 | 2 | 4620 | OMU | O4-C4 | -2.96 | 1.18 | 1.24 |
| 2 | 2 | 2401 | A2M | O3'-C3' | 2.95 | 1.49 | 1.43 |
| 2 | 2 | 3867 | A2M | O3'-C3' | 2.95 | 1.49 | 1.43 |
| 2 | 2 | 4872 | 2MG | C5-C4 | -2.94 | 1.35 | 1.43 |
| 2 | 2 | 3718 | A2M | O3'-C3' | 2.92 | 1.49 | 1.43 |
| 2 | 2 | 1524 | A2M | O3'-C3' | 2.92 | 1.49 | 1.43 |
| 2 | 2 | 4083 | 5MU | O4-C4 | -2.92 | 1.18 | 1.23 |
| 2 | 2 | 1534 | A2M | O3'-C3' | 2.91 | 1.49 | 1.43 |
| 2 | 2 | 398 | A2M | O3'-C3' | 2.90 | 1.49 | 1.43 |
| 2 | 2 | 3897 | B8K | C5-C4 | 2.90 | 1.47 | 1.38 |
| 2 | 2 | 3899 | BGH | O3'-C3' | -2.87 | 1.36 | 1.43 |
| 2 | 2 | 1659 | I4U | O4-C41 | -2.86 | 1.40 | 1.47 |
| 2 | 2 | 4571 | A2M | O3'-C3' | 2.86 | 1.49 | 1.43 |
| 2 | 2 | 3825 | A2M | O3'-C3' | 2.86 | 1.49 | 1.43 |
| 2 | 2 | 2363 | A2M | O3'-C3' | 2.85 | 1.49 | 1.43 |
| 2 | 2 | 4523 | A2M | O3'-C3' | 2.83 | 1.49 | 1.43 |
| 2 | 2 | 1326 | A2M | O3'-C3' | 2.83 | 1.49 | 1.43 |
| 2 | 2 | 1871 | A2M | O3'-C3' | 2.82 | 1.49 | 1.43 |
| 2 | 2 | 3723 | A2M | O3'-C3' | 2.82 | 1.49 | 1.43 |
| 2 | 2 | 1574 | B9B | C5-C4 | -2.82 | 1.33 | 1.40 |
| 2 | 2 | 4690 | B8K | C5-C4 | 2.82 | 1.47 | 1.38 |
| 2 | 2 | 4483 | B8T | O2-C2 | -2.79 | 1.18 | 1.23 |
| 2 | 2 | 1883 | OMG | O6-C6 | -2.78 | 1.17 | 1.23 |
| 2 | 2 | 4623 | OMG | O6-C6 | -2.78 | 1.17 | 1.23 |
| 2 | 2 | 4637 | OMG | O6-C6 | -2.78 | 1.17 | 1.23 |
| 2 | 2 | 4870 | OMG | O6-C6 | -2.77 | 1.17 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | 2 | 1316 | OMG | O6-C6 | -2.76 | 1.17 | 1.23 |
| 2 | 2 | 1517 | 2MG | C5-C4 | -2.76 | 1.36 | 1.43 |
| 2 | 2 | 373 | OMG | O6-C6 | -2.76 | 1.17 | 1.23 |
| 2 | 2 | 978 | 2MG | C5-C4 | -2.76 | 1.36 | 1.43 |
| 2 | 2 | 2380 | B8W | C5-C4 | -2.75 | 1.33 | 1.40 |
| 2 | 2 | 4671 | B8T | O2-C2 | -2.75 | 1.18 | 1.23 |
| 2 | 2 | 2050 | OMG | O6-C6 | -2.75 | 1.17 | 1.23 |
| 2 | 2 | 2364 | OMG | O6-C6 | -2.75 | 1.17 | 1.23 |
| 2 | 2 | 4620 | OMU | C6-N1 | 2.75 | 1.44 | 1.38 |
| 2 | 2 | 3909 | OMC | C5-C4 | 2.74 | 1.49 | 1.42 |
| 2 | 2 | 2804 | OMC | O2-C2 | -2.73 | 1.18 | 1.23 |
| 2 | 2 | 2422 | OMC | O2-C2 | -2.73 | 1.18 | 1.23 |
| 2 | 2 | 4494 | OMG | O6-C6 | -2.73 | 1.17 | 1.23 |
| 2 | 2 | 1659 | I4U | O2-C2 | -2.72 | 1.18 | 1.23 |
| 2 | 2 | 2365 | OMC | O2-C2 | -2.72 | 1.18 | 1.23 |
| 2 | 2 | 1348 | P4U | O2-C2 | -2.71 | 1.18 | 1.23 |
| 2 | 2 | 2424 | OMG | O6-C6 | -2.71 | 1.17 | 1.23 |
| 2 | 2 | 1522 | OMG | O6-C6 | -2.70 | 1.17 | 1.23 |
| 2 | 2 | 4185 | B8W | C5-C4 | -2.70 | 1.33 | 1.40 |
| 5 | 8 | 14 | OMU | C6-N1 | 2.69 | 1.44 | 1.38 |
| 2 | 2 | 2363 | A2M | O2'-C2' | -2.69 | 1.35 | 1.42 |
| 2 | 2 | 3899 | BGH | O6-C6 | -2.69 | 1.18 | 1.23 |
| 2 | 2 | 237 | B9B | C5-C4 | -2.69 | 1.33 | 1.40 |
| 2 | 2 | 2754 | B9B | C5-C4 | -2.68 | 1.33 | 1.40 |
| 2 | 2 | 1524 | A2M | O2'-C2' | -2.68 | 1.35 | 1.42 |
| 2 | 2 | 2773 | OMG | O6-C6 | -2.68 | 1.17 | 1.23 |
| 2 | 2 | 729 | 2MG | C5-C4 | -2.66 | 1.36 | 1.43 |
| 2 | 2 | 1534 | A2M | O2'-C2' | -2.66 | 1.35 | 1.42 |
| 2 | 2 | 4529 | B8W | C5-C4 | -2.65 | 1.33 | 1.40 |
| 2 | 2 | 2401 | A2M | C5-C4 | -2.64 | 1.33 | 1.40 |
| 2 | 2 | 1534 | A2M | C5-C4 | -2.62 | 1.34 | 1.40 |
| 2 | 2 | 2401 | A2M | O2'-C2' | -2.62 | 1.35 | 1.42 |
| 2 | 2 | 1625 | OMG | O6-C6 | -2.62 | 1.18 | 1.23 |
| 2 | 2 | 3867 | A2M | C5-C4 | -2.62 | 1.34 | 1.40 |
| 2 | 2 | 4083 | 5MU | O2-C2 | -2.62 | 1.18 | 1.23 |
| 2 | 2 | 4472 | B8W | C5-C4 | -2.62 | 1.34 | 1.40 |
| 2 | 2 | 3723 | A2M | C5-C4 | -2.61 | 1.34 | 1.40 |
| 2 | 2 | 4523 | A2M | O2'-C2' | -2.61 | 1.35 | 1.42 |
| 2 | 2 | 3825 | A2M | C5-C4 | -2.61 | 1.34 | 1.40 |
| 2 | 2 | 398 | A2M | O2'-C2' | -2.61 | 1.35 | 1.42 |
| 2 | 2 | 3869 | OMC | O2-C2 | -2.61 | 1.18 | 1.23 |
| 2 | 2 | 2363 | A2M | C5-C4 | -2.60 | 1.34 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | 2 | 3701 | OMC | O2-C2 | -2.60 | 1.18 | 1.23 |
| 2 | 2 | 398 | A2M | C5-C4 | -2.60 | 1.34 | 1.40 |
| 2 | 2 | 3825 | A2M | O2'-C2' | -2.60 | 1.36 | 1.42 |
| 2 | 2 | 3718 | A2M | O2'-C2' | -2.59 | 1.36 | 1.42 |
| 2 | 2 | 1326 | A2M | C5-C4 | -2.59 | 1.34 | 1.40 |
| 2 | 2 | 3701 | OMC | C5-C4 | 2.59 | 1.48 | 1.42 |
| 2 | 2 | 1871 | A2M | C5-C4 | -2.58 | 1.34 | 1.40 |
| 2 | 2 | 1524 | A2M | C5-C4 | -2.58 | 1.34 | 1.40 |
| 2 | 2 | 3718 | A2M | C5-C4 | -2.58 | 1.34 | 1.40 |
| 2 | 2 | 4571 | A2M | C5-C4 | -2.58 | 1.34 | 1.40 |
| 2 | 2 | 2522 | 7MG | O6-C6 | -2.57 | 1.18 | 1.23 |
| 2 | 2 | 1659 | I4U | O4-C4 | 2.57 | 1.40 | 1.35 |
| 2 | 2 | 4523 | A2M | C5-C4 | -2.57 | 1.34 | 1.40 |
| 2 | 2 | 2861 | OMC | O2-C2 | -2.56 | 1.19 | 1.23 |
| 2 | 2 | 4536 | OMC | O2-C2 | -2.55 | 1.19 | 1.23 |
| 2 | 2 | 3887 | OMC | O2-C2 | -2.54 | 1.19 | 1.23 |
| 2 | 2 | 4637 | OMG | C2-N1 | 2.52 | 1.43 | 1.37 |
| 2 | 2 | 373 | OMG | C2-N1 | 2.52 | 1.43 | 1.37 |
| 2 | 2 | 1605 | 7MG | O6-C6 | -2.51 | 1.18 | 1.23 |
| 2 | 2 | 2773 | OMG | C2-N1 | 2.51 | 1.43 | 1.37 |
| 2 | 2 | 4623 | OMG | C2-N1 | 2.51 | 1.43 | 1.37 |
| 2 | 2 | 3723 | A2M | O2'-C2' | -2.50 | 1.36 | 1.42 |
| 2 | 2 | 4550 | 7MG | O6-C6 | -2.50 | 1.18 | 1.23 |
| 2 | 2 | 1871 | A2M | O2'-C2' | -2.50 | 1.36 | 1.42 |
| 2 | 2 | 3867 | A2M | O2'-C2' | -2.50 | 1.36 | 1.42 |
| 2 | 2 | 2050 | OMG | C2-N1 | 2.49 | 1.43 | 1.37 |
| 2 | 2 | 1522 | OMG | C2-N1 | 2.49 | 1.43 | 1.37 |
| 2 | 2 | 4494 | OMG | C2-N1 | 2.49 | 1.43 | 1.37 |
| 2 | 2 | 2424 | OMG | C2-N1 | 2.49 | 1.43 | 1.37 |
| 2 | 2 | 1625 | OMG | C2-N1 | 2.49 | 1.43 | 1.37 |
| 2 | 2 | 2364 | OMG | C2-N1 | 2.48 | 1.43 | 1.37 |
| 2 | 2 | 4870 | OMG | C2-N1 | 2.47 | 1.43 | 1.37 |
| 2 | 2 | 1316 | OMG | C2-N1 | 2.47 | 1.43 | 1.37 |
| 2 | 2 | 4571 | A2M | O2'-C2' | -2.47 | 1.36 | 1.42 |
| 2 | 2 | 1883 | OMG | C2-N1 | 2.46 | 1.43 | 1.37 |
| 2 | 2 | 2297 | E7G | O6-C6 | -2.45 | 1.18 | 1.23 |
| 5 | 8 | 14 | OMU | O2-C2 | -2.45 | 1.18 | 1.23 |
| 2 | 2 | 4571 | A2M | C2-N3 | 2.44 | 1.36 | 1.32 |
| 2 | 2 | 2861 | OMC | C5-C4 | 2.43 | 1.48 | 1.42 |
| 2 | 2 | 1326 | A2M | C2-N3 | 2.43 | 1.36 | 1.32 |
| 2 | 2 | 2422 | OMC | C5-C4 | 2.42 | 1.48 | 1.42 |
| 2 | 2 | 1456 | B8Q | C6-N1 | 2.41 | 1.43 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | 2 | 3887 | OMC | C5-C4 | 2.41 | 1.48 | 1.42 |
| 2 | 2 | 2804 | OMC | C5-C4 | 2.41 | 1.48 | 1.42 |
| 2 | 2 | 2363 | A2M | C2-N3 | 2.41 | 1.36 | 1.32 |
| 2 | 2 | 4620 | OMU | O2-C2 | -2.39 | 1.18 | 1.23 |
| 2 | 2 | 3825 | A2M | C2-N3 | 2.39 | 1.35 | 1.32 |
| 2 | 2 | 2365 | OMC | C5-C4 | 2.39 | 1.48 | 1.42 |
| 2 | 2 | 4623 | OMG | C5-C4 | -2.38 | 1.37 | 1.43 |
| 2 | 2 | 4523 | A2M | C2-N3 | 2.38 | 1.35 | 1.32 |
| 2 | 2 | 3867 | A2M | C2-N3 | 2.37 | 1.35 | 1.32 |
| 2 | 2 | 373 | OMG | C5-C4 | -2.37 | 1.37 | 1.43 |
| 2 | 2 | 1326 | A2M | O2'-C2' | -2.36 | 1.36 | 1.42 |
| 2 | 2 | 4620 | OMU | C5-C4 | 2.36 | 1.48 | 1.43 |
| 5 | 8 | 14 | OMU | C5-C4 | 2.35 | 1.48 | 1.43 |
| 2 | 2 | 1534 | A2M | C2-N3 | 2.35 | 1.35 | 1.32 |
| 2 | 2 | 4530 | UR3 | C4-N3 | 2.34 | 1.46 | 1.40 |
| 2 | 2 | 4597 | UR3 | C5-C4 | 2.33 | 1.49 | 1.43 |
| 2 | 2 | 3718 | A2M | C2-N3 | 2.32 | 1.35 | 1.32 |
| 2 | 2 | 3723 | A2M | C2-N3 | 2.32 | 1.35 | 1.32 |
| 2 | 2 | 1883 | OMG | C5-C4 | -2.32 | 1.37 | 1.43 |
| 2 | 2 | 1871 | A2M | C2-N3 | 2.30 | 1.35 | 1.32 |
| 2 | 2 | 1524 | A2M | C2-N3 | 2.30 | 1.35 | 1.32 |
| 2 | 2 | 3869 | OMC | C5-C4 | 2.30 | 1.48 | 1.42 |
| 2 | 2 | 4536 | OMC | C5-C4 | 2.29 | 1.48 | 1.42 |
| 2 | 2 | 2401 | A2M | C2-N3 | 2.28 | 1.35 | 1.32 |
| 2 | 2 | 4637 | OMG | C5-C4 | -2.28 | 1.37 | 1.43 |
| 2 | 2 | 3909 | OMC | O2-C2 | -2.28 | 1.19 | 1.23 |
| 2 | 2 | 398 | A2M | C2-N3 | 2.28 | 1.35 | 1.32 |
| 2 | 2 | 1316 | OMG | C5-C4 | -2.24 | 1.37 | 1.43 |
| 2 | 2 | 4530 | UR3 | C5-C4 | 2.24 | 1.49 | 1.43 |
| 2 | 2 | 2050 | OMG | C5-C4 | -2.23 | 1.37 | 1.43 |
| 2 | 2 | 2364 | OMG | C5-C4 | -2.22 | 1.37 | 1.43 |
| 2 | 2 | 4597 | UR3 | C4-N3 | 2.19 | 1.45 | 1.40 |
| 2 | 2 | 3899 | BGH | C5-C4 | 2.18 | 1.45 | 1.38 |
| 2 | 2 | 1522 | OMG | C5-C4 | -2.13 | 1.37 | 1.43 |
| 2 | 2 | 4870 | OMG | C5-C4 | -2.11 | 1.37 | 1.43 |
| 2 | 2 | 4494 | OMG | C5-C4 | -2.10 | 1.37 | 1.43 |
| 2 | 2 | 2773 | OMG | C5-C4 | -2.09 | 1.37 | 1.43 |
| 2 | 2 | 1625 | OMG | C5-C4 | -2.08 | 1.37 | 1.43 |
| 2 | 2 | 4690 | B8K | O6-C6 | -2.08 | 1.19 | 1.23 |
| 2 | 2 | 2424 | OMG | C5-C4 | -2.04 | 1.37 | 1.43 |
| 2 | 2 | 1456 | B8Q | O2-C2 | -2.02 | 1.18 | 1.22 |
| 2 | 2 | 1871 | A2M | O5'-C5' | -2.01 | 1.39 | 1.44 |

