



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 02:58 PM BST

PDB ID : 4KZZ
Title : Rabbit 40S ribosomal subunit in complex with mRNA, initiator tRNA and eIF1A
Authors : Lomakin, I.B.; Steitz, T.A.
Deposited on : 2013-05-30
Resolution : 7.03 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.13 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.13 |

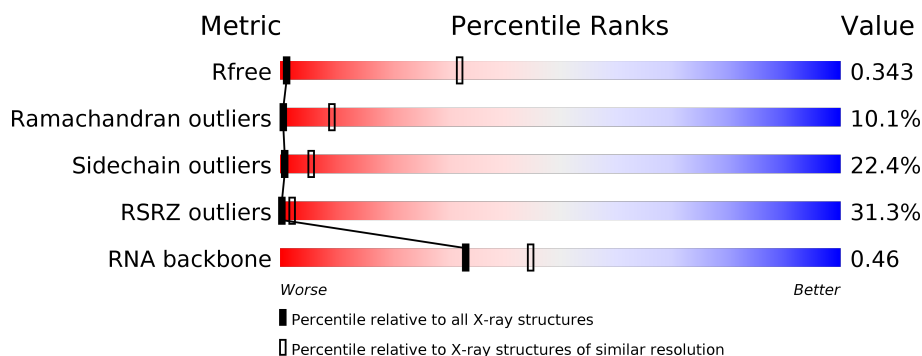
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.03 Å.

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



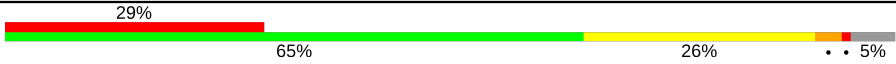



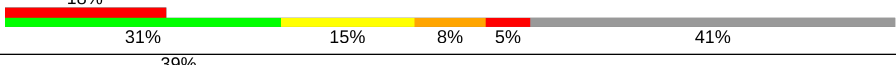
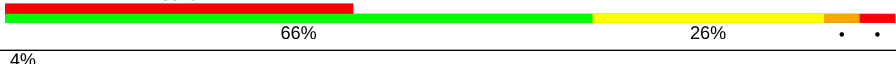
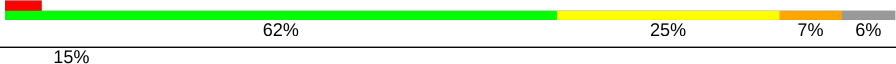

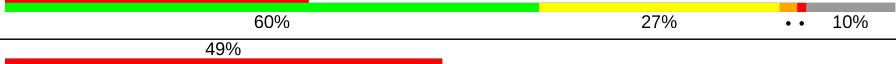


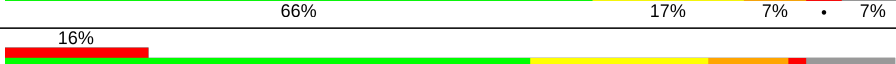



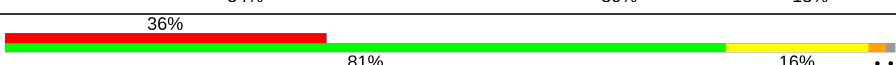
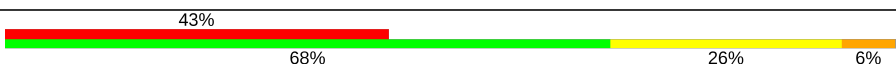
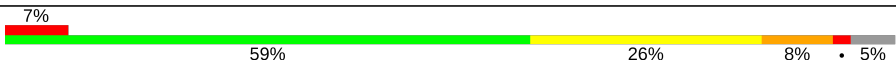
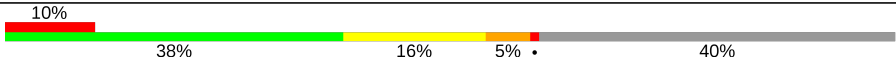


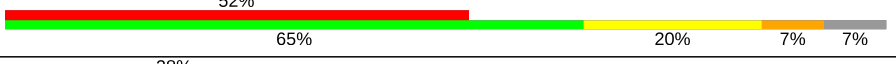
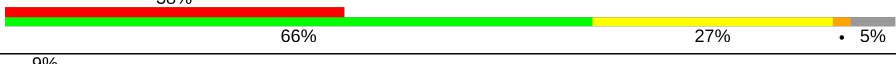


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1004 (10.00-3.90) |
| Ramachandran outliers | 138981 | 1002 (10.00-3.90) |
| Sidechain outliers | 138945 | 1002 (10.00-3.86) |
| RSRZ outliers | 127900 | 1004 (9.50-3.80) |
| RNA backbone | 3102 | 1078 (10.00-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 295 | <div> <div>14%</div> <div> <div>46%</div> <div>20%</div> <div>• •</div> <div>29%</div> </div> </div> |
| 2 | B | 264 | <div> <div>28%</div> <div> <div>55%</div> <div>23%</div> <div>•</div> <div>19%</div> </div> </div> |
| 3 | C | 278 | <div> <div>39%</div> <div> <div>58%</div> <div>20%</div> <div>• •</div> <div>19%</div> </div> </div> |
| 4 | D | 243 | <div> <div>68%</div> <div> <div>63%</div> <div>26%</div> <div>5%</div> <div>7%</div> </div> </div> |
| 5 | E | 263 | <div> <div>51%</div> <div> <div>66%</div> <div>29%</div> <div>•</div> </div> </div> |
| 6 | F | 204 | <div> <div>75%</div> <div> <div>66%</div> <div>21%</div> <div>• •</div> <div>6%</div> </div> </div> |


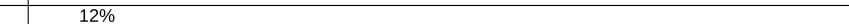

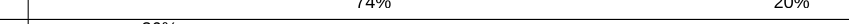

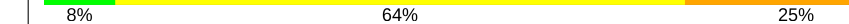
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 7 | G | 249 |  |
| 8 | H | 194 |  |
| 9 | I | 208 |  |
| 10 | J | 194 |  |
| 11 | K | 165 |  |
| 12 | L | 158 |  |
| 13 | M | 132 |  |
| 14 | N | 151 |  |
| 15 | O | 151 |  |
| 16 | P | 145 |  |
| 17 | Q | 146 |  |
| 18 | R | 135 |  |
| 19 | S | 152 |  |
| 20 | T | 145 |  |
| 21 | U | 119 |  |
| 22 | V | 83 |  |
| 23 | W | 130 |  |
| 24 | X | 143 |  |
| 25 | Y | 133 |  |
| 26 | Z | 125 |  |
| 27 | a | 115 |  |
| 28 | b | 84 |  |
| 29 | c | 69 |  |
| 30 | d | 56 |  |
| 31 | e | 133 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 32 | f | 156 |  |
| 33 | g | 317 |  |
| 34 | i | 1863 |  |
| 35 | j | 75 |  |
| 36 | k | 24 |  |
| 37 | n | 144 |  |

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 79048 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S Ribosomal Protein SA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1642 | 1045 | 289 | 300 | 8 | | | |

- Molecule 2 is a protein called 40S Ribosomal Protein S3A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 215 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1741 | 1107 | 309 | 310 | 15 | | | |

- Molecule 3 is a protein called 40S Ribosomal Protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 226 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1742 | 1127 | 300 | 306 | 9 | | | |

- Molecule 4 is a protein called 40S Ribosomal Protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | D | 227 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1764 | 1124 | 317 | 315 | 8 | | | |

- Molecule 5 is a protein called 40S Ribosomal Protein S4X.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5 | E | 263 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2083 | 1329 | 385 | 359 | 10 | | | |

- Molecule 6 is a protein called 40S Ribosomal Protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 191 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1509 | 943 | 286 | 273 | 7 | | | |

- Molecule 7 is a protein called 40S Ribosomal Protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7 | G | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1923 | 1200 | 387 | 329 | 7 | | | |

- Molecule 8 is a protein called 40S Ribosomal Protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | H | 190 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1530 | 975 | 281 | 273 | 1 | | | |

- Molecule 9 is a protein called 40S Ribosomal Protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 9 | I | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1679 | 1054 | 329 | 291 | 5 | | | |

- Molecule 10 is a protein called 40S Ribosomal Protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | J | 182 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1498 | 952 | 300 | 244 | 2 | | | |

- Molecule 11 is a protein called 40S Ribosomal Protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | K | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 827 | 539 | 148 | 134 | 6 | | | |

- Molecule 12 is a protein called 40S Ribosomal Protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | L | 158 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1296 | 827 | 241 | 221 | 7 | | | |

- Molecule 13 is a protein called 40S Ribosomal Protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | M | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 950 | 594 | 169 | 179 | 8 | | | |

- Molecule 14 is a protein called 40S Ribosomal Protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | N | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1208 | 773 | 229 | 205 | 1 | | | |

- Molecule 15 is a protein called 40S Ribosomal Protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | O | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1016 | 621 | 199 | 190 | 6 | | | |

- Molecule 16 is a protein called 40S Ribosomal Protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | P | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1060 | 673 | 201 | 179 | 7 | | | |

- Molecule 17 is a protein called 40S Ribosomal Protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | Q | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1124 | 715 | 212 | 194 | 3 | | | |

- Molecule 18 is a protein called 40S Ribosomal Protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | R | 126 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1019 | 639 | 188 | 187 | 5 | | | |

- Molecule 19 is a protein called 40S Ribosomal Protein S18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | S | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1139 | 714 | 231 | 193 | 1 | | | |

- Molecule 20 is a protein called 40S Ribosomal Protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | T | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 701 | 213 | 195 | 3 | | | |

- Molecule 21 is a protein called 40S Ribosomal Protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | U | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 822 | 514 | 156 | 148 | 4 | | | |

- Molecule 22 is a protein called 40S Ribosomal Protein S21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | V | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 619 | 378 | 117 | 119 | 5 | | | |

- Molecule 23 is a protein called 40S Ribosomal Protein S15A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | W | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1034 | 659 | 193 | 176 | 6 | | | |

- Molecule 24 is a protein called 40S Ribosomal Protein S23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | X | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1106 | 698 | 220 | 184 | 4 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| X | 1 | MET | ALA | SEE REMARK 999 | UNP G1SZ47 |

- Molecule 25 is a protein called 40S Ribosomal Protein S24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | Y | 126 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 645 | 198 | 173 | 5 | | | |

- Molecule 26 is a protein called 40S Ribosomal Protein S25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | Z | 75 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 598 | 382 | 111 | 104 | 1 | | | |

- Molecule 27 is a protein called 40S Ribosomal Protein S26.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | a | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 844 | 527 | 173 | 138 | 6 | | | |

- Molecule 28 is a protein called 40S Ribosomal Protein S27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | b | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 659 | 413 | 122 | 116 | 8 | | | |

- Molecule 29 is a protein called 40S Ribosomal Protein S28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 29 | c | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 506 | 308 | 102 | 94 | 2 | | | |

- Molecule 30 is a protein called 40S Ribosomal Protein S29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | d | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 445 | 278 | 90 | 72 | 5 | | | |

- Molecule 31 is a protein called 40S Ribosomal Protein S30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 31 | e | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 473 | 293 | 104 | 75 | 1 | | | |

- Molecule 32 is a protein called 40S Ribosomal Protein S27A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32 | f | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 367 | 109 | 98 | 7 | | | |

- Molecule 33 is a protein called 40S Ribosomal Protein RACK1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 33 | g | 313 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2436 | 1535 | 424 | 465 | 12 | | | |

- Molecule 34 is a RNA chain called 18S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 34 | i | 1797 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37514 | 16712 | 6634 | 12372 | 1796 | | | |