All (307) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 2 | 2 | 2754 | B9B | O6-C6-N1 | -29.66 | 94.52 | 120.12 |
| 2 | 2 | 1574 | B9B | O6-C6-N1 | -29.32 | 94.82 | 120.12 |
| 2 | 2 | 237 | B9B | O6-C6-N1 | -29.25 | 94.87 | 120.12 |
| 2 | 2 | 4564 | M7A | C5-C6-N6 | 13.86 | 147.40 | 123.74 |
| 2 | 2 | 4564 | M7A | N6-C6-N1 | -11.73 | 92.66 | 118.35 |
| 2 | 2 | 1534 | A2M | C5-C6-N6 | 10.52 | 136.34 | 120.35 |
| 2 | 2 | 1871 | A2M | C5-C6-N6 | 10.50 | 136.31 | 120.35 |
| 2 | 2 | 4523 | A2M | C5-C6-N6 | 10.46 | 136.24 | 120.35 |
| 2 | 2 | 3825 | A2M | C5-C6-N6 | 10.40 | 136.16 | 120.35 |
| 2 | 2 | 398 | A2M | C5-C6-N6 | 10.39 | 136.15 | 120.35 |
| 2 | 2 | 2363 | A2M | C5-C6-N6 | 10.38 | 136.13 | 120.35 |
| 2 | 2 | 3723 | A2M | C5-C6-N6 | 10.37 | 136.11 | 120.35 |
| 2 | 2 | 2401 | A2M | C5-C6-N6 | 10.31 | 136.02 | 120.35 |
| 2 | 2 | 1524 | A2M | C5-C6-N6 | 10.30 | 136.01 | 120.35 |
| 2 | 2 | 3718 | A2M | C5-C6-N6 | 10.30 | 136.01 | 120.35 |
| 2 | 2 | 3867 | A2M | C5-C6-N6 | 10.30 | 136.00 | 120.35 |
| 2 | 2 | 4083 | 5MU | C5-C4-N3 | 10.26 | 124.07 | 115.31 |
| 2 | 2 | 4571 | A2M | C5-C6-N6 | 10.25 | 135.92 | 120.35 |
| 2 | 2 | 1326 | A2M | C5-C6-N6 | 10.24 | 135.91 | 120.35 |
| 2 | 2 | 4083 | 5MU | C5-C6-N1 | -7.94 | 115.17 | 123.34 |
| 2 | 2 | 1534 | A2M | N6-C6-N1 | -7.48 | 103.05 | 118.57 |
| 2 | 2 | 4597 | UR3 | C4-N3-C2 | -7.43 | 117.57 | 124.56 |
| 2 | 2 | 2363 | A2M | N6-C6-N1 | -7.36 | 103.30 | 118.57 |
| 2 | 2 | 1871 | A2M | N6-C6-N1 | -7.35 | 103.31 | 118.57 |
| 2 | 2 | 3825 | A2M | N6-C6-N1 | -7.32 | 103.37 | 118.57 |
| 2 | 2 | 4523 | A2M | N6-C6-N1 | -7.31 | 103.40 | 118.57 |
| 2 | 2 | 3723 | A2M | N6-C6-N1 | -7.28 | 103.47 | 118.57 |
| 2 | 2 | 398 | A2M | N6-C6-N1 | -7.27 | 103.49 | 118.57 |
| 2 | 2 | 2401 | A2M | N6-C6-N1 | -7.26 | 103.51 | 118.57 |
| 2 | 2 | 3867 | A2M | N6-C6-N1 | -7.22 | 103.60 | 118.57 |
| 2 | 2 | 1326 | A2M | N6-C6-N1 | -7.19 | 103.64 | 118.57 |
| 2 | 2 | 4571 | A2M | N6-C6-N1 | -7.18 | 103.66 | 118.57 |
| 2 | 2 | 3718 | A2M | N6-C6-N1 | -7.17 | 103.69 | 118.57 |
| 2 | 2 | 1524 | A2M | N6-C6-N1 | -7.16 | 103.72 | 118.57 |
| 2 | 2 | 4083 | 5MU | C4-N3-C2 | -6.99 | 118.31 | 127.35 |
| 2 | 2 | 4690 | B8K | C72-C71-N7 | 6.55 | 128.72 | 118.86 |
| 2 | 2 | 3723 | A2M | N3-C2-N1 | -6.37 | 118.72 | 128.68 |
| 2 | 2 | 2401 | A2M | N3-C2-N1 | -6.34 | 118.77 | 128.68 |
| 2 | 2 | 1534 | A2M | N3-C2-N1 | -6.33 | 118.78 | 128.68 |
| 2 | 2 | 1871 | A2M | N3-C2-N1 | -6.33 | 118.78 | 128.68 |
| 2 | 2 | 3825 | A2M | N3-C2-N1 | -6.33 | 118.79 | 128.68 |
| 2 | 2 | 398 | A2M | N3-C2-N1 | -6.31 | 118.82 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | 2 | 4523 | A2M | N3-C2-N1 | -6.30 | 118.83 | 128.68 |
| 2 | 2 | 1326 | A2M | N3-C2-N1 | -6.28 | 118.87 | 128.68 |
| 2 | 2 | 3867 | A2M | N3-C2-N1 | -6.24 | 118.93 | 128.68 |
| 2 | 2 | 1524 | A2M | N3-C2-N1 | -6.21 | 118.97 | 128.68 |
| 2 | 2 | 4571 | A2M | N3-C2-N1 | -6.20 | 118.98 | 128.68 |
| 2 | 2 | 2363 | A2M | N3-C2-N1 | -6.19 | 119.01 | 128.68 |
| 2 | 2 | 3718 | A2M | N3-C2-N1 | -6.18 | 119.03 | 128.68 |
| 2 | 2 | 4564 | M7A | N3-C2-N1 | -6.13 | 119.01 | 128.60 |
| 2 | 2 | 3899 | BGH | C72-C71-N7 | 6.07 | 127.99 | 118.86 |
| 2 | 2 | 3897 | B8K | C72-C71-N7 | 6.02 | 127.92 | 118.86 |
| 2 | 2 | 4690 | B8K | C5-C6-N1 | 6.02 | 121.59 | 110.99 |
| 2 | 2 | 4185 | B8W | N2-C2-N3 | 5.78 | 127.22 | 117.79 |
| 2 | 2 | 2380 | B8W | N2-C2-N3 | 5.73 | 127.12 | 117.79 |
| 2 | 2 | 3899 | BGH | C5-C6-N1 | 5.72 | 121.06 | 110.99 |
| 2 | 2 | 3897 | B8K | C5-C6-N1 | 5.67 | 120.98 | 110.99 |
| 2 | 2 | 1456 | B8Q | N3-C2-N1 | 5.63 | 123.75 | 117.13 |
| 2 | 2 | 2786 | B9H | C31-N3-C2 | 5.57 | 124.17 | 117.21 |
| 2 | 2 | 4529 | B8W | O6-C6-N1 | 5.56 | 126.74 | 119.03 |
| 2 | 2 | 3909 | OMC | O2-C2-N3 | -5.53 | 113.34 | 122.33 |
| 2 | 2 | 4529 | B8W | N2-C2-N3 | 5.51 | 126.77 | 117.79 |
| 2 | 2 | 237 | B9B | N3-C2-N1 | -5.46 | 119.94 | 127.22 |
| 2 | 2 | 4472 | B8W | N3-C2-N1 | -5.44 | 119.97 | 127.22 |
| 2 | 2 | 2754 | B9B | N3-C2-N1 | -5.42 | 119.99 | 127.22 |
| 2 | 2 | 1909 | P7G | C4-C5-N7 | 5.40 | 109.52 | 106.67 |
| 5 | 8 | 14 | OMU | C4-N3-C2 | -5.38 | 119.48 | 126.58 |
| 2 | 2 | 4185 | B8W | N3-C2-N1 | -5.36 | 120.08 | 127.22 |
| 2 | 2 | 2380 | B8W | N3-C2-N1 | -5.33 | 120.11 | 127.22 |
| 2 | 2 | 1574 | B9B | N3-C2-N1 | -5.28 | 120.17 | 127.22 |
| 2 | 2 | 4620 | OMU | C4-N3-C2 | -5.23 | 119.68 | 126.58 |
| 2 | 2 | 4472 | B8W | N2-C2-N3 | 5.19 | 126.26 | 117.79 |
| 2 | 2 | 4529 | B8W | N3-C2-N1 | -5.16 | 120.34 | 127.22 |
| 2 | 2 | 3899 | BGH | C2-N3-C4 | 5.12 | 121.43 | 112.30 |
| 2 | 2 | 1456 | B8Q | C31-N3-C4 | 5.09 | 121.91 | 114.25 |
| 2 | 2 | 2297 | E7G | C5-C6-N1 | 5.06 | 119.90 | 110.99 |
| 2 | 2 | 1605 | 7MG | C5-C6-N1 | 4.98 | 119.77 | 110.99 |
| 2 | 2 | 4564 | M7A | N3-C4-N9 | 4.98 | 133.16 | 126.87 |
| 2 | 2 | 4690 | B8K | C4-C5-N7 | 4.94 | 109.30 | 104.91 |
| 2 | 2 | 2297 | E7G | C4-C5-N7 | 4.93 | 109.29 | 104.91 |
| 2 | 2 | 3897 | B8K | C2-N3-C4 | 4.92 | 121.06 | 112.30 |
| 2 | 2 | 2522 | 7MG | C5-C6-N1 | 4.87 | 119.58 | 110.99 |
| 2 | 2 | 4550 | 7MG | C5-C6-N1 | 4.87 | 119.57 | 110.99 |
| 2 | 2 | 3880 | P7G | C4-C5-N7 | 4.85 | 109.23 | 106.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 237 | B9B | C2-N3-C4 | 4.82 | 120.86 | 115.36 |
| 2 | 2 | 2786 | B9H | C6-N1-C2 | -4.79 | 117.50 | 121.79 |
| 2 | 2 | 4083 | 5MU | N3-C2-N1 | 4.77 | 121.22 | 114.89 |
| 2 | 2 | 4690 | B8K | C2-N3-C4 | 4.76 | 120.78 | 112.30 |
| 2 | 2 | 4472 | B8W | C2-N3-C4 | 4.71 | 120.73 | 115.36 |
| 2 | 2 | 2754 | B9B | C2-N3-C4 | 4.67 | 120.69 | 115.36 |
| 2 | 2 | 4083 | 5MU | C5M-C5-C6 | -4.62 | 116.68 | 122.85 |
| 2 | 2 | 1456 | B8Q | O2-C2-N3 | -4.59 | 116.20 | 122.95 |
| 2 | 2 | 4530 | UR3 | C4-N3-C2 | -4.59 | 120.24 | 124.56 |
| 2 | 2 | 4690 | B8K | N9-C8-N7 | 4.58 | 109.47 | 103.33 |
| 2 | 2 | 2754 | B9B | N2-C2-N3 | 4.55 | 125.20 | 117.79 |
| 2 | 2 | 2297 | E7G | C2-N3-C4 | 4.47 | 120.26 | 112.30 |
| 2 | 2 | 1605 | 7MG | C2-N3-C4 | 4.46 | 120.25 | 112.30 |
| 2 | 2 | 237 | B9B | N2-C2-N3 | 4.46 | 125.06 | 117.79 |
| 2 | 2 | 4185 | B8W | C2-N3-C4 | 4.46 | 120.45 | 115.36 |
| 2 | 2 | 1574 | B9B | C2-N3-C4 | 4.42 | 120.40 | 115.36 |
| 2 | 2 | 4550 | 7MG | C2-N3-C4 | 4.41 | 120.16 | 112.30 |
| 2 | 2 | 3897 | B8K | C5-C4-N9 | 4.33 | 111.97 | 106.35 |
| 2 | 2 | 2522 | 7MG | C2-N3-C4 | 4.31 | 119.98 | 112.30 |
| 2 | 2 | 4185 | B8W | O6-C6-N1 | 4.21 | 124.86 | 119.03 |
| 2 | 2 | 2380 | B8W | C2-N3-C4 | 4.19 | 120.14 | 115.36 |
| 2 | 2 | 3909 | OMC | O2-C2-N1 | 4.14 | 127.43 | 118.89 |
| 2 | 2 | 3899 | BGH | C4-C5-N7 | 4.13 | 108.58 | 104.91 |
| 2 | 2 | 3899 | BGH | N9-C8-N7 | 4.11 | 108.85 | 103.33 |
| 2 | 2 | 2380 | B8W | C1'-N9-C4 | -4.10 | 119.43 | 126.64 |
| 2 | 2 | 4083 | 5MU | O4-C4-C5 | -4.06 | 120.19 | 124.90 |
| 2 | 2 | 3899 | BGH | C5-C4-N9 | 4.04 | 111.60 | 106.35 |
| 2 | 2 | 4529 | B8W | C2-N3-C4 | 3.98 | 119.91 | 115.36 |
| 2 | 2 | 1574 | B9B | N2-C2-N3 | 3.92 | 124.18 | 117.79 |
| 2 | 2 | 4690 | B8K | C5-C4-N9 | 3.85 | 111.34 | 106.35 |
| 2 | 2 | 1659 | I4U | C5-C4-N3 | -3.81 | 119.11 | 124.91 |
| 2 | 2 | 3897 | B8K | C4-C5-N7 | 3.79 | 108.28 | 104.91 |
| 2 | 2 | 3897 | B8K | N9-C8-N7 | 3.78 | 108.40 | 103.33 |
| 2 | 2 | 4620 | OMU | N3-C2-N1 | 3.77 | 119.90 | 114.89 |
| 2 | 2 | 4872 | 2MG | CM2-N2-C2 | -3.77 | 115.54 | 123.86 |
| 2 | 2 | 1605 | 7MG | C5-C4-N3 | -3.73 | 121.03 | 128.13 |
| 2 | 2 | 2297 | E7G | C5-C4-N3 | -3.73 | 121.03 | 128.13 |
| 2 | 2 | 4550 | 7MG | C5-C4-N3 | -3.70 | 121.08 | 128.13 |
| 2 | 2 | 3899 | BGH | C5-C4-N3 | -3.70 | 121.08 | 128.13 |
| 2 | 2 | 1456 | B8Q | C6-N1-C2 | -3.69 | 118.48 | 121.79 |
| 2 | 2 | 1605 | 7MG | C5-C4-N9 | 3.68 | 111.12 | 106.35 |
| 2 | 2 | 4472 | B8W | C1'-N9-C4 | -3.67 | 120.20 | 126.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 4083 | 5MU | C5M-C5-C4 | 3.64 | 122.77 | 118.77 |
| 2 | 2 | 2380 | B8W | O6-C6-N1 | 3.63 | 124.06 | 119.03 |
| 2 | 2 | 1517 | 2MG | C5-C6-N1 | 3.63 | 120.36 | 113.95 |
| 2 | 2 | 1883 | OMG | C5-C6-N1 | 3.60 | 120.31 | 113.95 |
| 2 | 2 | 373 | OMG | C5-C6-N1 | 3.59 | 120.29 | 113.95 |
| 2 | 2 | 729 | 2MG | C5-C6-N1 | 3.53 | 120.19 | 113.95 |
| 5 | 8 | 14 | OMU | N3-C2-N1 | 3.53 | 119.57 | 114.89 |
| 2 | 2 | 4550 | 7MG | C5-C4-N9 | 3.52 | 110.92 | 106.35 |
| 2 | 2 | 4564 | M7A | C2-N3-C4 | 3.52 | 120.07 | 111.75 |
| 2 | 2 | 2424 | OMG | C5-C6-N1 | 3.50 | 120.14 | 113.95 |
| 2 | 2 | 2297 | E7G | C5-C4-N9 | 3.50 | 110.89 | 106.35 |
| 2 | 2 | 1348 | P4U | C5-C4-N3 | -3.50 | 119.59 | 124.91 |
| 2 | 2 | 978 | 2MG | C5-C6-N1 | 3.49 | 120.12 | 113.95 |
| 5 | 8 | 14 | OMU | C5-C4-N3 | 3.48 | 120.05 | 114.84 |
| 2 | 2 | 4870 | OMG | C5-C6-N1 | 3.47 | 120.08 | 113.95 |
| 2 | 2 | 2364 | OMG | C5-C6-N1 | 3.46 | 120.06 | 113.95 |
| 2 | 2 | 4623 | OMG | C5-C6-N1 | 3.45 | 120.05 | 113.95 |
| 2 | 2 | 2522 | 7MG | C5-C4-N3 | -3.45 | 121.56 | 128.13 |
| 2 | 2 | 4872 | 2MG | C5-C6-N1 | 3.45 | 120.04 | 113.95 |
| 2 | 2 | 2522 | 7MG | C5-C4-N9 | 3.44 | 110.81 | 106.35 |
| 2 | 2 | 1316 | OMG | C5-C6-N1 | 3.43 | 120.01 | 113.95 |
| 2 | 2 | 4637 | OMG | C5-C6-N1 | 3.41 | 119.97 | 113.95 |
| 2 | 2 | 4494 | OMG | C5-C6-N1 | 3.41 | 119.97 | 113.95 |
| 2 | 2 | 2050 | OMG | C5-C6-N1 | 3.40 | 119.96 | 113.95 |
| 2 | 2 | 1625 | OMG | C5-C6-N1 | 3.40 | 119.95 | 113.95 |
| 2 | 2 | 1522 | OMG | C5-C6-N1 | 3.39 | 119.93 | 113.95 |
| 2 | 2 | 2773 | OMG | C5-C6-N1 | 3.38 | 119.92 | 113.95 |
| 2 | 2 | 4620 | OMU | C5-C4-N3 | 3.38 | 119.89 | 114.84 |
| 2 | 2 | 4690 | B8K | C6-C5-C4 | -3.25 | 115.93 | 122.62 |
| 2 | 2 | 3897 | B8K | C5-C4-N3 | -3.19 | 122.05 | 128.13 |
| 2 | 2 | 1909 | P7G | N9-C8-N7 | 3.17 | 107.92 | 103.38 |
| 2 | 2 | 3897 | B8K | C6-C5-C4 | -3.17 | 116.08 | 122.62 |
| 2 | 2 | 2050 | OMG | C2-N1-C6 | -3.17 | 119.27 | 125.10 |
| 2 | 2 | 4185 | B8W | C1'-N9-C4 | -3.16 | 121.09 | 126.64 |
| 2 | 2 | 2364 | OMG | C2-N1-C6 | -3.16 | 119.28 | 125.10 |
| 2 | 2 | 4637 | OMG | C2-N1-C6 | -3.13 | 119.33 | 125.10 |
| 2 | 2 | 1883 | OMG | C2-N1-C6 | -3.12 | 119.35 | 125.10 |
| 2 | 2 | 2861 | OMC | O2-C2-N3 | -3.12 | 117.25 | 122.33 |
| 2 | 2 | 4536 | OMC | O2-C2-N3 | -3.11 | 117.27 | 122.33 |
| 2 | 2 | 2424 | OMG | C2-N1-C6 | -3.11 | 119.37 | 125.10 |
| 2 | 2 | 4690 | B8K | C5-C4-N3 | -3.10 | 122.22 | 128.13 |
| 2 | 2 | 4494 | OMG | C2-N1-C6 | -3.10 | 119.39 | 125.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | 2 | 1316 | OMG | C2-N1-C6 | -3.08 | 119.43 | 125.10 |
| 2 | 2 | 1625 | OMG | C2-N1-C6 | -3.07 | 119.44 | 125.10 |
| 2 | 2 | 4623 | OMG | C2-N1-C6 | -3.06 | 119.47 | 125.10 |
| 2 | 2 | 4472 | B8W | O6-C6-N1 | 3.06 | 123.27 | 119.03 |
| 2 | 2 | 2522 | 7MG | N9-C8-N7 | 3.04 | 107.72 | 103.38 |
| 2 | 2 | 373 | OMG | C2-N1-C6 | -3.03 | 119.51 | 125.10 |
| 2 | 2 | 4083 | 5MU | C6-C5-C4 | 3.01 | 120.55 | 118.03 |
| 5 | 8 | 14 | OMU | O4-C4-C5 | -3.01 | 119.87 | 125.16 |
| 2 | 2 | 1522 | OMG | C2-N1-C6 | -2.99 | 119.59 | 125.10 |
| 2 | 2 | 2773 | OMG | C2-N1-C6 | -2.97 | 119.62 | 125.10 |
| 2 | 2 | 4870 | OMG | C2-N1-C6 | -2.95 | 119.67 | 125.10 |
| 2 | 2 | 4185 | B8W | N2-C2-N1 | -2.92 | 112.71 | 117.25 |
| 2 | 2 | 4597 | UR3 | C6-N1-C2 | -2.92 | 119.17 | 121.79 |
| 2 | 2 | 4483 | B8T | O2-C2-N3 | -2.91 | 117.60 | 122.33 |
| 2 | 2 | 3899 | BGH | C6-C5-C4 | -2.89 | 116.66 | 122.62 |
| 2 | 2 | 2380 | B8W | N2-C2-N1 | -2.89 | 112.76 | 117.25 |
| 2 | 2 | 2522 | 7MG | C4-C5-N7 | 2.89 | 109.54 | 105.53 |
| 2 | 2 | 1574 | B9B | C61-O6-C6 | -2.88 | 112.12 | 117.51 |
| 2 | 2 | 3887 | OMC | O2-C2-N3 | -2.87 | 117.66 | 122.33 |
| 2 | 2 | 4620 | OMU | O4-C4-C5 | -2.84 | 120.17 | 125.16 |
| 2 | 2 | 4483 | B8T | O3'-C3'-C2' | 2.82 | 120.94 | 111.82 |
| 2 | 2 | 1605 | 7MG | N9-C8-N7 | 2.81 | 107.40 | 103.38 |
| 2 | 2 | 4529 | B8W | N2-C2-N1 | -2.80 | 112.89 | 117.25 |
| 2 | 2 | 3909 | OMC | C5-C4-N4 | 2.80 | 124.98 | 120.57 |
| 2 | 2 | 2363 | A2M | C1'-N9-C4 | 2.77 | 131.52 | 126.64 |
| 2 | 2 | 3899 | BGH | O6-C6-N1 | -2.77 | 114.81 | 120.12 |
| 2 | 2 | 4671 | B8T | C6-C5-C4 | 2.75 | 120.32 | 116.96 |
| 2 | 2 | 2422 | OMC | O2-C2-N3 | -2.74 | 117.87 | 122.33 |
| 2 | 2 | 1883 | OMG | O6-C6-C5 | -2.73 | 119.04 | 124.37 |
| 2 | 2 | 4597 | UR3 | C3U-N3-C2 | 2.72 | 122.09 | 117.31 |
| 2 | 2 | 4571 | A2M | C1'-N9-C4 | 2.71 | 131.40 | 126.64 |
| 2 | 2 | 1909 | P7G | C71-N7-C5 | 2.71 | 130.93 | 124.52 |
| 2 | 2 | 4529 | B8W | C1'-N9-C4 | -2.69 | 121.92 | 126.64 |
| 2 | 2 | 3897 | B8K | O6-C6-N1 | -2.68 | 114.98 | 120.12 |
| 2 | 2 | 2297 | E7G | N9-C8-N7 | 2.68 | 107.20 | 103.38 |
| 2 | 2 | 978 | 2MG | C8-N7-C5 | 2.67 | 108.08 | 102.99 |
| 2 | 2 | 4872 | 2MG | C8-N7-C5 | 2.65 | 108.04 | 102.99 |
| 2 | 2 | 4083 | 5MU | O2-C2-N1 | -2.63 | 119.29 | 122.79 |
| 2 | 2 | 4690 | B8K | C2-N1-C6 | -2.61 | 120.34 | 125.10 |
| 2 | 2 | 3867 | A2M | C1'-N9-C4 | 2.61 | 131.22 | 126.64 |
| 2 | 2 | 4550 | 7MG | C4-C5-N7 | 2.59 | 109.12 | 105.53 |
| 2 | 2 | 1605 | 7MG | C4-C5-N7 | 2.59 | 109.12 | 105.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | 2 | 3909 | OMC | C4-N3-C2 | 2.58 | 124.42 | 120.25 |
| 2 | 2 | 4550 | 7MG | N9-C8-N7 | 2.58 | 107.07 | 103.38 |
| 2 | 2 | 3909 | OMC | C1'-N1-C2 | 2.58 | 124.18 | 118.42 |
| 2 | 2 | 237 | B9B | C61-O6-C6 | -2.55 | 112.76 | 117.51 |
| 2 | 2 | 729 | 2MG | C8-N7-C5 | 2.52 | 107.78 | 102.99 |
| 2 | 2 | 1605 | 7MG | C2-N1-C6 | -2.48 | 120.57 | 125.10 |
| 2 | 2 | 2297 | E7G | C2-N1-C6 | -2.48 | 120.58 | 125.10 |
| 2 | 2 | 2754 | B9B | C61-O6-C6 | -2.46 | 112.91 | 117.51 |
| 2 | 2 | 1517 | 2MG | C8-N7-C5 | 2.46 | 107.68 | 102.99 |
| 2 | 2 | 1517 | 2MG | O6-C6-C5 | -2.46 | 119.56 | 124.37 |
| 2 | 2 | 4623 | OMG | C8-N7-C5 | 2.45 | 107.66 | 102.99 |
| 2 | 2 | 4564 | M7A | C5-C4-N3 | -2.44 | 120.90 | 126.62 |
| 2 | 2 | 2786 | B9H | O3'-C3'-C4' | 2.43 | 118.09 | 111.05 |
| 2 | 2 | 373 | OMG | C8-N7-C5 | 2.43 | 107.61 | 102.99 |
| 2 | 2 | 3880 | P7G | N9-C8-N7 | 2.43 | 106.85 | 103.38 |
| 2 | 2 | 2861 | OMC | C1'-N1-C2 | 2.42 | 123.82 | 118.42 |
| 2 | 2 | 4472 | B8W | C2-N1-C6 | 2.41 | 119.95 | 116.08 |
| 2 | 2 | 3909 | OMC | C5-C4-N3 | -2.41 | 117.23 | 121.33 |
| 2 | 2 | 3869 | OMC | O2-C2-N3 | -2.40 | 118.43 | 122.33 |
| 2 | 2 | 2786 | B9H | O2-C2-N1 | -2.38 | 117.15 | 122.72 |
| 2 | 2 | 4483 | B8T | O3'-C3'-C4' | 2.37 | 117.90 | 111.05 |
| 2 | 2 | 1316 | OMG | C8-N7-C5 | 2.37 | 107.50 | 102.99 |
| 2 | 2 | 1456 | B8Q | C31-N3-C2 | 2.36 | 121.22 | 117.79 |
| 2 | 2 | 3897 | B8K | C2-N1-C6 | -2.36 | 120.80 | 125.10 |
| 2 | 2 | 3899 | BGH | N1-C2-N3 | -2.35 | 118.94 | 123.32 |
| 2 | 2 | 4870 | OMG | C8-N7-C5 | 2.35 | 107.46 | 102.99 |
| 2 | 2 | 3718 | A2M | C1'-N9-C4 | 2.34 | 130.76 | 126.64 |
| 2 | 2 | 373 | OMG | O6-C6-C5 | -2.34 | 119.80 | 124.37 |
| 2 | 2 | 3899 | BGH | C2-N1-C6 | -2.34 | 120.83 | 125.10 |
| 2 | 2 | 1326 | A2M | C1'-N9-C4 | 2.33 | 130.73 | 126.64 |
| 2 | 2 | 4550 | 7MG | C2-N1-C6 | -2.32 | 120.86 | 125.10 |
| 2 | 2 | 2364 | OMG | O6-C6-C5 | -2.32 | 119.85 | 124.37 |
| 2 | 2 | 3897 | B8K | N1-C2-N3 | -2.30 | 119.03 | 123.32 |
| 2 | 2 | 2424 | OMG | O6-C6-C5 | -2.30 | 119.89 | 124.37 |
| 2 | 2 | 1522 | OMG | O6-C6-C5 | -2.29 | 119.89 | 124.37 |
| 2 | 2 | 1625 | OMG | O6-C6-C5 | -2.29 | 119.89 | 124.37 |
| 2 | 2 | 4623 | OMG | N2-C2-N1 | 2.29 | 121.59 | 116.71 |
| 2 | 2 | 4083 | 5MU | O4-C4-N3 | -2.28 | 115.74 | 120.12 |
| 2 | 2 | 4530 | UR3 | C6-N1-C2 | -2.28 | 119.74 | 121.79 |
| 2 | 2 | 4494 | OMG | O6-C6-C5 | -2.28 | 119.91 | 124.37 |
| 5 | 8 | 14 | OMU | C1'-N1-C2 | 2.27 | 121.68 | 117.57 |
| 2 | 2 | 4637 | OMG | O6-C6-C5 | -2.26 | 119.96 | 124.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | 2 | 1456 | B8Q | C1'-N1-C2 | 2.26 | 120.80 | 116.99 |
| 2 | 2 | 4872 | 2MG | O6-C6-C5 | -2.26 | 119.97 | 124.37 |
| 2 | 2 | 729 | 2MG | O6-C6-C5 | -2.25 | 119.97 | 124.37 |
| 2 | 2 | 4564 | M7A | C4-N9-C1' | -2.25 | 121.25 | 126.60 |
| 2 | 2 | 4637 | OMG | N2-C2-N1 | 2.25 | 121.50 | 116.71 |
| 2 | 2 | 4690 | B8K | N1-C2-N3 | -2.24 | 119.14 | 123.32 |
| 2 | 2 | 4472 | B8W | N2-C2-N1 | -2.24 | 113.77 | 117.25 |
| 2 | 2 | 1316 | OMG | O6-C6-C5 | -2.23 | 120.01 | 124.37 |
| 2 | 2 | 3909 | OMC | C6-N1-C2 | -2.23 | 116.62 | 120.49 |
| 2 | 2 | 2380 | B8W | C2-N1-C6 | 2.23 | 119.66 | 116.08 |
| 2 | 2 | 978 | 2MG | O6-C6-C5 | -2.22 | 120.03 | 124.37 |
| 5 | 8 | 14 | OMU | CM2-O2'-C2' | 2.22 | 120.35 | 114.52 |
| 2 | 2 | 4623 | OMG | O6-C6-C5 | -2.22 | 120.04 | 124.37 |
| 2 | 2 | 4690 | B8K | O6-C6-C5 | -2.22 | 122.10 | 127.54 |
| 2 | 2 | 2522 | 7MG | C2-N1-C6 | -2.21 | 121.07 | 125.10 |
| 2 | 2 | 4637 | OMG | C8-N7-C5 | 2.21 | 107.20 | 102.99 |
| 2 | 2 | 1522 | OMG | C8-N7-C5 | 2.20 | 107.19 | 102.99 |
| 2 | 2 | 2773 | OMG | C8-N7-C5 | 2.20 | 107.18 | 102.99 |
| 2 | 2 | 2050 | OMG | C8-N7-C5 | 2.20 | 107.18 | 102.99 |
| 2 | 2 | 2050 | OMG | O6-C6-C5 | -2.20 | 120.08 | 124.37 |
| 2 | 2 | 2773 | OMG | O6-C6-C5 | -2.19 | 120.10 | 124.37 |
| 2 | 2 | 4536 | OMC | C1'-N1-C2 | 2.17 | 123.26 | 118.42 |
| 2 | 2 | 4870 | OMG | O6-C6-C5 | -2.16 | 120.14 | 124.37 |
| 2 | 2 | 1524 | A2M | C1'-N9-C4 | 2.15 | 130.42 | 126.64 |
| 2 | 2 | 4529 | B8W | C2-N1-C6 | 2.15 | 119.53 | 116.08 |
| 2 | 2 | 2424 | OMG | C8-N7-C5 | 2.14 | 107.08 | 102.99 |
| 2 | 2 | 2364 | OMG | C8-N7-C5 | 2.14 | 107.06 | 102.99 |
| 2 | 2 | 3723 | A2M | C1'-N9-C4 | 2.13 | 130.39 | 126.64 |
| 2 | 2 | 1883 | OMG | C8-N7-C5 | 2.12 | 107.04 | 102.99 |
| 2 | 2 | 4483 | B8T | C6-C5-C4 | 2.12 | 119.56 | 116.96 |
| 2 | 2 | 2522 | 7MG | C6-C5-C4 | -2.12 | 118.25 | 122.62 |
| 2 | 2 | 4185 | B8W | C2-N1-C6 | 2.10 | 119.46 | 116.08 |
| 2 | 2 | 1659 | I4U | O2-C2-N3 | -2.09 | 118.93 | 122.33 |
| 2 | 2 | 4483 | B8T | C5-C4-N3 | -2.09 | 119.23 | 122.59 |
| 2 | 2 | 1625 | OMG | C8-N7-C5 | 2.09 | 106.97 | 102.99 |
| 2 | 2 | 2786 | B9H | C21-O2'-C2' | 2.08 | 119.98 | 114.52 |
| 2 | 2 | 2522 | 7MG | O6-C6-C5 | -2.08 | 122.44 | 127.54 |
| 2 | 2 | 3825 | A2M | C1'-N9-C4 | 2.08 | 130.29 | 126.64 |
| 2 | 2 | 4620 | OMU | O2-C2-N1 | -2.07 | 120.03 | 122.79 |
| 2 | 2 | 4529 | B8W | O6-C6-C5 | -2.07 | 113.05 | 116.01 |
| 2 | 2 | 2861 | OMC | O2-C2-N1 | 2.07 | 123.17 | 118.89 |
| 2 | 2 | 2422 | OMC | C1'-N1-C2 | 2.07 | 123.04 | 118.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | 2 | 4536 | OMC | O2-C2-N1 | 2.07 | 123.16 | 118.89 |
| 2 | 2 | 1605 | 7MG | O6-C6-C5 | -2.06 | 122.49 | 127.54 |
| 2 | 2 | 2297 | E7G | C6-C5-C4 | -2.05 | 118.39 | 122.62 |
| 2 | 2 | 4483 | B8T | C6-N1-C2 | -2.05 | 116.94 | 120.49 |
| 2 | 2 | 4523 | A2M | C1'-N9-C4 | 2.03 | 130.21 | 126.64 |
| 2 | 2 | 1348 | P4U | O2-C2-N3 | -2.03 | 119.03 | 122.33 |
| 2 | 2 | 2364 | OMG | N2-C2-N1 | 2.02 | 121.01 | 116.71 |
| 2 | 2 | 2297 | E7G | O6-C6-C5 | -2.02 | 122.59 | 127.54 |
| 2 | 2 | 2522 | 7MG | N1-C2-N3 | -2.02 | 119.56 | 123.32 |
| 2 | 2 | 4494 | OMG | C8-N7-C5 | 2.02 | 106.83 | 102.99 |
| 2 | 2 | 373 | OMG | N2-C2-N1 | 2.02 | 121.00 | 116.71 |
| 2 | 2 | 1316 | OMG | N2-C2-N1 | 2.01 | 120.98 | 116.71 |
| 2 | 2 | 2050 | OMG | N2-C2-N1 | 2.00 | 120.98 | 116.71 |