- Molecule 35 is a RNA chain called initiator Met-RNA-i.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 35 | j | 75 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1607 | 717 | 298 | 517 | 75 | | | |

- Molecule 36 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 36 | k | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 273 | 123 | 47 | 90 | 13 | | | |

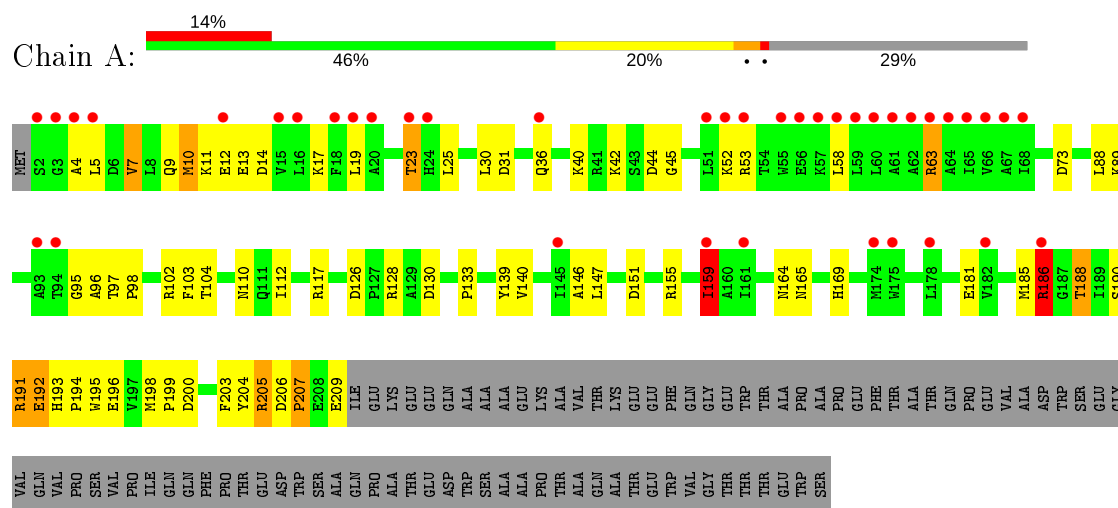
- Molecule 37 is a protein called human initiation factor eIF1A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | n | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 407 | 119 | 118 | 4 | | | |