There are no chirality outliers.

All (75) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 5 | 8 | 14 | OMU | C1'-C2'-O2'-CM2 |
| 2 | 2 | 237 | B9B | C5-C6-O6-C61 |
| 2 | 2 | 237 | B9B | N1-C6-O6-C61 |
| 2 | 2 | 237 | B9B | C3'-C4'-C5'-O5' |
| 2 | 2 | 237 | B9B | O4'-C4'-C5'-O5' |
| 2 | 2 | 398 | A2M | O4'-C4'-C5'-O5' |
| 2 | 2 | 1348 | P4U | N3-C4-O4-C41 |
| 2 | 2 | 1574 | B9B | C5-C6-O6-C61 |
| 2 | 2 | 1574 | B9B | N1-C6-O6-C61 |
| 2 | 2 | 1574 | B9B | C62-C61-O6-C6 |
| 2 | 2 | 1625 | OMG | C3'-C4'-C5'-O5' |
| 2 | 2 | 1871 | A2M | O4'-C4'-C5'-O5' |
| 2 | 2 | 1871 | A2M | C3'-C4'-C5'-O5' |
| 2 | 2 | 1883 | OMG | C3'-C4'-C5'-O5' |
| 2 | 2 | 2364 | OMG | C1'-C2'-O2'-CM2 |
| 2 | 2 | 2380 | B8W | C5-C6-O6-C61 |
| 2 | 2 | 2380 | B8W | N1-C6-O6-C61 |
| 2 | 2 | 2424 | OMG | O4'-C4'-C5'-O5' |
| 2 | 2 | 2424 | OMG | C3'-C4'-C5'-O5' |
| 2 | 2 | 2754 | B9B | C5-C6-O6-C61 |
| 2 | 2 | 2754 | B9B | N1-C6-O6-C61 |
| 2 | 2 | 2754 | B9B | C62-C61-O6-C6 |
| 2 | 2 | 2786 | B9H | C1'-C2'-O2'-C21 |
| 2 | 2 | 4185 | B8W | C5-C6-O6-C61 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 2 | 2 | 4472 | B8W | C5-C6-O6-C61 |
| 2 | 2 | 4472 | B8W | N1-C6-O6-C61 |
| 2 | 2 | 4550 | 7MG | O4'-C4'-C5'-O5' |
| 2 | 2 | 4550 | 7MG | C3'-C4'-C5'-O5' |
| 2 | 2 | 4637 | OMG | O4'-C4'-C5'-O5' |
| 2 | 2 | 4637 | OMG | C1'-C2'-O2'-CM2 |
| 2 | 2 | 4870 | OMG | O4'-C4'-C5'-O5' |
| 2 | 2 | 4870 | OMG | C3'-C4'-C5'-O5' |
| 2 | 2 | 4872 | 2MG | O4'-C4'-C5'-O5' |
| 2 | 2 | 398 | A2M | C3'-C4'-C5'-O5' |
| 2 | 2 | 1883 | OMG | O4'-C4'-C5'-O5' |
| 2 | 2 | 2364 | OMG | O4'-C4'-C5'-O5' |
| 2 | 2 | 3867 | A2M | C3'-C4'-C5'-O5' |
| 2 | 2 | 3897 | B8K | O4'-C4'-C5'-O5' |
| 2 | 2 | 4529 | B8W | C3'-C4'-C5'-O5' |
| 2 | 2 | 4529 | B8W | O4'-C4'-C5'-O5' |
| 2 | 2 | 4637 | OMG | C3'-C4'-C5'-O5' |
| 2 | 2 | 4872 | 2MG | C3'-C4'-C5'-O5' |
| 2 | 2 | 237 | B9B | O6-C61-C62-C63 |
| 2 | 2 | 1625 | OMG | O4'-C4'-C5'-O5' |
| 2 | 2 | 1909 | P7G | O4'-C4'-C5'-O5' |
| 2 | 2 | 2364 | OMG | C3'-C4'-C5'-O5' |
| 2 | 2 | 3867 | A2M | O4'-C4'-C5'-O5' |
| 2 | 2 | 3897 | B8K | C3'-C4'-C5'-O5' |
| 2 | 2 | 3880 | P7G | O4'-C4'-C5'-O5' |
| 2 | 2 | 1909 | P7G | C3'-C4'-C5'-O5' |
| 2 | 2 | 3701 | OMC | C3'-C4'-C5'-O5' |
| 2 | 2 | 3701 | OMC | O4'-C4'-C5'-O5' |
| 2 | 2 | 3880 | P7G | C3'-C4'-C5'-O5' |
| 2 | 2 | 2297 | E7G | C72-C71-N7-C8 |
| 2 | 2 | 2754 | B9B | O6-C61-C62-C63 |
| 2 | 2 | 1534 | A2M | C4'-C5'-O5'-P |
| 2 | 2 | 237 | B9B | C62-C61-O6-C6 |
| 2 | 2 | 4185 | B8W | N1-C6-O6-C61 |
| 2 | 2 | 3867 | A2M | C4'-C5'-O5'-P |
| 2 | 2 | 373 | OMG | C4'-C5'-O5'-P |
| 2 | 2 | 3887 | OMC | C4'-C5'-O5'-P |
| 2 | 2 | 4523 | A2M | C4'-C5'-O5'-P |
| 2 | 2 | 1625 | OMG | C4'-C5'-O5'-P |
| 2 | 2 | 4637 | OMG | C4'-C5'-O5'-P |
| 2 | 2 | 3897 | B8K | C4'-C5'-O5'-P |
| 2 | 2 | 2422 | OMC | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 2 | 2 | 4870 | OMG | C4'-C5'-O5'-P |
| 2 | 2 | 1909 | P7G | C72-C71-N7-C8 |
| 2 | 2 | 1517 | 2MG | C4'-C5'-O5'-P |
| 2 | 2 | 3909 | OMC | O4'-C4'-C5'-O5' |
| 2 | 2 | 729 | 2MG | O4'-C4'-C5'-O5' |
| 2 | 2 | 1534 | A2M | O4'-C4'-C5'-O5' |
| 2 | 2 | 3909 | OMC | C2'-C1'-N1-C2 |
| 2 | 2 | 1659 | I4U | C43-C41-O4-C4 |
| 2 | 2 | 3899 | BGH | 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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 | $\# Z > 2$ |
| 60 | GTP | w | 801 | 61,36 | 26,34,34 | 1.13 | 2 (7%) | 32,54,54 | 1.56 | 7 (21%) |

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. '2' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|------------|---------|
| 60 | GTP | w | 801 | 61,36 | - | 5/18/38/38 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 60 | w | 801 | GTP | C5-C6 | -3.97 | 1.39 | 1.47 |
| 60 | w | 801 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 60 | w | 801 | GTP | PA-O3A-PB | -3.29 | 121.53 | 132.83 |
| 60 | w | 801 | GTP | C5-C6-N1 | 3.29 | 119.76 | 113.95 |
| 60 | w | 801 | GTP | C8-N7-C5 | 3.07 | 108.83 | 102.99 |
| 60 | w | 801 | GTP | C2-N1-C6 | -2.92 | 119.73 | 125.10 |
| 60 | w | 801 | GTP | C3'-C2'-C1' | 2.82 | 105.23 | 100.98 |
| 60 | w | 801 | GTP | PB-O3B-PG | -2.70 | 123.56 | 132.83 |
| 60 | w | 801 | GTP | O6-C6-C5 | -2.12 | 120.24 | 124.37 |

There are no chirality outliers.

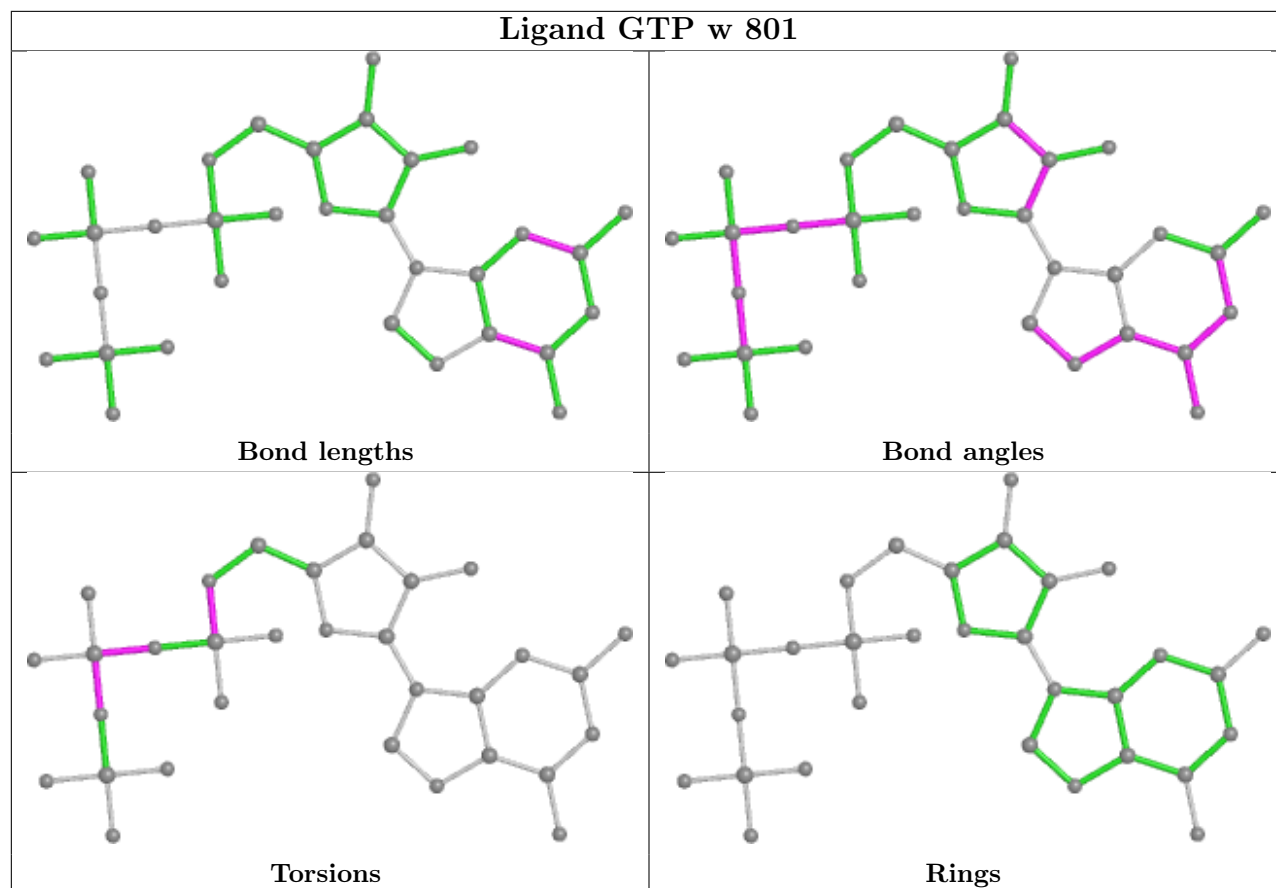
All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 60 | w | 801 | GTP | C5'-O5'-PA-O3A |
| 60 | w | 801 | GTP | PA-O3A-PB-O1B |
| 60 | w | 801 | GTP | C5'-O5'-PA-O2A |
| 60 | w | 801 | GTP | PG-O3B-PB-O3A |
| 60 | w | 801 | GTP | PG-O3B-PB-O2B |

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.

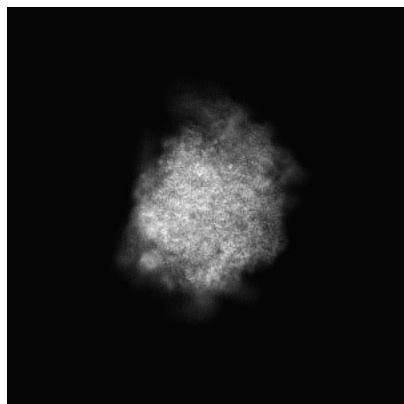
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35651. These allow visual inspection of the internal detail of the map and identification of artifacts.

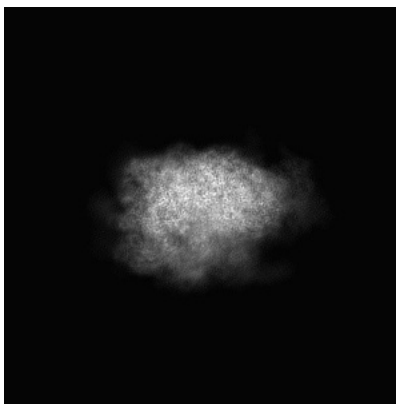
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

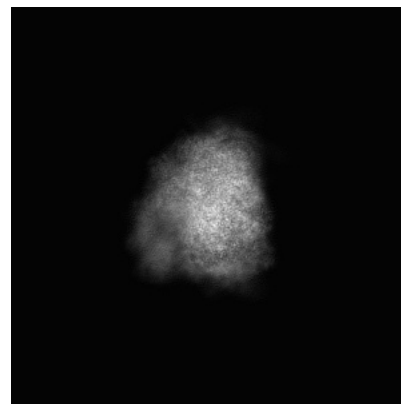
6.1.1 Primary map



X

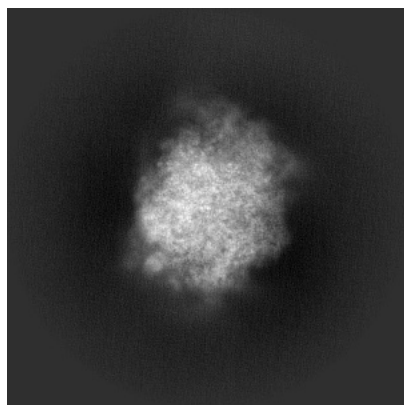


Y

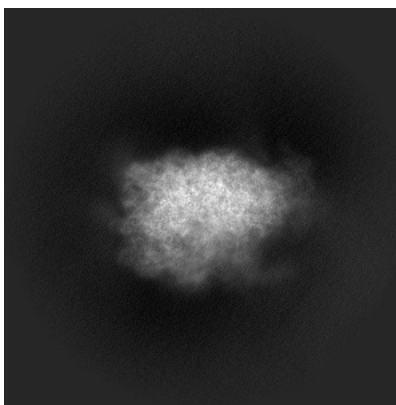


Z

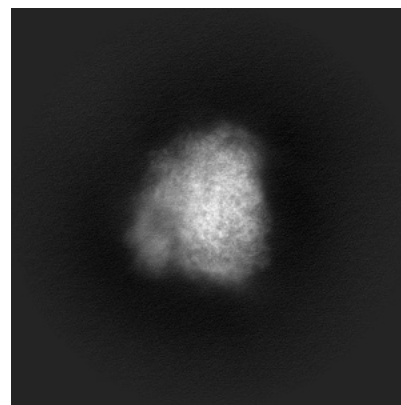
6.1.2 Raw map



X



Y

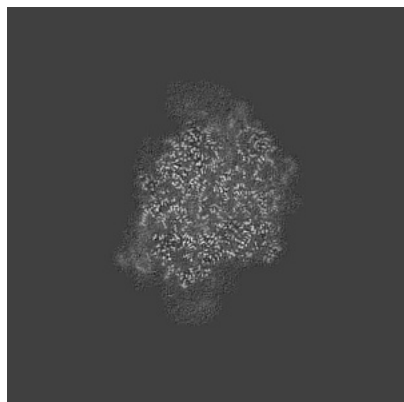


Z

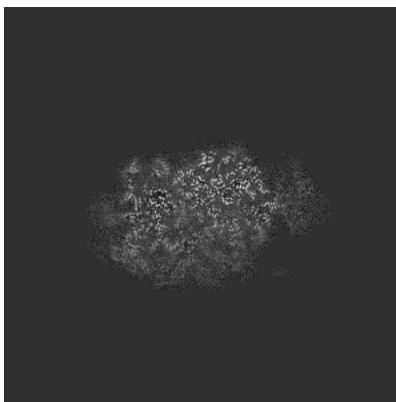
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