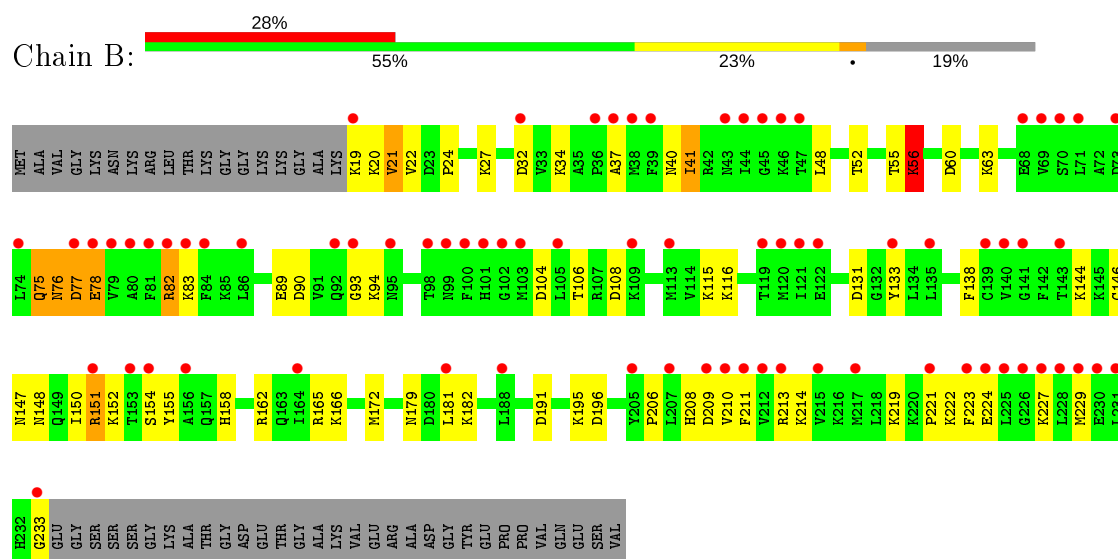
3 Residue-property plots

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

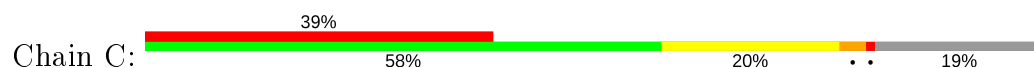
- Molecule 1: 40S Ribosomal Protein SA

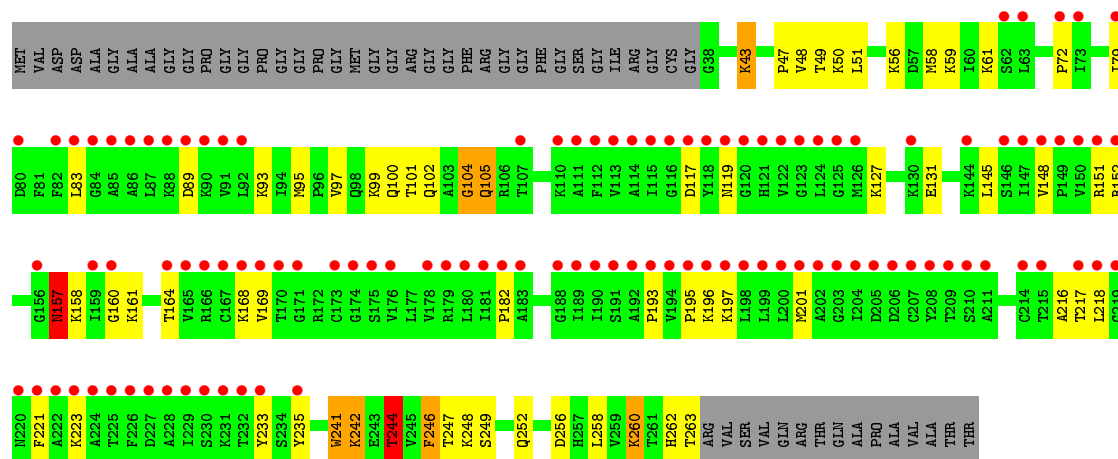


- Molecule 2: 40S Ribosomal Protein S3A

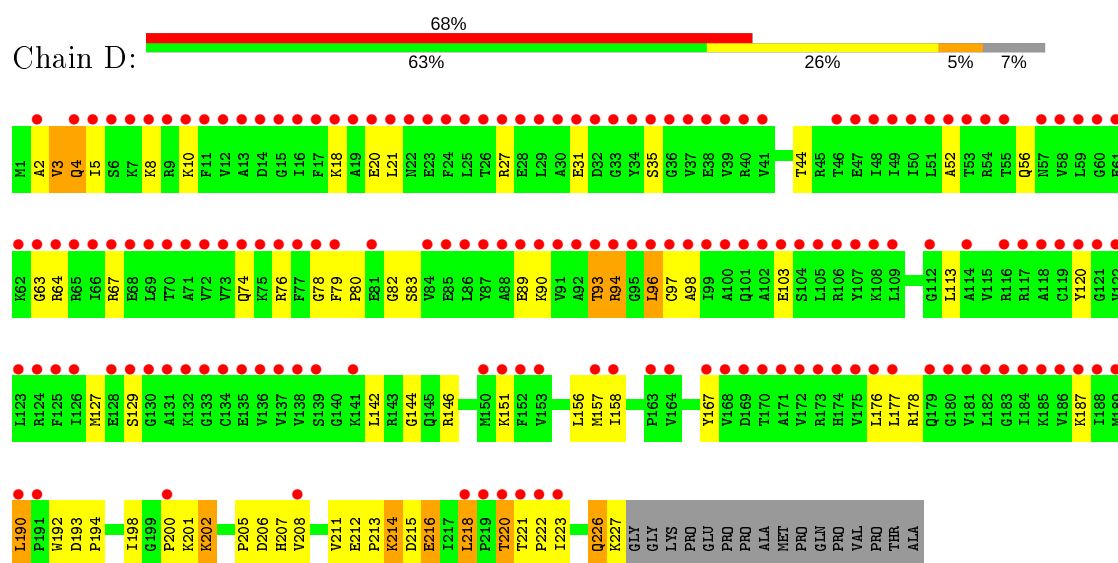


- Molecule 3: 40S Ribosomal Protein S2

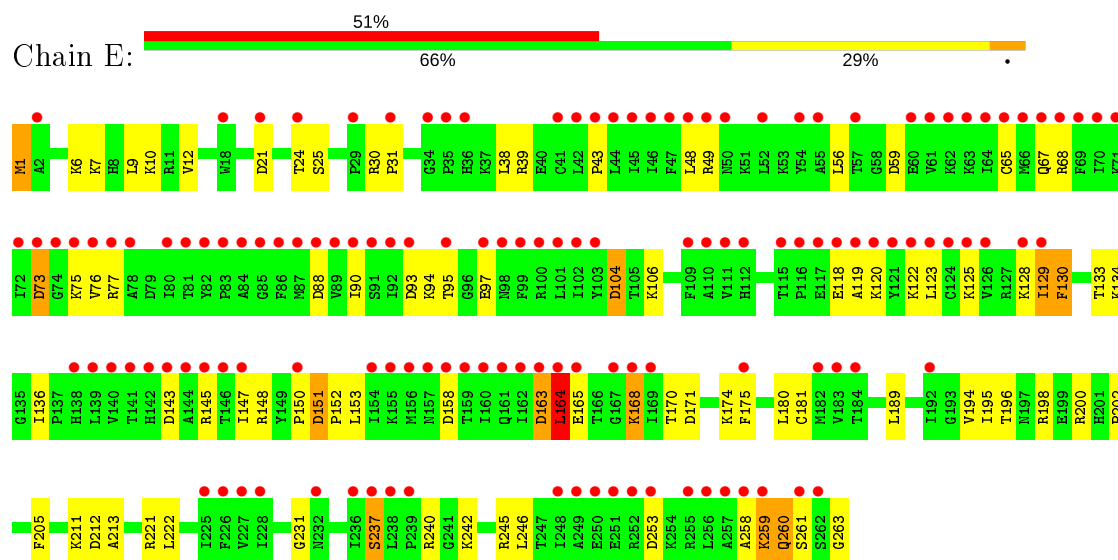




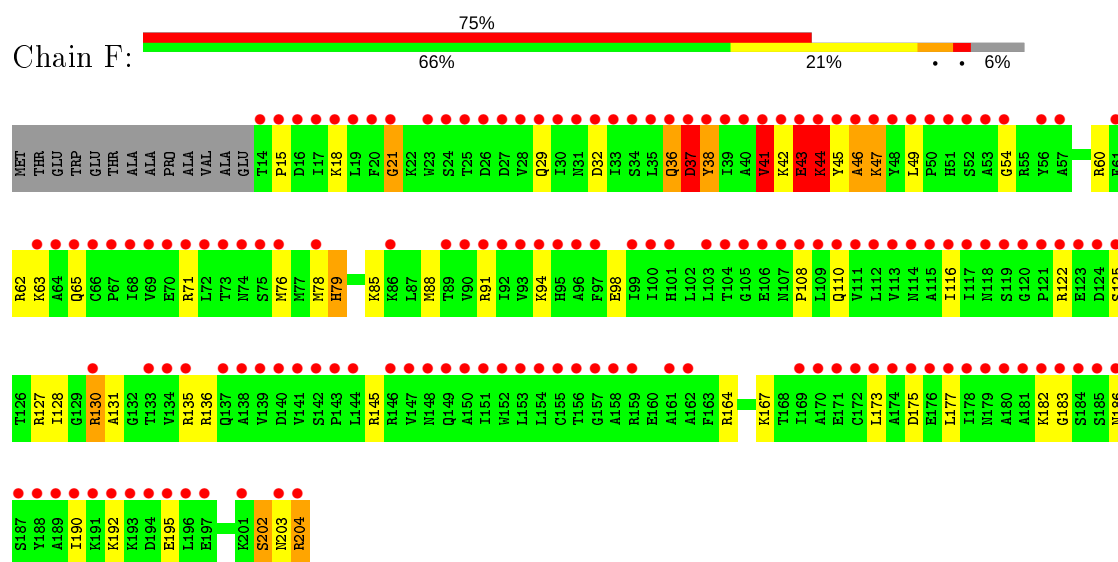
• Molecule 4: 40S Ribosomal Protein S3



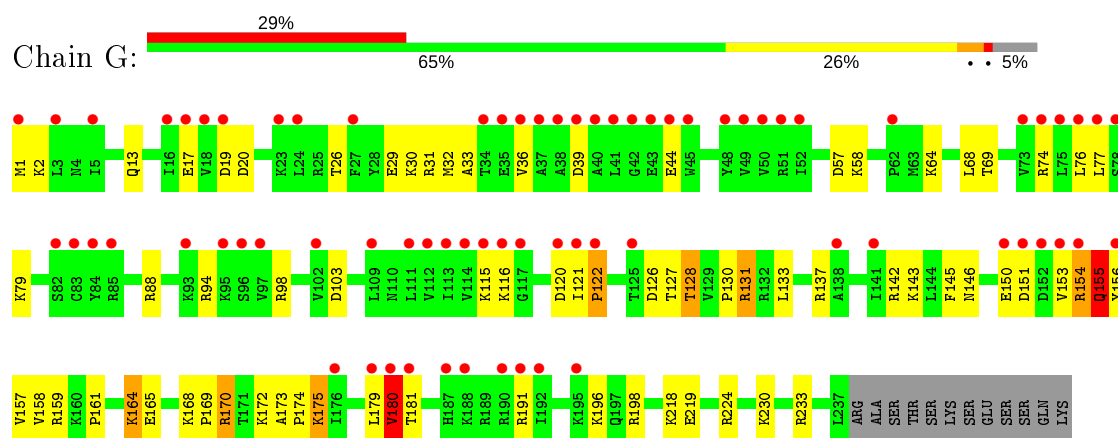
• Molecule 5: 40S Ribosomal Protein S4X



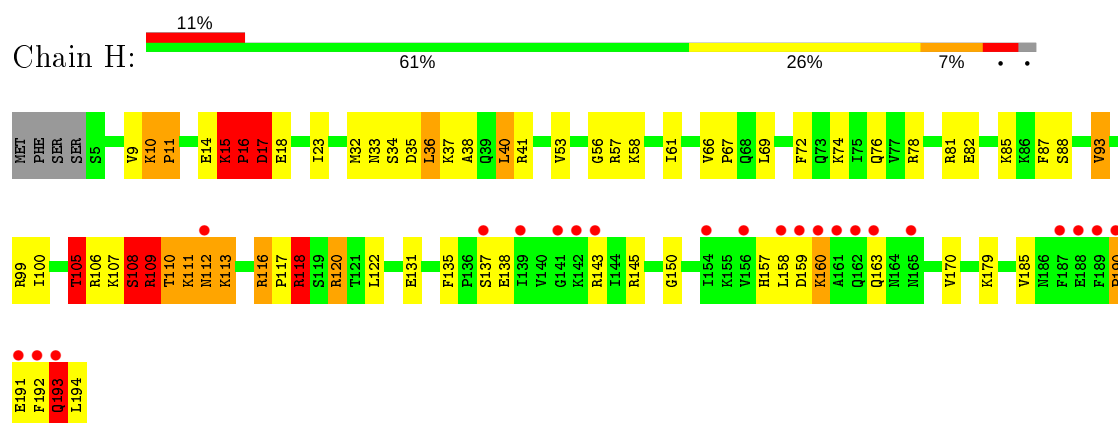
• Molecule 6: 40S Ribosomal Protein S5



- Molecule 7: 40S Ribosomal Protein S6

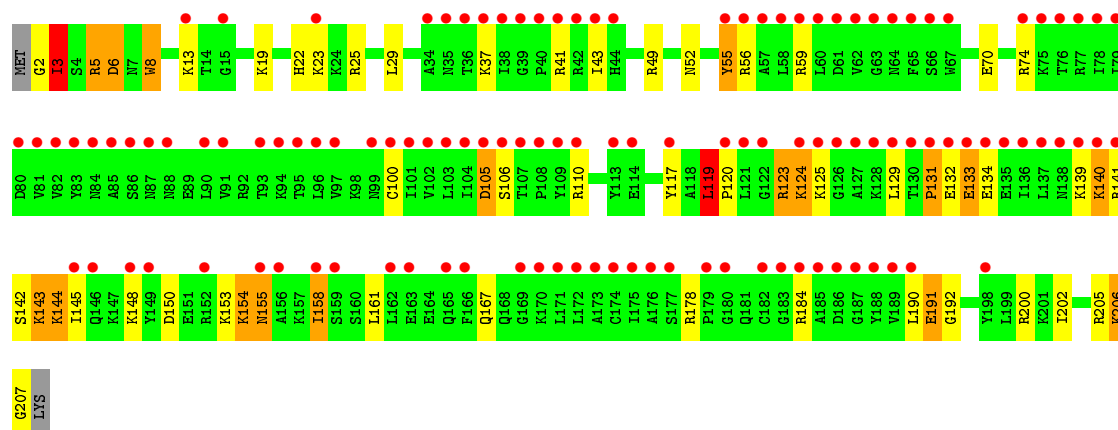


- Molecule 8: 40S Ribosomal Protein S7

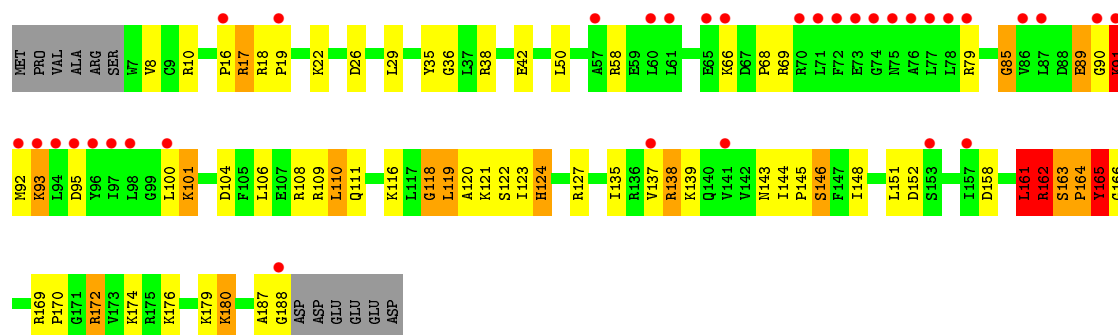


- Molecule 9: 40S Ribosomal Protein S8

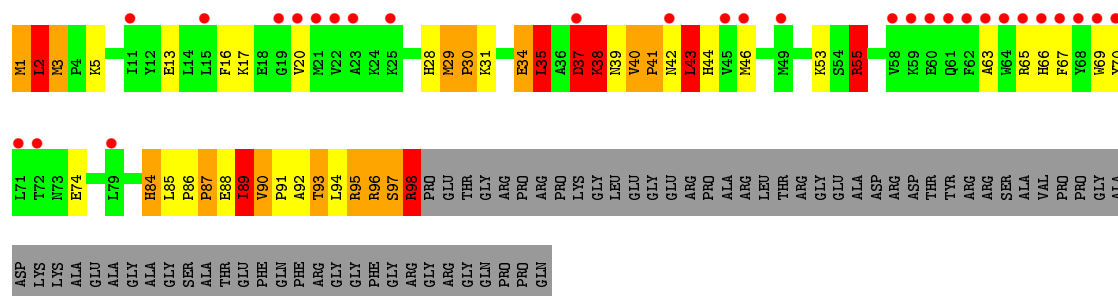
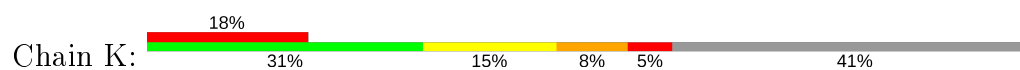




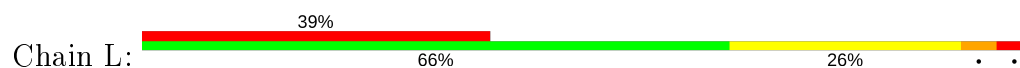
• Molecule 10: 40S Ribosomal Protein S9

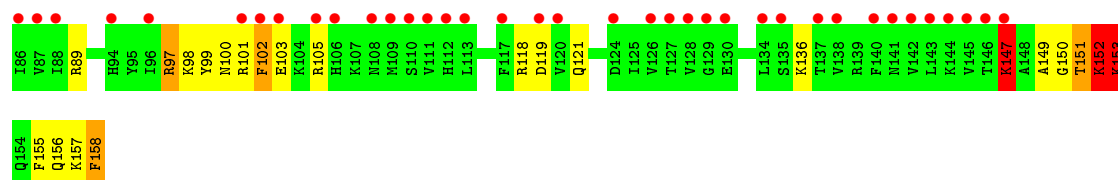


• Molecule 11: 40S Ribosomal Protein S10

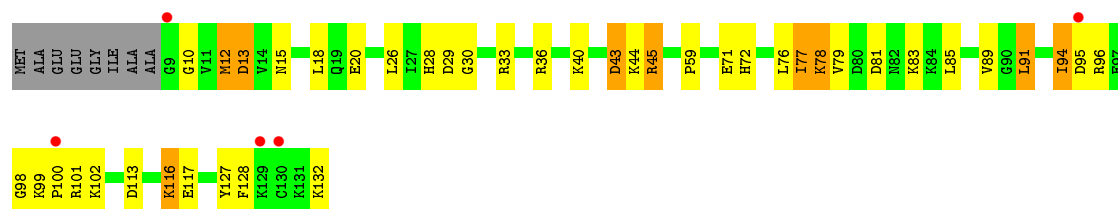


• Molecule 12: 40S Ribosomal Protein S11

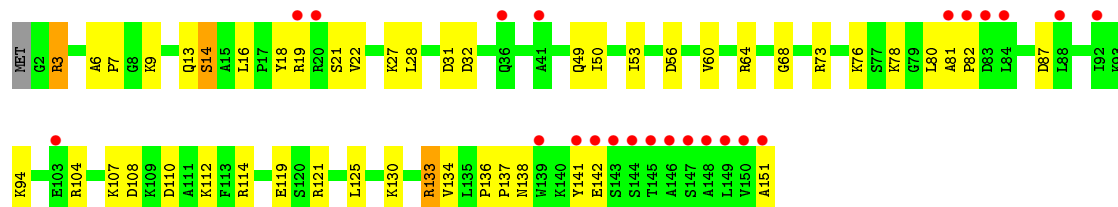




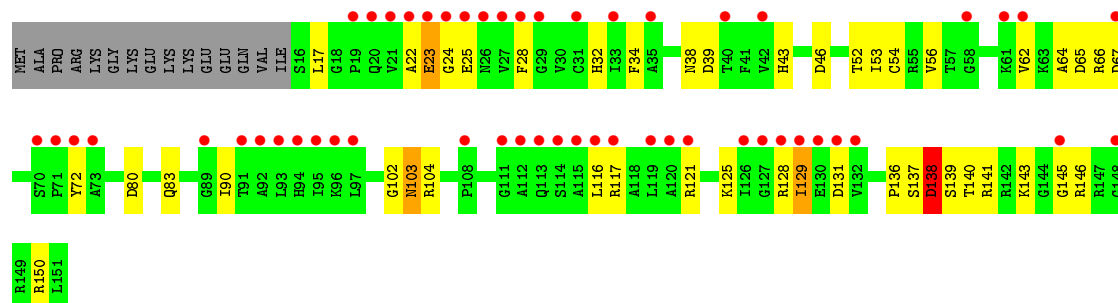
• Molecule 13: 40S Ribosomal Protein S12