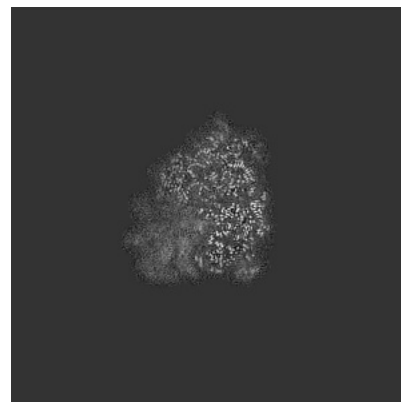
6.2.1 Primary map



X Index: 200

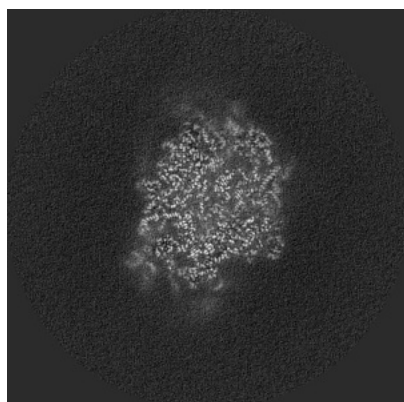


Y Index: 200

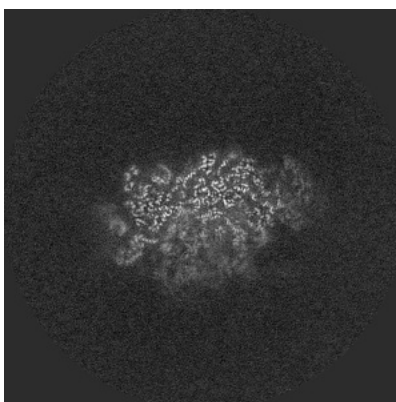


Z Index: 200

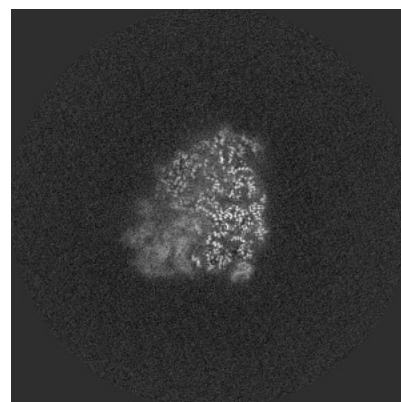
6.2.2 Raw map



X Index: 200



Y Index: 200

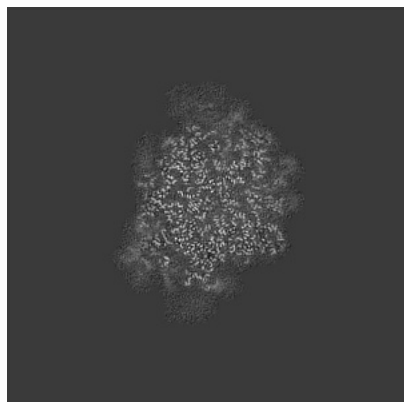


Z Index: 200

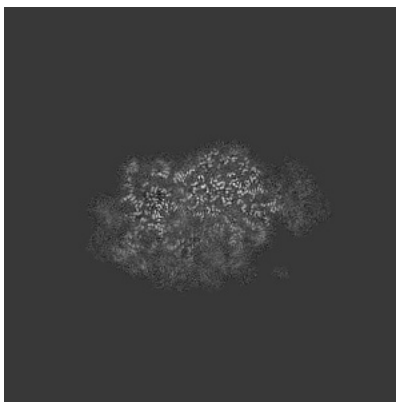
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

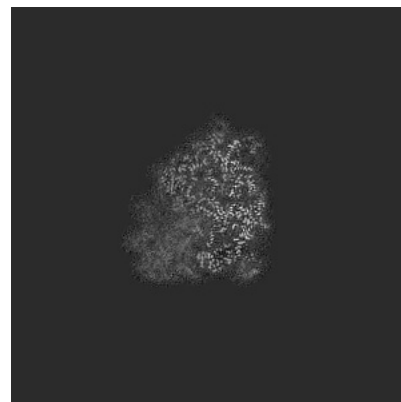
6.3.1 Primary map



X Index: 206

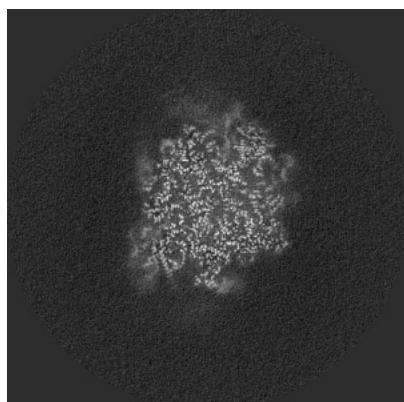


Y Index: 199

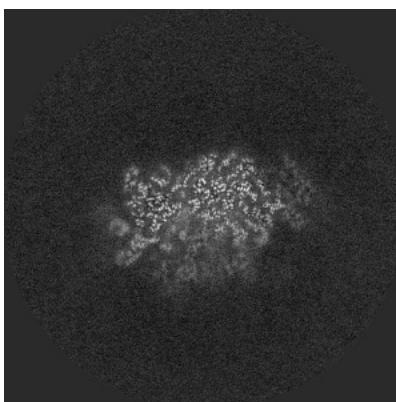


Z Index: 198

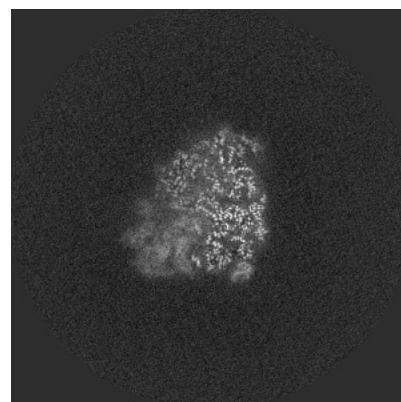
6.3.2 Raw map



X Index: 206



Y Index: 199

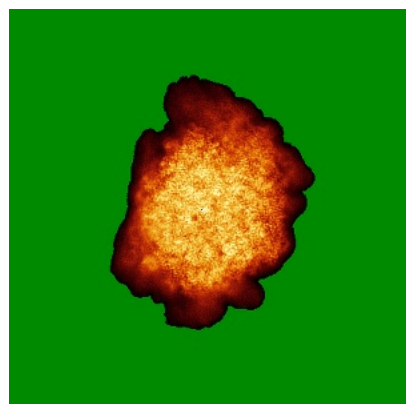


Z Index: 200

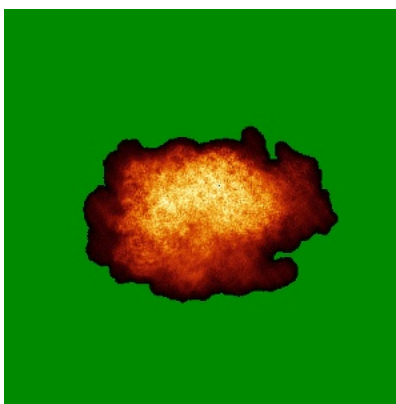
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

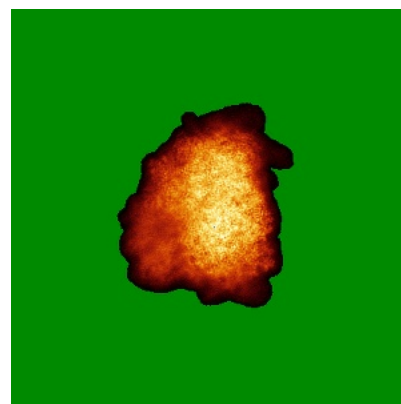
6.4.1 Primary map



X

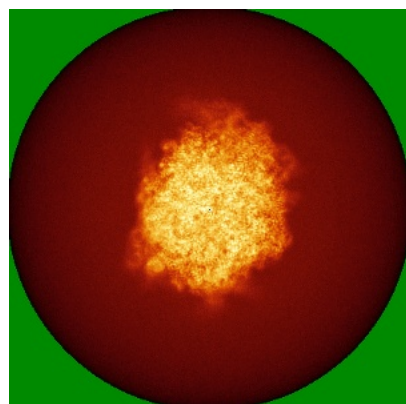


Y

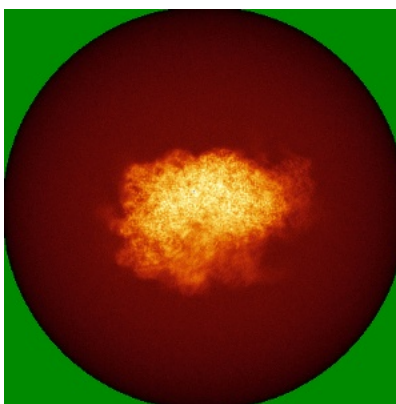


Z

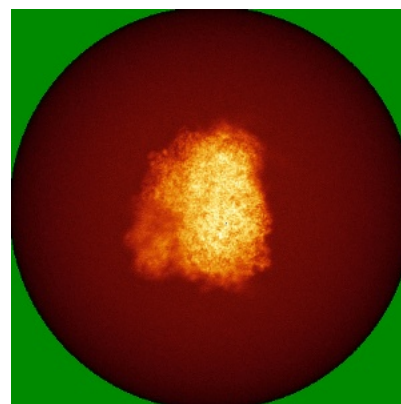
6.4.2 Raw map



X



Y

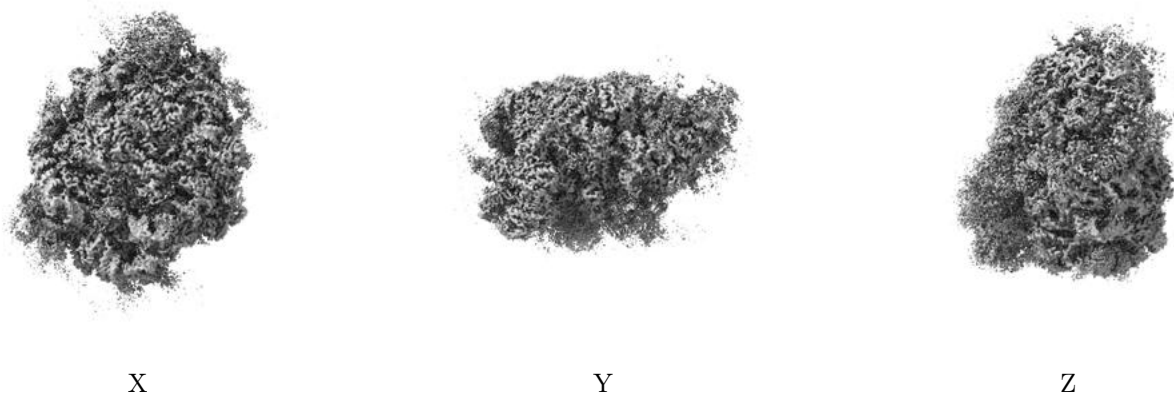


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

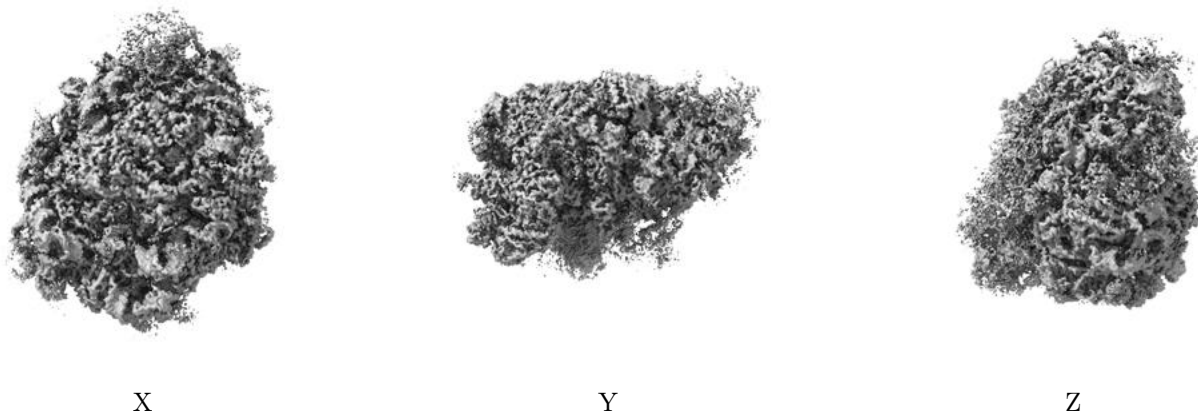
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

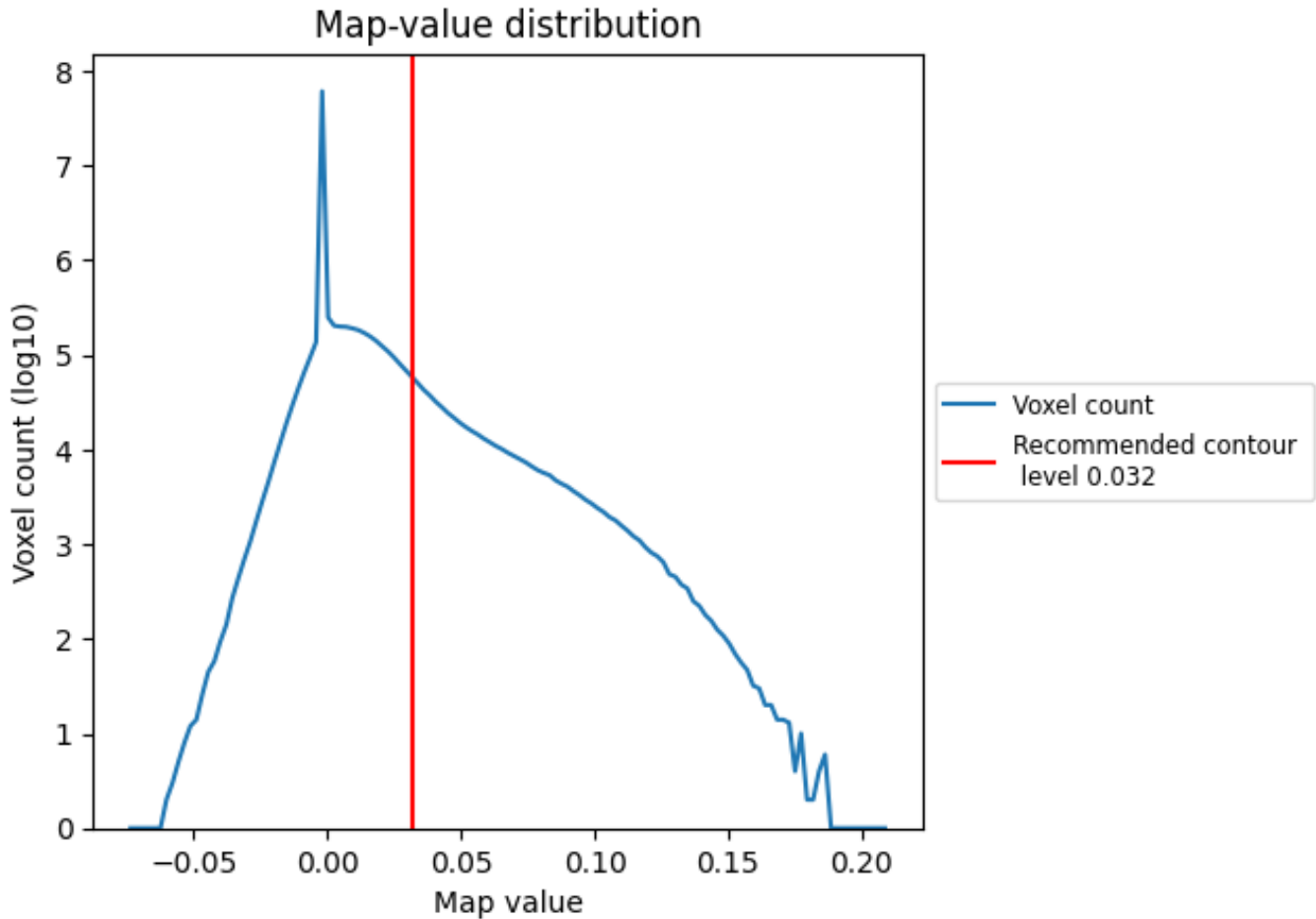
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

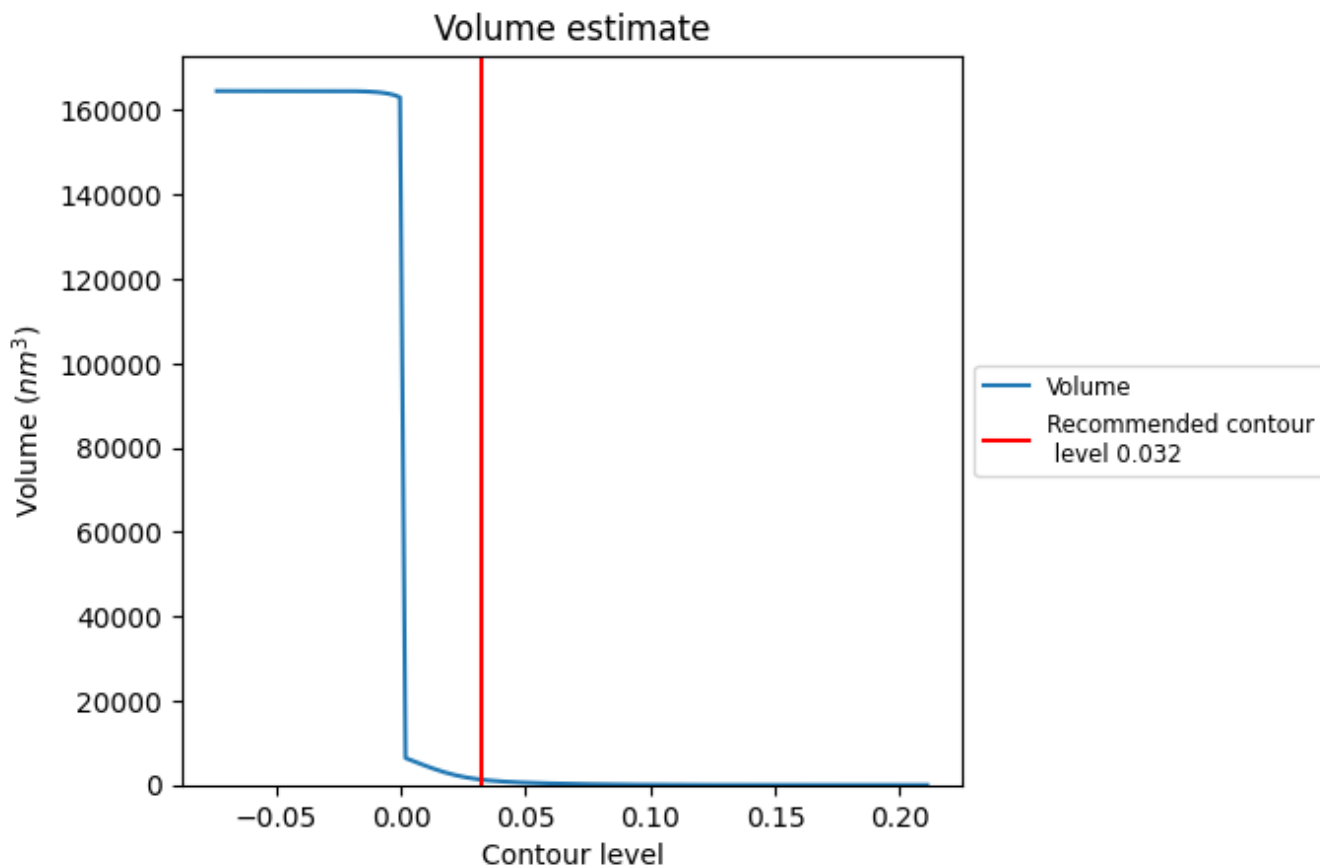
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

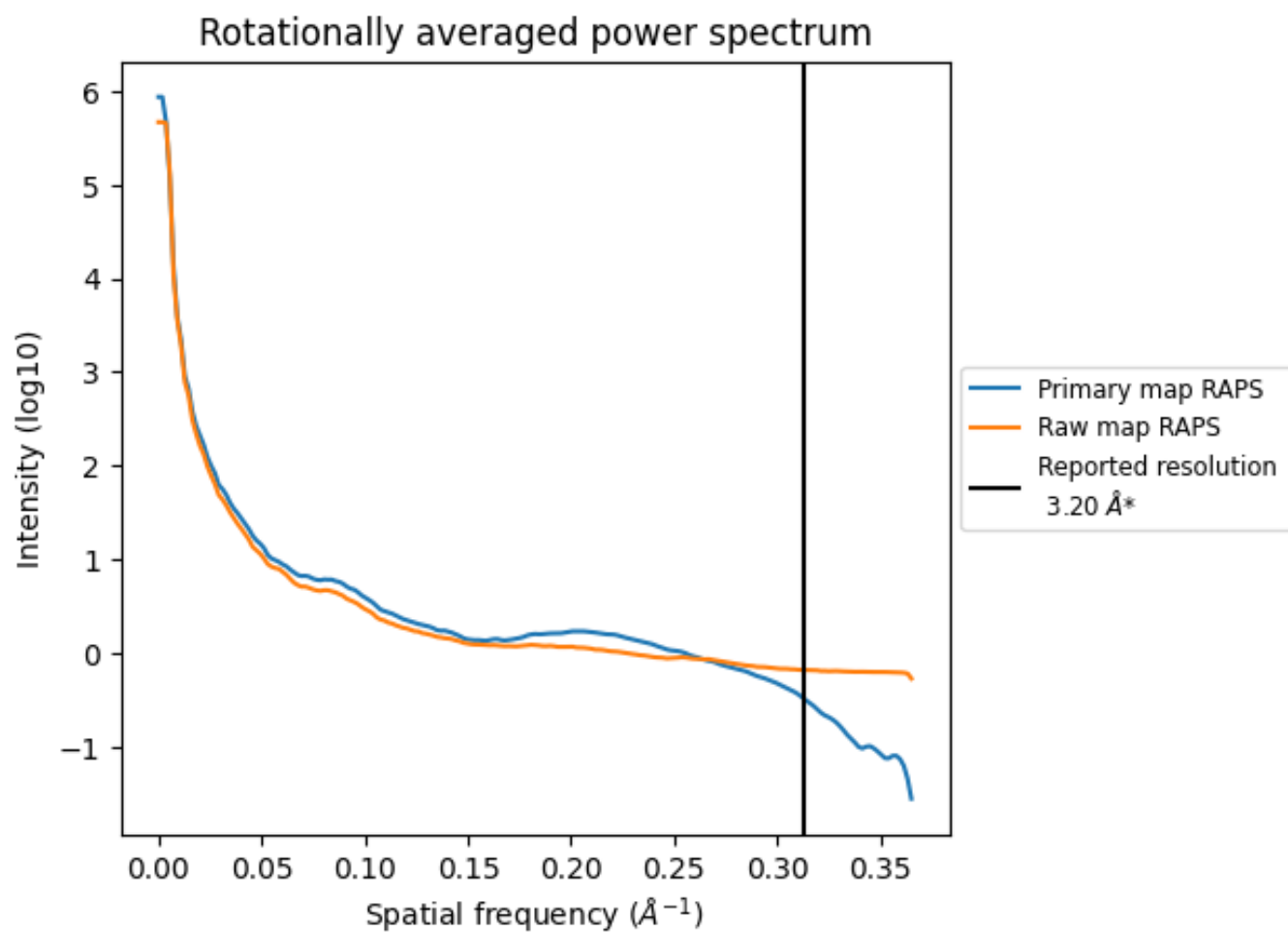
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1286 nm³; this corresponds to an approximate mass of 1162 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