• Molecule 14: 40S Ribosomal Protein S13

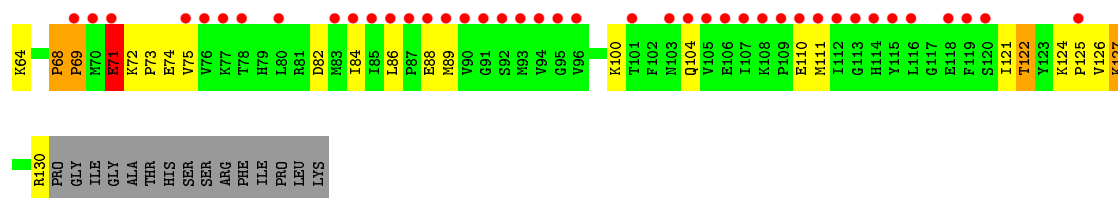


• Molecule 15: 40S Ribosomal Protein S14

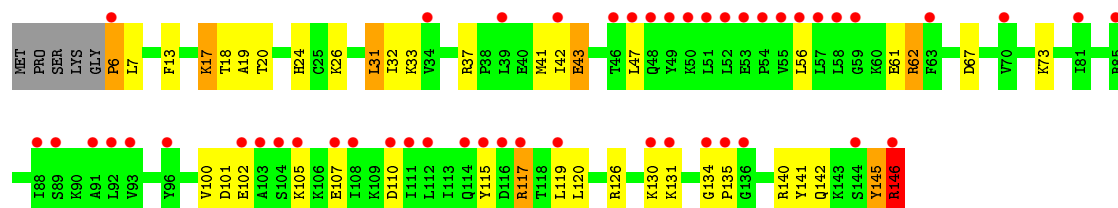


• Molecule 16: 40S Ribosomal Protein S15

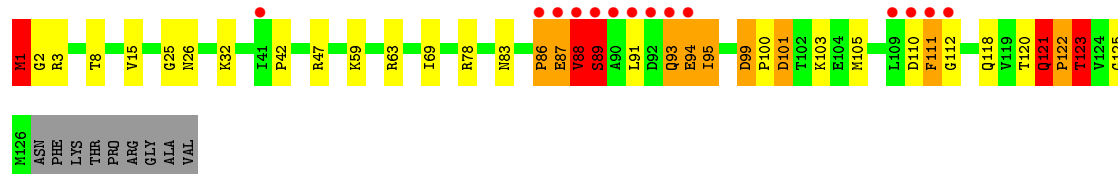




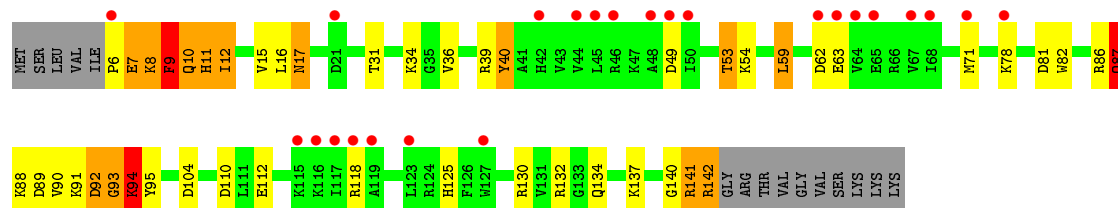
- Molecule 17: 40S Ribosomal Protein S16



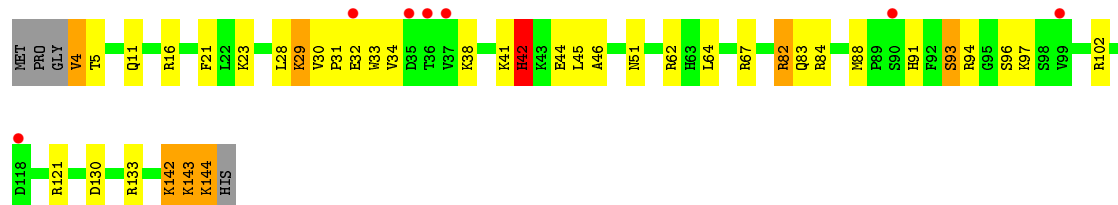
- Molecule 18: 40S Ribosomal Protein S17



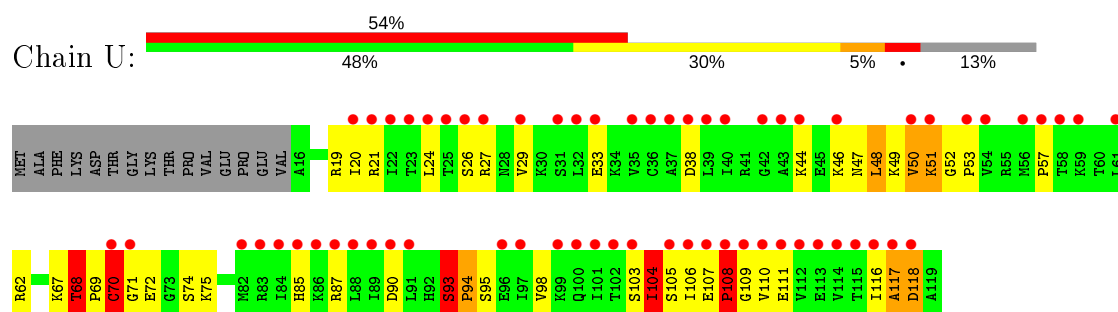
- Molecule 19: 40S Ribosomal Protein S18



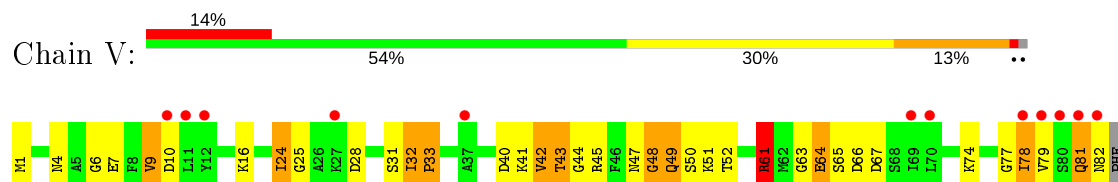
- Molecule 20: 40S Ribosomal Protein S19



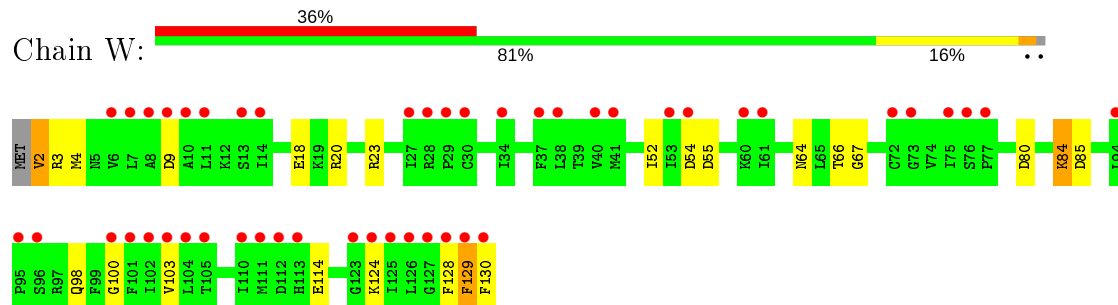
- Molecule 21: 40S Ribosomal Protein S20



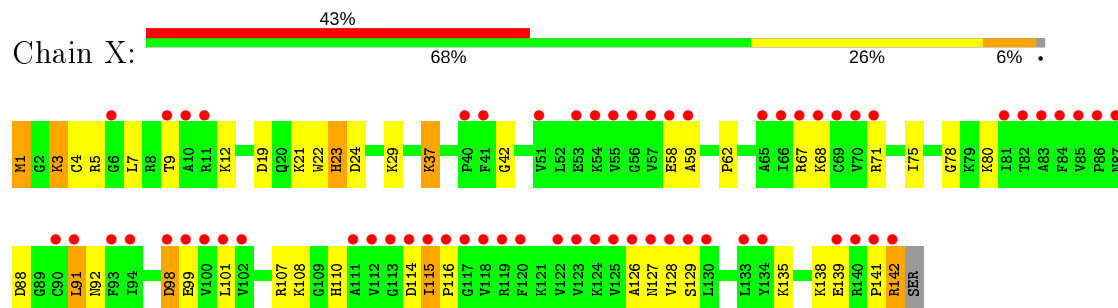
- Molecule 22: 40S Ribosomal Protein S21



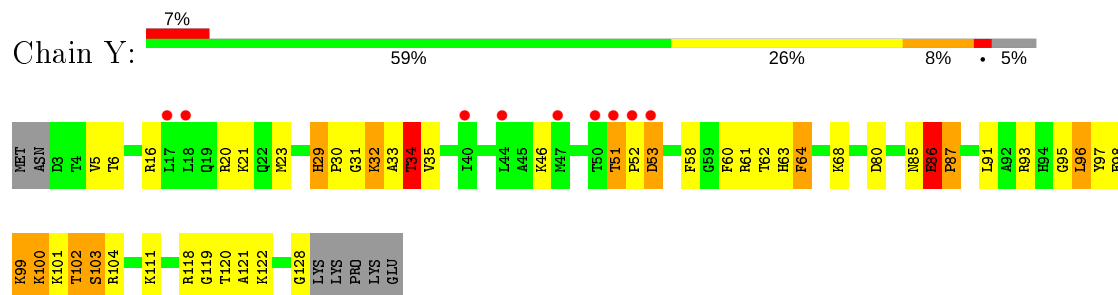
- Molecule 23: 40S Ribosomal Protein S15A



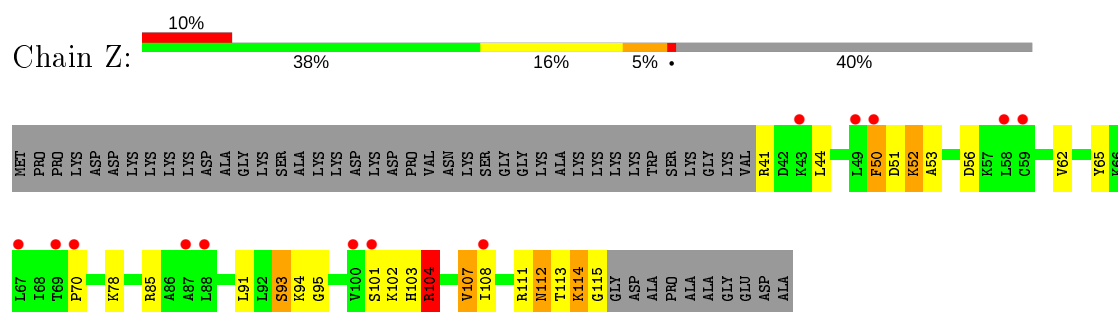
- Molecule 24: 40S Ribosomal Protein S23



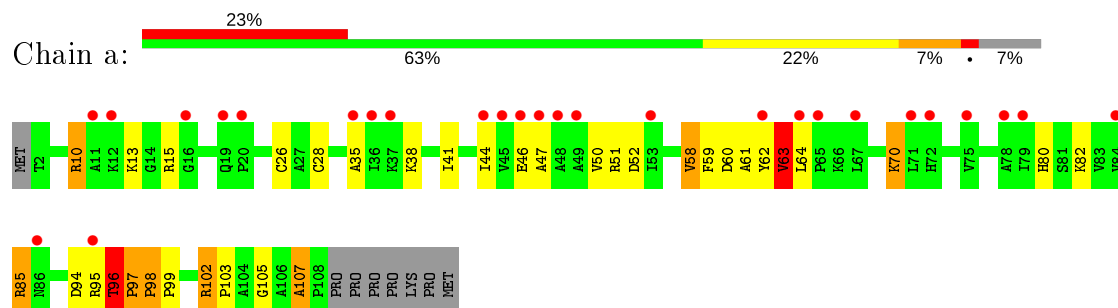
- Molecule 25: 40S Ribosomal Protein S24



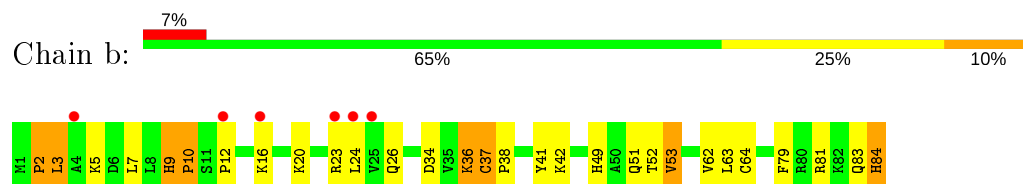
- Molecule 26: 40S Ribosomal Protein S25



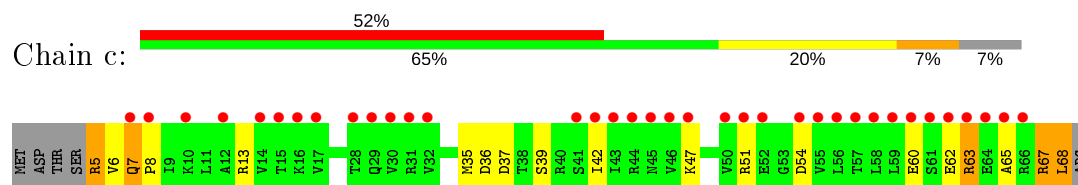
- Molecule 27: 40S Ribosomal Protein S26



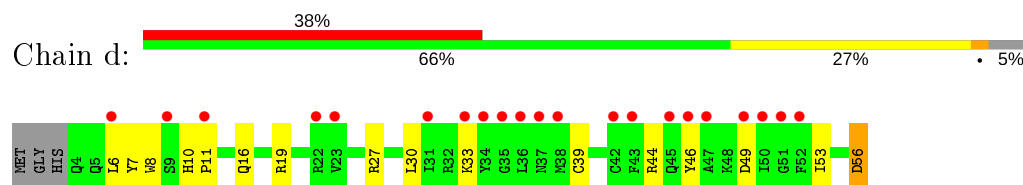
- Molecule 28: 40S Ribosomal Protein S27



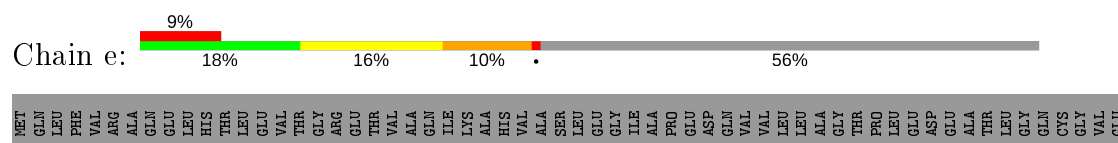
- Molecule 29: 40S Ribosomal Protein S28

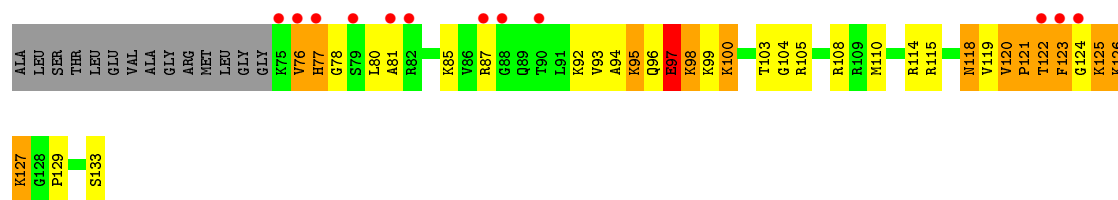


- Molecule 30: 40S Ribosomal Protein S29

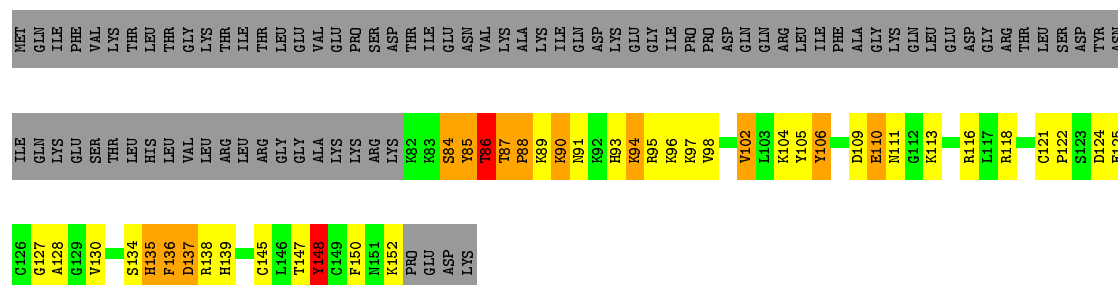
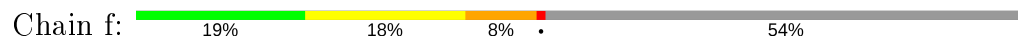


- Molecule 31: 40S Ribosomal Protein S30

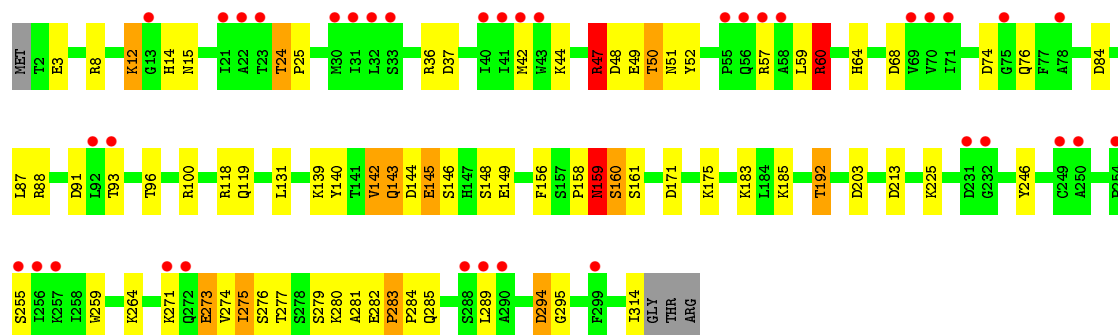
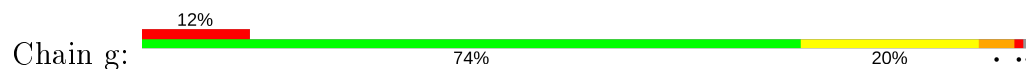




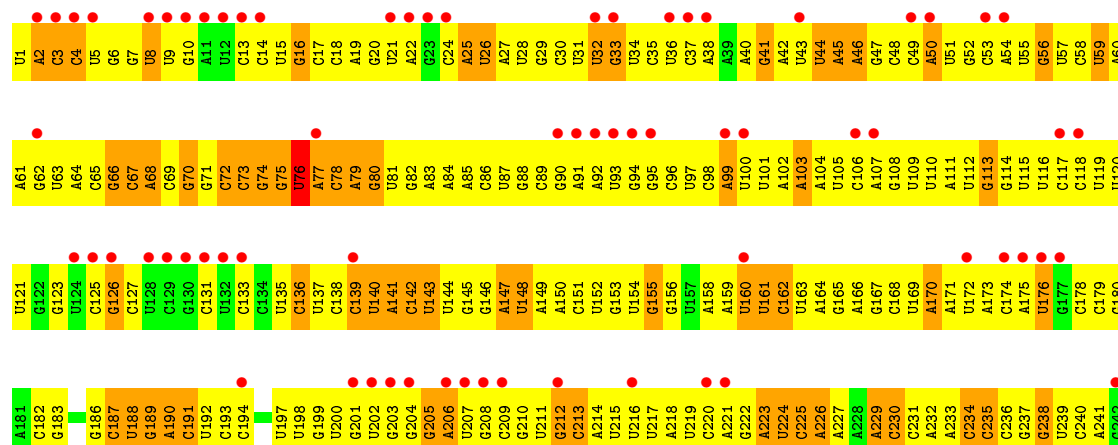
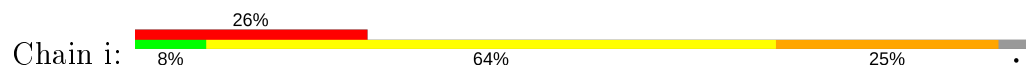
• Molecule 32: 40S Ribosomal Protein S27A