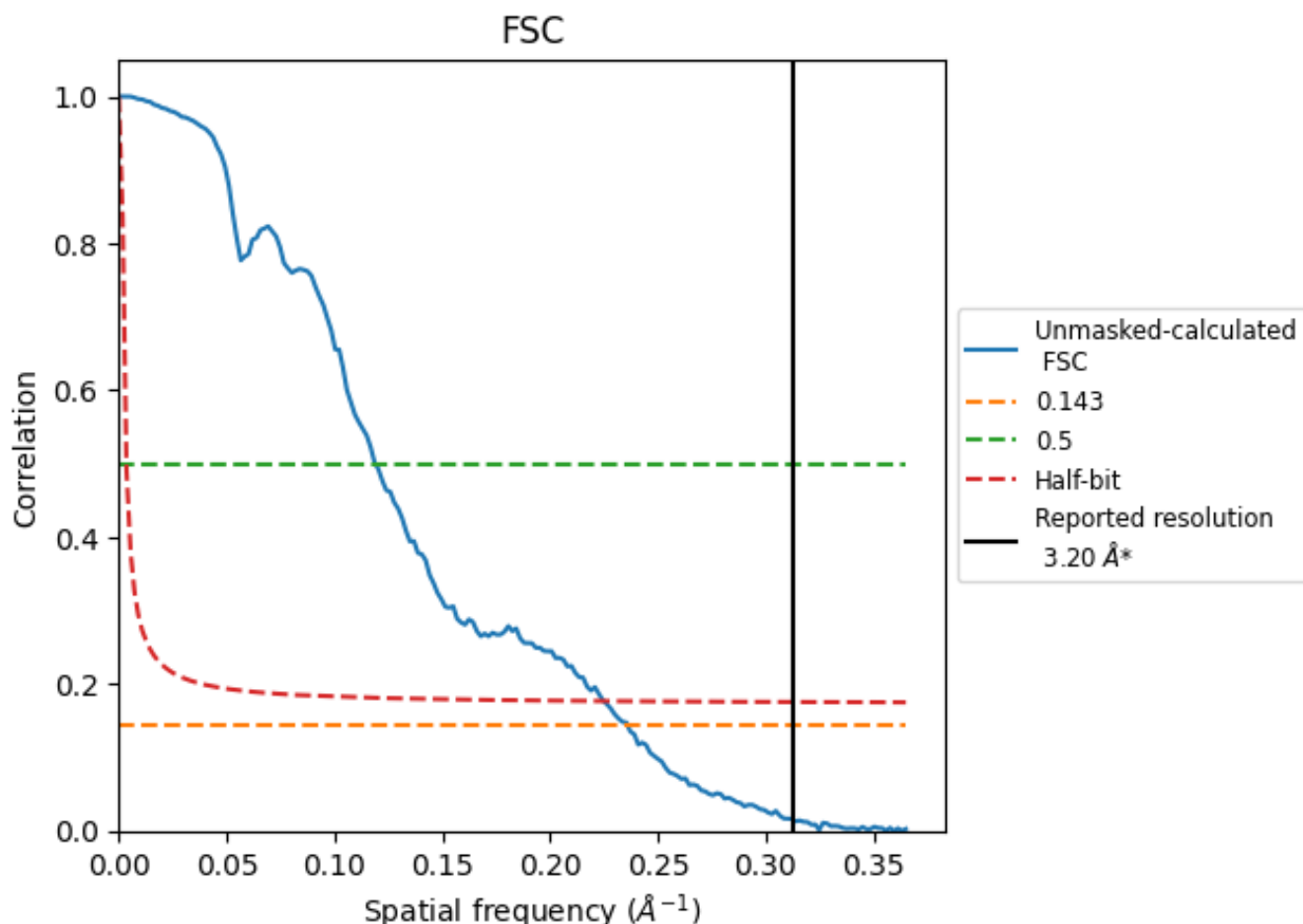


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

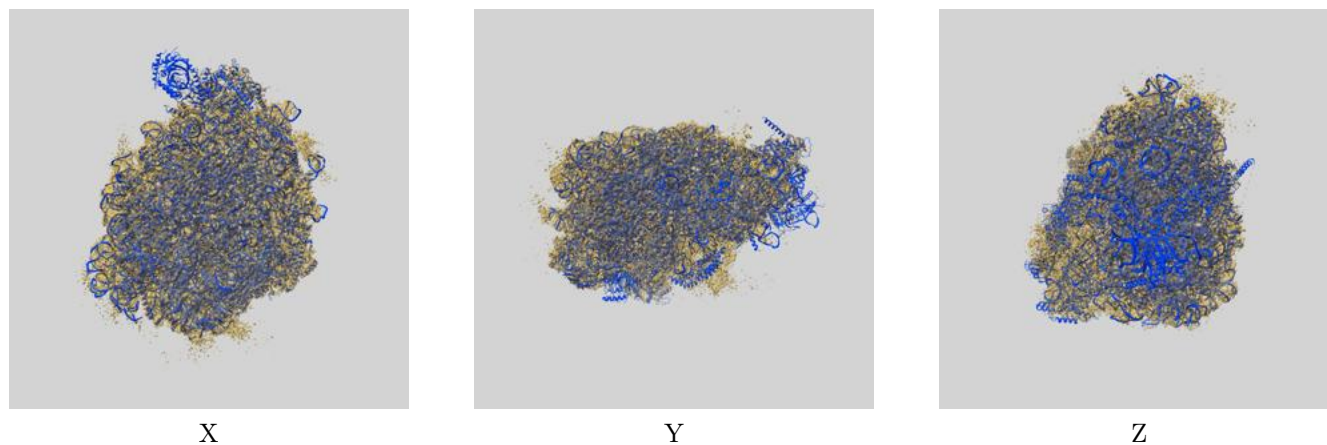
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.20 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 4.24 | 8.41 | 4.45 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

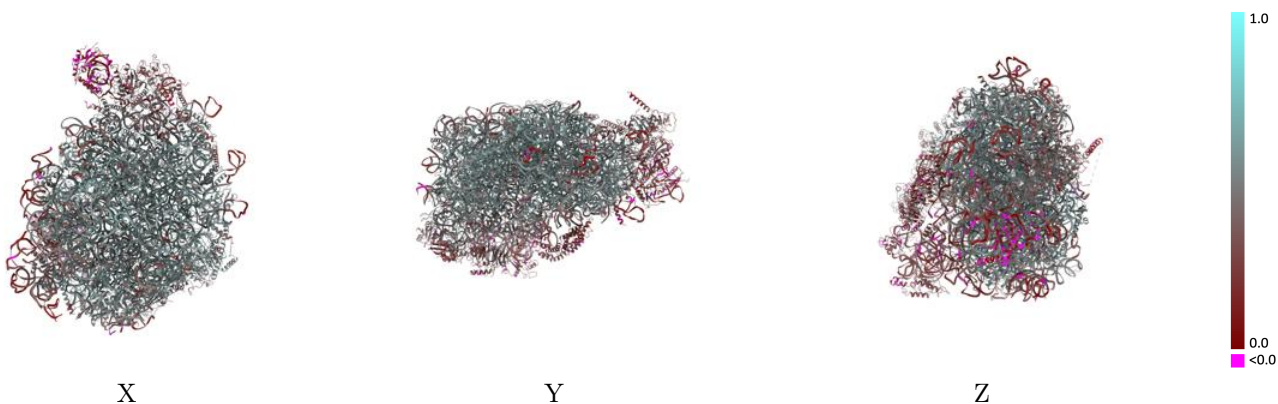
This section contains information regarding the fit between EMDB map EMD-35651 and PDB model 8IPY. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



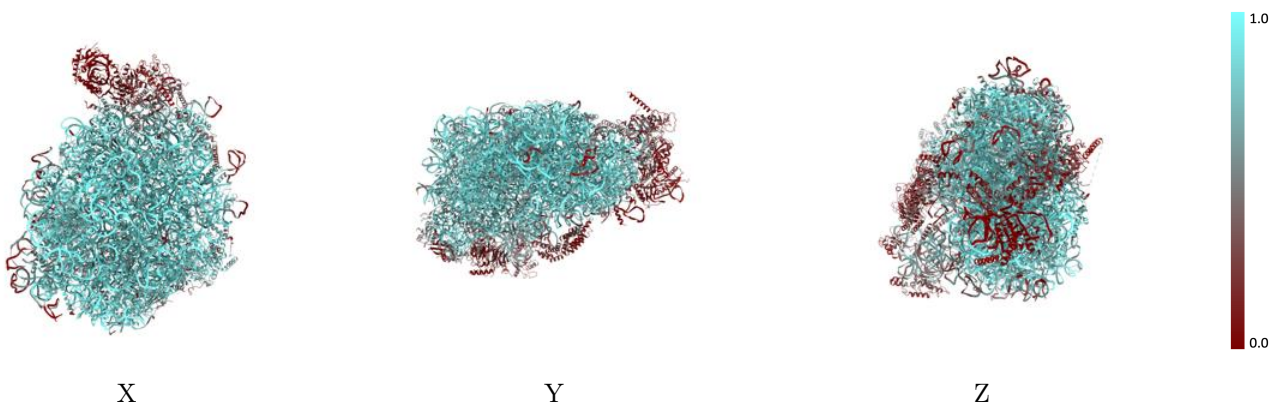
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



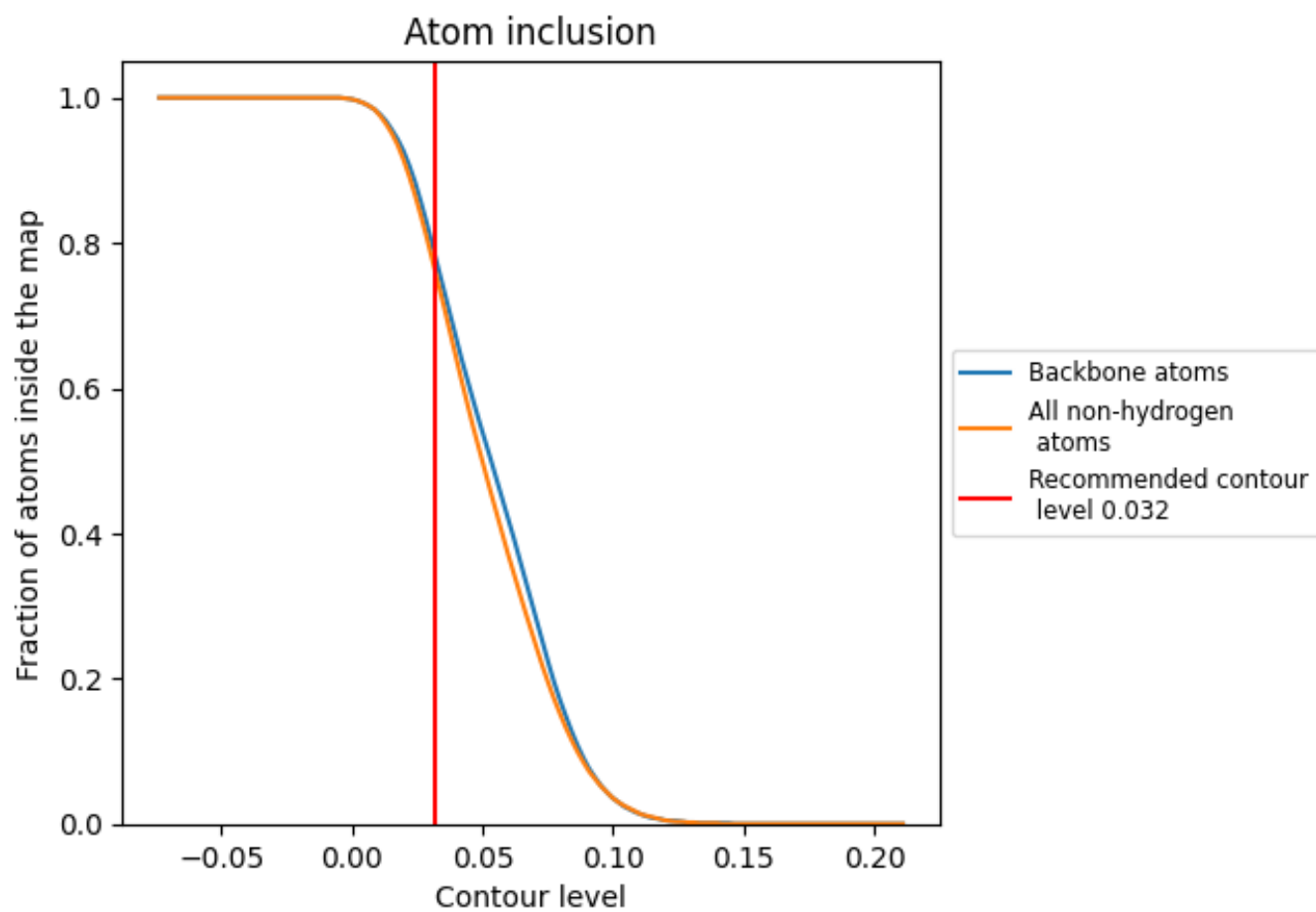
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



















































The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7590 |  0.4550 |
| 1 |  0.1910 |  0.3760 |
| 2 |  0.8690 |  0.4650 |
| 3 |  0.7220 |  0.2860 |
| 4 |  0.7210 |  0.4550 |
| 6 |  0.7640 |  0.4940 |
| 7 |  0.8360 |  0.5340 |
| 8 |  0.9400 |  0.5330 |
| 9 |  0.6160 |  0.4430 |
| A |  0.5310 |  0.3820 |
| B |  0.9000 |  0.5510 |
| C |  0.2390 |  0.2200 |
| D |  0.9190 |  0.5520 |
| E |  0.6830 |  0.4780 |
| F |  0.8660 |  0.5320 |
| G |  0.7080 |  0.4640 |
| H |  0.8610 |  0.5290 |
| I |  0.8250 |  0.5220 |
| J |  0.7560 |  0.4930 |
| K |  0.8250 |  0.4970 |
| L |  0.8970 |  0.5490 |
| M |  0.9570 |  0.5650 |
| N |  0.1680 |  0.2300 |
| O |  0.7180 |  0.5040 |
| P |  0.9720 |  0.5700 |
| Q |  0.8290 |  0.5100 |
| R |  0.2500 |  0.2090 |
| S |  0.8860 |  0.5270 |
| T |  0.5770 |  0.3150 |
| U |  0.8960 |  0.5420 |
| V |  0.8970 |  0.5380 |
| W |  0.1220 |  0.3400 |
| X |  0.7960 |  0.5140 |
| Y |  0.8650 |  0.5350 |
| Z |  0.9280 |  0.5600 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| a |  0.8740 |  0.5190 |
| b |  0.9190 |  0.5480 |
| c |  0.0030 |  0.1510 |
| d |  0.7750 |  0.5030 |
| e |  0.9050 |  0.5430 |
| f |  0.3610 |  0.3410 |
| g |  0.7730 |  0.4970 |
| h |  0.8790 |  0.5370 |
| i |  0.7890 |  0.4960 |
| j |  0.8370 |  0.5250 |
| k |  0.9470 |  0.5680 |
| l |  0.9280 |  0.5570 |
| m |  0.8640 |  0.5280 |
| n |  0.9510 |  0.5670 |
| o |  0.7930 |  0.4870 |
| p |  0.9040 |  0.5370 |
| q |  0.3710 |  0.4000 |
| r |  0.3250 |  0.3040 |
| t |  0.0870 |  0.2720 |
| u |  0.4560 |  0.3610 |
| v |  0.5690 |  0.4210 |
| w |  0.7280 |  0.4680 |
| x |  0.0020 |  0.1540 |
| y |  0.3500 |  0.3070 |
| z |  0.6580 |  0.4570 |