• Molecule 33: 40S Ribosomal Protein RACK1



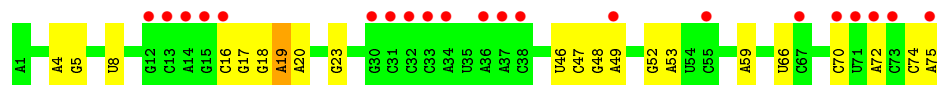
• Molecule 34: 18S Ribosomal RNA



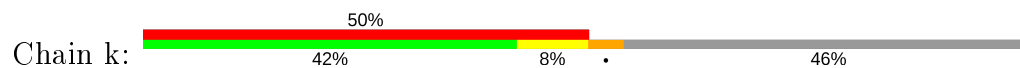


| | | | | | | | | | |
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| A1816 | G1756 | A1636 | A1574 | G1454 | G1334 | A1274 | G1214 | U1152 | G1092 |
| A1817 | G1757 | U1637 | A1575 | G1455 | U1335 | C1275 | C1215 | G1153 | G1093 |
| A1818 | G1698 | U1638 | A1576 | G1456 | U1336 | C1276 | A1216 | G1154 | C1094 |
| A1819 | C1699 | C1639 | C1577 | G1457 | A1517 | G1277 | G1217 | | G1095 |
| G1820 | C1760 | C1640 | C1578 | U1458 | A1398 | U1338 | G1218 | U1157 | A1096 |
| G1821 | C1761 | C1641 | C1579 | U1459 | U1339 | C1278 | A1219 | C1158 | U1097 |
| G1822 | A1762 | A1642 | U1580 | C1460 | U1340 | A1279 | G1220 | C1159 | G1098 |
| G1823 | G1763 | G1643 | U1581 | C1461 | G1341 | A1280 | U1221 | G1160 | C1099 |
| G1824 | G1764 | U1644 | G1582 | G1462 | U1342 | G1281 | G1222 | G1161 | G1100 |
| A1825 | G1765 | A1645 | C1583 | C1463 | U1343 | A1283 | G1223 | G1162 | G1101 |
| A1826 | C1766 | A1646 | A1584 | C1464 | G1344 | U1284 | A1224 | G1163 | C1102 |
| A1827 | G1767 | G1647 | C1585 | A1465 | G1345 | U1285 | G1225 | G1164 | G1103 |
| A1828 | U1648 | U1648 | C1586 | C1466 | U1346 | G1286 | G1226 | G1165 | G1104 |
| A1829 | G1649 | G1649 | C1587 | C1467 | G1347 | A1287 | C1227 | A1166 | C1105 |
| G1830 | G1770 | C1650 | A1588 | C1468 | G1348 | C1288 | U1228 | G1167 | G1106 |
| G1831 | G1771 | G1651 | A1589 | C1469 | U1349 | A1289 | G1229 | U1168 | U1107 |
| U1832 | C1772 | G1652 | U1590 | A1470 | A1410 | G1290 | C1230 | A1169 | U1108 |
| U1833 | G1773 | G1653 | U1591 | C1471 | C1411 | A1291 | G1231 | U1170 | A1109 |
| U1834 | G1774 | U1654 | C1592 | A1472 | C1412 | U1292 | G1232 | G1171 | U1110 |
| C1835 | A1775 | C1655 | G1593 | U1473 | C1413 | U1293 | C1233 | G1172 | U1111 |
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| G1837 | C1777 | U1657 | G1595 | G1475 | U1355 | A1295 | U1235 | U1174 | C1113 |
| U1838 | G1778 | A1658 | A1596 | A1476 | U1356 | U1296 | A1236 | G1175 | C1114 |
| A1839 | C1779 | A1659 | U1597 | G1477 | G1357 | A1297 | A1237 | C1176 | A1115 |
| G1840 | U1780 | G1660 | G1598 | C1478 | U1358 | G1298 | U1238 | A1177 | U1116 |
| G1841 | G1781 | C1661 | G1599 | A1479 | C1359 | C1299 | U1239 | G1178 | G1117 |
| U1842 | A1782 | U1662 | G1600 | U1480 | U1360 | U1300 | U1240 | | A1118 |
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| A1845 | G1785 | C1665 | G1603 | C1483 | C1363 | U1303 | C1243 | G1183 | C1121 |
| C1846 | G1786 | G1666 | U1604 | C1484 | U1364 | U1304 | U1244 | A1184 | G1122 |
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| G1849 | G1789 | G1669 | G1607 | G1487 | C1367 | C1307 | A1247 | C1187 | G1125 |
| C1850 | G1790 | A1670 | U1608 | U1488 | G1368 | G1308 | C1248 | U1188 | G1126 |
| G1851 | U1791 | U1671 | A1609 | C1489 | C1369 | A1309 | A1249 | U1189 | G1127 |
| G1852 | G1792 | U1672 | U1610 | U1490 | C1370 | U1310 | C1250 | A1190 | C1128 |
| A1853 | G1793 | A1673 | A1611 | G1491 | G1371 | U1311 | G1251 | A1191 | A1129 |
| A1854 | A1794 | U1674 | C1552 | U1492 | A1372 | C1312 | G1252 | A1192 | G1130 |
| G1855 | A1795 | G1675 | C1553 | G1493 | U1373 | U1313 | G1253 | G1193 | C1131 |
| G1856 | C1796 | U1676 | A1554 | A1494 | A1374 | G1314 | A1254 | G1194 | U1132 |
| A1857 | U1797 | C1677 | U1555 | U1495 | U1375 | U1315 | A1255 | A1195 | U1133 |
| U1858 | U1798 | C1678 | A1556 | G1496 | C1376 | G1316 | A1256 | A1196 | G1134 |
| C1859 | G1799 | C1679 | C1557 | C1497 | G1377 | G1317 | C1257 | U1197 | C1135 |
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| U1861 | C1801 | G1681 | C1559 | C1499 | A1379 | U1319 | U1259 | G1199 | G1137 |
| U1862 | U1802 | C1682 | C1560 | U1500 | C1380 | G1320 | C1260 | A1200 | G1138 |
| A1863 | A1803 | C1683 | G1561 | U1501 | U1441 | G1321 | A1261 | C1201 | A1139 |
| | U1804 | C1684 | C1624 | A1502 | A1442 | U1322 | C1262 | G1202 | A1140 |
| | C1805 | U1685 | G1563 | G1503 | G1443 | G1323 | C1263 | G1203 | A1141 |
| | U1806 | U1686 | A1564 | A1504 | A1383 | G1324 | C1264 | A1204 | C1142 |
| | G1746 | U1687 | G1627 | U1505 | A1384 | U1325 | G1265 | A1205 | C1143 |
| | A1807 | G1688 | A1628 | G1506 | C1385 | G1326 | G1266 | G1206 | A1144 |
| | G1808 | C1689 | C1567 | U1507 | U1386 | C1327 | C1267 | G1207 | A1145 |
| | A1809 | U1689 | A1529 | C1508 | U1387 | A1328 | G1268 | G1208 | A1146 |
| | G1810 | A1690 | G1630 | G1509 | U1388 | U1329 | C1269 | C1209 | G1147 |
| | G1811 | C1691 | G1631 | G1510 | C1389 | G1330 | G1270 | A1210 | U1148 |
| | A1812 | A1692 | A1632 | G1511 | G1390 | G1331 | G1271 | C1211 | C1149 |
| | A1813 | G1693 | G1633 | G1512 | A1391 | C1332 | A1272 | C1212 | U1150 |
| | G1814 | A1694 | G1634 | G1513 | C1392 | C1333 | | A1213 | U1151 |
| | U1815 | C1695 | U1573 | C1513 | U1393 | | | | |

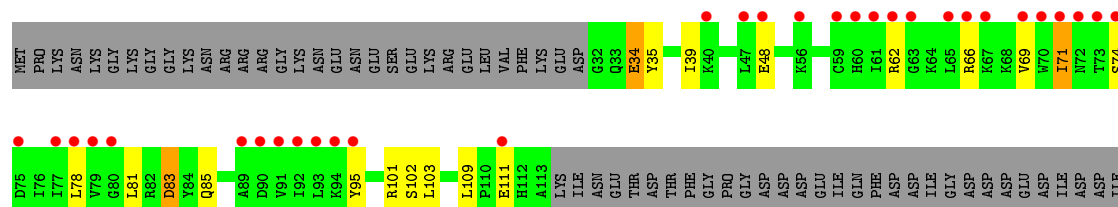
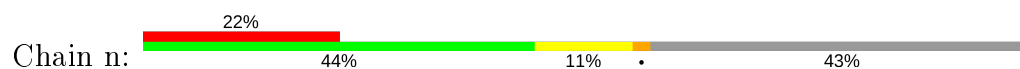
- Molecule 35: initiator Met-RNA-i



- Molecule 36: mRNA



- Molecule 37: human initiation factor eIF1A



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 31 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 297.75Å 297.75Å 485.16Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 77.53 – 7.03 77.53 – 7.03 | Depositor EDS |
| % Data completeness (in resolution range) | 98.3 (77.53-7.03) 98.7 (77.53-7.03) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.98 (at 6.72Å) | Xtriage |
| Refinement program | PHENIX 1.7.3_928 | Depositor |
| R, R_{free} | 0.345 , 0.359 0.339 , 0.343 | Depositor DCC |
| R_{free} test set | 1946 reflections (5.01%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 566.4 | Xtriage |
| Anisotropy | 0.159 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.22 , 125.0 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$ | Xtriage |
| Estimated twinning fraction | 0.055 for -h,-k,l | Xtriage |
| F_o, F_c correlation | 0.86 | EDS |
| Total number of atoms | 79048 | wwPDB-VP |
| Average B, all atoms (Å ²) | 179.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|-------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.76 | 2/1679 (0.1%) | 1.06 | 17/2283 (0.7%) |
| 2 | B | 0.79 | 7/1769 (0.4%) | 1.08 | 22/2367 (0.9%) |
| 3 | C | 0.97 | 7/1778 (0.4%) | 1.19 | 18/2399 (0.8%) |
| 4 | D | 1.03 | 6/1792 (0.3%) | 1.30 | 22/2412 (0.9%) |
| 5 | E | 0.76 | 5/2125 (0.2%) | 0.98 | 23/2856 (0.8%) |
| 6 | F | 0.99 | 5/1531 (0.3%) | 1.21 | 17/2059 (0.8%) |
| 7 | G | 0.97 | 15/1946 (0.8%) | 1.23 | 25/2590 (1.0%) |
| 8 | H | 1.09 | 7/1553 (0.5%) | 2.19 | 29/2079 (1.4%) |
| 9 | I | 1.11 | 7/1708 (0.4%) | 1.51 | 33/2278 (1.4%) |
| 10 | J | 1.27 | 19/1522 (1.2%) | 1.51 | 42/2031 (2.1%) |
| 11 | K | 1.21 | 6/851 (0.7%) | 1.78 | 31/1147 (2.7%) |
| 12 | L | 1.10 | 6/1319 (0.5%) | 1.40 | 17/1761 (1.0%) |
| 13 | M | 1.00 | 3/960 (0.3%) | 1.23 | 7/1287 (0.5%) |
| 14 | N | 0.83 | 4/1232 (0.3%) | 1.01 | 12/1656 (0.7%) |
| 15 | O | 0.61 | 0/1029 | 1.05 | 12/1380 (0.9%) |
| 16 | P | 0.75 | 1/1079 (0.1%) | 1.43 | 32/1437 (2.2%) |
| 17 | Q | 0.71 | 3/1142 (0.3%) | 1.11 | 15/1528 (1.0%) |
| 18 | R | 1.23 | 10/1031 (1.0%) | 1.64 | 30/1383 (2.2%) |
| 19 | S | 1.21 | 10/1157 (0.9%) | 1.61 | 36/1548 (2.3%) |
| 20 | T | 0.95 | 3/1132 (0.3%) | 1.26 | 13/1517 (0.9%) |
| 21 | U | 0.96 | 1/832 (0.1%) | 1.59 | 29/1117 (2.6%) |
| 22 | V | 0.75 | 1/626 (0.2%) | 1.39 | 15/839 (1.8%) |
| 23 | W | 0.85 | 4/1051 (0.4%) | 0.86 | 9/1406 (0.6%) |
| 24 | X | 1.00 | 8/1124 (0.7%) | 1.24 | 21/1500 (1.4%) |
| 25 | Y | 0.93 | 3/1038 (0.3%) | 1.42 | 21/1380 (1.5%) |
| 26 | Z | 1.04 | 5/604 (0.8%) | 1.35 | 17/810 (2.1%) |
| 27 | a | 0.89 | 4/860 (0.5%) | 1.60 | 21/1156 (1.8%) |
| 28 | b | 1.02 | 2/673 (0.3%) | 1.36 | 12/902 (1.3%) |
| 29 | c | 0.80 | 1/508 (0.2%) | 1.18 | 8/680 (1.2%) |
| 30 | d | 0.90 | 2/455 (0.4%) | 0.79 | 3/603 (0.5%) |
| 31 | e | 1.47 | 5/478 (1.0%) | 1.43 | 11/628 (1.8%) |
| 32 | f | 1.10 | 4/593 (0.7%) | 1.49 | 16/786 (2.0%) |
| 33 | g | 0.91 | 1/2493 (0.0%) | 1.29 | 27/3394 (0.8%) |
| 34 | i | 2.41 | 1848/41879 (4.4%) | 2.21 | 2565/65157 (3.9%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 35 | j | 0.67 | 5/1798 (0.3%) | 0.82 | 0/2802 |
| 36 | k | 1.64 | 1/304 (0.3%) | 1.35 | 3/470 (0.6%) |
| 37 | n | 0.40 | 0/657 | 0.38 | 0/881 |
| All | All | 1.83 | 2021/84308 (2.4%) | 1.84 | 3231/122509 (2.6%) |

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 |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 11 |
| 2 | B | 0 | 4 |
| 3 | C | 1 | 5 |
| 4 | D | 0 | 5 |
| 5 | E | 1 | 2 |
| 6 | F | 0 | 3 |
| 7 | G | 0 | 1 |
| 8 | H | 0 | 10 |
| 9 | I | 0 | 8 |
| 10 | J | 1 | 11 |
| 11 | K | 0 | 11 |
| 12 | L | 0 | 7 |
| 13 | M | 0 | 1 |
| 14 | N | 0 | 4 |
| 15 | O | 0 | 1 |
| 16 | P | 0 | 10 |
| 17 | Q | 0 | 4 |
| 18 | R | 1 | 5 |
| 19 | S | 1 | 10 |
| 20 | T | 1 | 6 |
| 21 | U | 0 | 8 |
| 22 | V | 0 | 9 |
| 23 | W | 0 | 2 |
| 24 | X | 0 | 4 |
| 25 | Y | 1 | 6 |
| 26 | Z | 0 | 6 |
| 27 | a | 0 | 2 |
| 28 | b | 0 | 3 |
| 31 | e | 0 | 5 |
| 32 | f | 0 | 6 |
| 33 | g | 0 | 13 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 34 | i | 6 | 0 |
| All | All | 13 | 183 |

All (2021) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 36 | k | 22 | C | C1'-N1 | 28.08 | 1.90 | 1.48 |
| 34 | i | 1322 | U | C2'-C1' | -25.56 | 1.25 | 1.53 |
| 34 | i | 66 | G | C2'-C1' | -24.65 | 1.26 | 1.53 |
| 34 | i | 652 | G | C2'-C1' | -23.81 | 1.27 | 1.53 |
| 34 | i | 858 | A | C2'-C1' | -23.76 | 1.27 | 1.53 |
| 34 | i | 1307 | C | C2'-C1' | -22.20 | 1.28 | 1.53 |
| 34 | i | 521 | A | C2'-C1' | -22.14 | 1.28 | 1.53 |
| 34 | i | 1037 | G | C2'-C1' | -21.86 | 1.29 | 1.53 |
| 34 | i | 145 | G | C2'-C1' | -21.62 | 1.29 | 1.53 |
| 34 | i | 1233 | C | C2'-C1' | -21.47 | 1.29 | 1.53 |
| 34 | i | 287 | U | C2'-C1' | -21.27 | 1.29 | 1.53 |
| 4 | D | 5 | ILE | C-N | 21.22 | 1.82 | 1.34 |
| 34 | i | 1327 | C | C2'-C1' | -20.67 | 1.30 | 1.53 |
| 34 | i | 1393 | U | C2'-C1' | -20.58 | 1.30 | 1.53 |
| 34 | i | 299 | G | C2'-C1' | -20.54 | 1.30 | 1.53 |
| 34 | i | 215 | U | C2'-C1' | -20.29 | 1.31 | 1.53 |
| 34 | i | 1503 | G | O4'-C1' | -19.98 | 1.15 | 1.41 |
| 34 | i | 630 | A | C2'-C1' | -19.72 | 1.31 | 1.53 |
| 34 | i | 343 | C | C2'-C1' | -19.71 | 1.31 | 1.53 |
| 34 | i | 1407 | G | C2'-C1' | -19.57 | 1.31 | 1.53 |
| 34 | i | 612 | C | C2'-C1' | -19.42 | 1.31 | 1.53 |
| 34 | i | 1855 | G | C2'-C1' | -19.41 | 1.31 | 1.53 |
| 34 | i | 1738 | G | C2'-C1' | -19.35 | 1.32 | 1.53 |
| 34 | i | 956 | U | C2'-C1' | -19.28 | 1.32 | 1.53 |
| 34 | i | 1308 | G | C2'-C1' | -19.27 | 1.32 | 1.53 |
| 34 | i | 684 | A | C2'-C1' | -18.94 | 1.32 | 1.53 |
| 34 | i | 1496 | G | C2'-C1' | -18.90 | 1.32 | 1.53 |
| 34 | i | 1159 | C | C2'-C1' | -18.73 | 1.32 | 1.53 |
| 34 | i | 1227 | C | C2'-C1' | -18.72 | 1.32 | 1.53 |
| 31 | e | 95 | LYS | C-N | 18.50 | 1.76 | 1.34 |
| 34 | i | 1194 | G | C2'-C1' | -18.46 | 1.33 | 1.53 |
| 34 | i | 518 | A | C2'-C1' | -18.41 | 1.33 | 1.53 |
| 34 | i | 1222 | G | C2'-C1' | -17.91 | 1.33 | 1.53 |
| 34 | i | 443 | C | C2'-C1' | -17.87 | 1.33 | 1.53 |
| 34 | i | 859 | U | C2'-C1' | -17.81 | 1.33 | 1.53 |
| 34 | i | 1774 | G | C2'-C1' | -17.75 | 1.33 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 1226 | C | C2'-C1' | -17.72 | 1.33 | 1.53 |
| 34 | i | 606 | A | C2'-C1' | -17.50 | 1.34 | 1.53 |
| 34 | i | 41 | G | C2'-C1' | -17.44 | 1.34 | 1.53 |
| 34 | i | 1199 | G | C2'-C1' | -17.43 | 1.34 | 1.53 |
| 34 | i | 1010 | G | C2'-C1' | -17.43 | 1.34 | 1.53 |
| 34 | i | 1279 | C | O4'-C1' | 17.42 | 1.64 | 1.41 |
| 34 | i | 389 | C | O4'-C1' | 17.37 | 1.64 | 1.41 |
| 34 | i | 1472 | A | O4'-C1' | -17.21 | 1.19 | 1.41 |
| 34 | i | 984 | C | O4'-C1' | 17.19 | 1.64 | 1.41 |
| 10 | J | 118 | GLY | C-N | 17.15 | 1.73 | 1.34 |
| 34 | i | 1214 | C | C2'-C1' | -17.07 | 1.34 | 1.53 |
| 34 | i | 1348 | G | C2'-C1' | -16.88 | 1.34 | 1.53 |
| 34 | i | 1258 | C | C2'-C1' | -16.87 | 1.34 | 1.53 |
| 34 | i | 1044 | G | C2'-C1' | -16.84 | 1.34 | 1.53 |
| 34 | i | 1233 | C | O4'-C1' | 16.77 | 1.63 | 1.41 |
| 10 | J | 85 | GLY | C-N | -16.75 | 0.95 | 1.34 |
| 34 | i | 1732 | G | C2'-C1' | -16.74 | 1.34 | 1.53 |
| 34 | i | 838 | C | C2'-C1' | -16.70 | 1.34 | 1.53 |
| 34 | i | 929 | G | C2'-C1' | -16.68 | 1.35 | 1.53 |
| 34 | i | 94 | G | C2'-C1' | -16.68 | 1.35 | 1.53 |
| 34 | i | 626 | C | O4'-C1' | 16.66 | 1.63 | 1.41 |
| 34 | i | 604 | G | C2'-C1' | -16.65 | 1.35 | 1.53 |
| 34 | i | 844 | U | C2'-C1' | -16.58 | 1.35 | 1.53 |
| 34 | i | 1467 | C | O4'-C1' | 16.57 | 1.63 | 1.41 |
| 34 | i | 1733 | C | O4'-C1' | 16.43 | 1.63 | 1.41 |
| 34 | i | 1308 | G | O4'-C1' | 16.43 | 1.63 | 1.41 |
| 34 | i | 435 | A | C2'-C1' | -16.41 | 1.35 | 1.53 |
| 18 | R | 1 | MET | N-CA | 16.34 | 1.79 | 1.46 |
| 34 | i | 1043 | C | O4'-C1' | 16.34 | 1.62 | 1.41 |
| 34 | i | 92 | A | C2'-C1' | -16.34 | 1.35 | 1.53 |
| 34 | i | 1325 | U | C2'-C1' | -16.28 | 1.35 | 1.53 |
| 34 | i | 689 | G | O4'-C1' | 16.27 | 1.62 | 1.41 |
| 34 | i | 611 | C | O4'-C1' | 16.26 | 1.62 | 1.41 |
| 34 | i | 1571 | G | C2'-C1' | -16.25 | 1.35 | 1.53 |
| 34 | i | 604 | G | O4'-C1' | 16.21 | 1.62 | 1.41 |
| 34 | i | 446 | C | C2'-C1' | -16.17 | 1.35 | 1.53 |
| 34 | i | 390 | C | O4'-C1' | 16.16 | 1.62 | 1.41 |
| 34 | i | 277 | U | O4'-C1' | 16.07 | 1.62 | 1.41 |
| 34 | i | 1847 | C | C2'-C1' | -16.03 | 1.35 | 1.53 |
| 34 | i | 1563 | C | C2'-C1' | -16.02 | 1.35 | 1.53 |
| 34 | i | 143 | U | C2'-C1' | -16.00 | 1.35 | 1.53 |
| 34 | i | 788 | C | C2'-C1' | -15.93 | 1.35 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 446 | C | O4'-C1' | 15.92 | 1.62 | 1.41 |
| 34 | i | 1666 | G | C2'-C1' | -15.92 | 1.35 | 1.53 |
| 34 | i | 1012 | U | O4'-C1' | 15.85 | 1.62 | 1.41 |
| 34 | i | 1305 | C | O4'-C1' | 15.83 | 1.62 | 1.41 |
| 34 | i | 225 | C | O4'-C1' | 15.81 | 1.62 | 1.41 |
| 34 | i | 792 | G | C2'-C1' | -15.81 | 1.35 | 1.53 |
| 34 | i | 581 | U | C2'-C1' | -15.77 | 1.35 | 1.53 |
| 34 | i | 830 | C | C2'-C1' | -15.74 | 1.36 | 1.53 |
| 34 | i | 1432 | C | O4'-C1' | 15.74 | 1.62 | 1.41 |
| 34 | i | 1660 | G | C2'-C1' | -15.71 | 1.36 | 1.53 |
| 34 | i | 179 | C | C2'-C1' | -15.70 | 1.36 | 1.53 |
| 34 | i | 1227 | C | O4'-C1' | 15.70 | 1.62 | 1.41 |
| 34 | i | 1683 | C | C2'-C1' | -15.70 | 1.36 | 1.53 |
| 34 | i | 594 | A | O4'-C1' | 15.69 | 1.62 | 1.41 |
| 34 | i | 794 | G | O4'-C1' | 15.66 | 1.62 | 1.41 |
| 34 | i | 541 | U | C2'-C1' | -15.61 | 1.36 | 1.53 |
| 34 | i | 1688 | G | C2'-C1' | -15.59 | 1.36 | 1.53 |
| 34 | i | 1452 | G | C2'-C1' | -15.55 | 1.36 | 1.53 |
| 34 | i | 1736 | U | C2'-C1' | -15.54 | 1.36 | 1.53 |
| 34 | i | 909 | A | O4'-C1' | 15.52 | 1.61 | 1.41 |
| 34 | i | 1766 | C | O4'-C1' | 15.52 | 1.61 | 1.41 |
| 34 | i | 741 | C | O4'-C1' | 15.48 | 1.61 | 1.41 |
| 34 | i | 286 | C | O4'-C1' | 15.47 | 1.61 | 1.41 |
| 34 | i | 179 | C | O4'-C1' | 15.38 | 1.61 | 1.41 |
| 34 | i | 877 | G | C2'-C1' | -15.37 | 1.36 | 1.53 |
| 34 | i | 1659 | A | C2'-C1' | -15.34 | 1.36 | 1.53 |
| 34 | i | 1393 | U | O4'-C1' | 15.34 | 1.61 | 1.41 |
| 34 | i | 1288 | C | O4'-C1' | 15.33 | 1.61 | 1.41 |
| 34 | i | 222 | G | C2'-C1' | -15.33 | 1.36 | 1.53 |
| 34 | i | 62 | G | C2'-C1' | -15.29 | 1.36 | 1.53 |
| 34 | i | 186 | G | C2'-C1' | -15.29 | 1.36 | 1.53 |
| 18 | R | 1 | MET | CA-CB | 15.29 | 1.87 | 1.53 |
| 34 | i | 730 | C | O4'-C1' | 15.28 | 1.61 | 1.41 |
| 34 | i | 657 | U | C2'-C1' | -15.27 | 1.36 | 1.53 |
| 34 | i | 1237 | A | O4'-C1' | 15.21 | 1.61 | 1.41 |
| 34 | i | 214 | A | O4'-C1' | 15.20 | 1.61 | 1.41 |
| 34 | i | 986 | A | C2'-C1' | -15.19 | 1.36 | 1.53 |
| 34 | i | 1524 | C | O4'-C1' | 15.18 | 1.61 | 1.41 |
| 34 | i | 1615 | A | C2'-C1' | -15.17 | 1.36 | 1.53 |
| 34 | i | 1012 | U | C2'-C1' | -15.15 | 1.36 | 1.53 |
| 34 | i | 1018 | U | C2'-C1' | -15.15 | 1.36 | 1.53 |
| 34 | i | 408 | A | C2'-C1' | -15.05 | 1.36 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 1171 | G | C2'-C1' | -15.05 | 1.36 | 1.53 |
| 34 | i | 225 | C | C2'-C1' | -15.00 | 1.36 | 1.53 |
| 34 | i | 734 | C | C2'-C1' | -14.93 | 1.36 | 1.53 |
| 34 | i | 164 | A | C2'-C1' | -14.91 | 1.36 | 1.53 |
| 34 | i | 1307 | C | O4'-C1' | 14.88 | 1.60 | 1.41 |
| 34 | i | 4 | C | C2'-C1' | -14.87 | 1.36 | 1.53 |
| 34 | i | 1406 | C | O4'-C1' | 14.87 | 1.60 | 1.41 |
| 34 | i | 538 | C | O4'-C1' | 14.82 | 1.60 | 1.41 |
| 34 | i | 838 | C | O4'-C1' | 14.82 | 1.60 | 1.41 |
| 34 | i | 970 | C | O4'-C1' | 14.78 | 1.60 | 1.41 |
| 34 | i | 188 | U | C2'-C1' | -14.77 | 1.37 | 1.53 |
| 34 | i | 1703 | C | O4'-C1' | 14.76 | 1.60 | 1.41 |
| 34 | i | 1413 | C | O4'-C1' | 14.74 | 1.60 | 1.41 |
| 34 | i | 1656 | A | C2'-C1' | -14.70 | 1.37 | 1.53 |
| 34 | i | 1610 | U | C2'-C1' | -14.70 | 1.37 | 1.53 |
| 34 | i | 1090 | C | O4'-C1' | 14.70 | 1.60 | 1.41 |
| 34 | i | 1289 | A | O4'-C1' | 14.68 | 1.60 | 1.41 |
| 34 | i | 1494 | A | C2'-C1' | -14.64 | 1.37 | 1.53 |
| 34 | i | 205 | G | C2'-C1' | -14.62 | 1.37 | 1.53 |
| 34 | i | 728 | U | C2'-C1' | -14.62 | 1.37 | 1.53 |
| 34 | i | 1142 | C | C2'-C1' | -14.61 | 1.37 | 1.53 |
| 10 | J | 188 | GLY | C-O | -14.60 | 1.00 | 1.23 |
| 34 | i | 873 | C | O4'-C1' | 14.60 | 1.60 | 1.41 |
| 34 | i | 1828 | A | C2'-C1' | -14.60 | 1.37 | 1.53 |
| 34 | i | 81 | U | C2'-C1' | -14.59 | 1.37 | 1.53 |
| 34 | i | 1587 | C | O4'-C1' | 14.59 | 1.60 | 1.41 |
| 9 | I | 207 | GLY | C-O | -14.57 | 1.00 | 1.23 |
| 26 | Z | 115 | GLY | C-O | -14.54 | 1.00 | 1.23 |
| 34 | i | 804 | A | C2'-C1' | -14.53 | 1.37 | 1.53 |
| 34 | i | 914 | U | C2'-C1' | -14.53 | 1.37 | 1.53 |
| 34 | i | 1230 | C | O4'-C1' | 14.52 | 1.60 | 1.41 |
| 34 | i | 1699 | C | O4'-C1' | 14.52 | 1.60 | 1.41 |
| 2 | B | 233 | GLY | C-O | -14.48 | 1.00 | 1.23 |
| 25 | Y | 128 | GLY | C-O | -14.47 | 1.00 | 1.23 |
| 34 | i | 1216 | A | C2'-C1' | -14.46 | 1.37 | 1.53 |
| 34 | i | 431 | C | O4'-C1' | 14.44 | 1.60 | 1.41 |
| 5 | E | 263 | GLY | C-O | -14.44 | 1.00 | 1.23 |
| 34 | i | 1376 | C | O4'-C1' | 14.43 | 1.60 | 1.41 |
| 34 | i | 1014 | U | C2'-C1' | -14.43 | 1.37 | 1.53 |
| 9 | I | 43 | ILE | C-N | 14.42 | 1.67 | 1.34 |
| 34 | i | 1611 | U | C2'-C1' | -14.41 | 1.37 | 1.53 |
| 34 | i | 215 | U | O4'-C1' | 14.40 | 1.60 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 1229 | G | C2'-C1' | -14.39 | 1.37 | 1.53 |
| 34 | i | 1263 | C | C2'-C1' | -14.39 | 1.37 | 1.53 |
| 21 | U | 93 | SER | C-N | 14.38 | 1.61 | 1.34 |
| 34 | i | 1738 | G | O4'-C1' | 14.35 | 1.60 | 1.41 |
| 34 | i | 1755 | U | C2'-C1' | -14.34 | 1.37 | 1.53 |
| 34 | i | 1144 | A | O4'-C1' | -14.29 | 1.23 | 1.41 |
| 34 | i | 845 | A | C2'-C1' | -14.28 | 1.37 | 1.53 |
| 34 | i | 438 | A | O4'-C1' | -14.27 | 1.23 | 1.41 |
| 34 | i | 35 | C | O4'-C1' | 14.24 | 1.60 | 1.41 |
| 34 | i | 1416 | G | C2'-C1' | -14.23 | 1.37 | 1.53 |
| 34 | i | 431 | C | C2'-C1' | -14.22 | 1.37 | 1.53 |
| 34 | i | 144 | U | O4'-C1' | 14.21 | 1.60 | 1.41 |
| 34 | i | 1691 | C | O4'-C1' | 14.11 | 1.59 | 1.41 |
| 34 | i | 1214 | C | O4'-C1' | 14.08 | 1.59 | 1.41 |
| 34 | i | 623 | C | C2'-C1' | -14.08 | 1.37 | 1.53 |
| 18 | R | 1 | MET | CA-C | -14.03 | 1.16 | 1.52 |
| 34 | i | 1587 | C | C2'-C1' | -14.02 | 1.38 | 1.53 |
| 34 | i | 1793 | G | C2'-C1' | -14.02 | 1.38 | 1.53 |
| 34 | i | 830 | C | O4'-C1' | 14.01 | 1.59 | 1.41 |
| 34 | i | 1801 | C | C2'-C1' | -13.99 | 1.38 | 1.53 |
| 34 | i | 1140 | A | C2'-C1' | -13.98 | 1.38 | 1.53 |
| 34 | i | 915 | A | C2'-C1' | -13.96 | 1.38 | 1.53 |
| 34 | i | 1557 | C | C2'-C1' | -13.96 | 1.38 | 1.53 |
| 34 | i | 852 | C | O4'-C1' | 13.94 | 1.59 | 1.41 |
| 34 | i | 1736 | U | O4'-C1' | 13.93 | 1.59 | 1.41 |
| 34 | i | 1184 | A | O4'-C1' | 13.93 | 1.59 | 1.41 |
| 34 | i | 1602 | A | C2'-C1' | -13.92 | 1.38 | 1.53 |
| 34 | i | 616 | G | O4'-C1' | 13.90 | 1.59 | 1.41 |
| 34 | i | 947 | C | O4'-C1' | 13.89 | 1.59 | 1.41 |
| 34 | i | 1520 | C | O4'-C1' | 13.89 | 1.59 | 1.41 |
| 34 | i | 1693 | C | O4'-C1' | 13.88 | 1.59 | 1.41 |
| 34 | i | 1433 | C | O4'-C1' | 13.88 | 1.59 | 1.41 |
| 34 | i | 1251 | G | C2'-C1' | -13.86 | 1.38 | 1.53 |
| 34 | i | 187 | C | O4'-C1' | 13.85 | 1.59 | 1.41 |
| 34 | i | 605 | C | O4'-C1' | 13.82 | 1.59 | 1.41 |
| 34 | i | 168 | C | O4'-C1' | 13.82 | 1.59 | 1.41 |
| 34 | i | 887 | G | C2'-C1' | -13.82 | 1.38 | 1.53 |
| 34 | i | 735 | C | O4'-C1' | 13.82 | 1.59 | 1.41 |
| 34 | i | 1003 | C | O4'-C1' | 13.79 | 1.59 | 1.41 |
| 34 | i | 852 | C | C2'-C1' | -13.79 | 1.38 | 1.53 |
| 34 | i | 312 | C | O4'-C1' | 13.76 | 1.59 | 1.41 |
| 34 | i | 1765 | G | C2'-C1' | -13.75 | 1.38 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 801 | U | O4'-C1' | 13.75 | 1.59 | 1.41 |
| 34 | i | 1400 | U | O4'-C1' | 13.73 | 1.59 | 1.41 |
| 34 | i | 734 | C | O4'-C1' | 13.72 | 1.59 | 1.41 |
| 34 | i | 1427 | G | C2'-C1' | -13.68 | 1.38 | 1.53 |
| 34 | i | 377 | C | O4'-C1' | 13.67 | 1.59 | 1.41 |
| 34 | i | 1419 | C | O4'-C1' | 13.67 | 1.59 | 1.41 |
| 34 | i | 1617 | U | O4'-C1' | 13.66 | 1.59 | 1.41 |
| 34 | i | 564 | A | O4'-C1' | 13.65 | 1.59 | 1.41 |
| 34 | i | 340 | C | O4'-C1' | 13.65 | 1.59 | 1.41 |
| 34 | i | 1263 | C | O4'-C1' | 13.63 | 1.59 | 1.41 |
| 34 | i | 1002 | C | O4'-C1' | 13.63 | 1.59 | 1.41 |
| 34 | i | 1436 | C | O4'-C1' | 13.63 | 1.59 | 1.41 |
| 34 | i | 884 | U | C2'-C1' | -13.60 | 1.38 | 1.53 |
| 34 | i | 1022 | C | O4'-C1' | 13.59 | 1.59 | 1.41 |
| 34 | i | 1411 | C | O4'-C1' | 13.59 | 1.59 | 1.41 |
| 34 | i | 13 | C | O4'-C1' | 13.57 | 1.59 | 1.41 |
| 34 | i | 1241 | G | C2'-C1' | -13.56 | 1.38 | 1.53 |
| 34 | i | 903 | G | C2'-C1' | -13.54 | 1.38 | 1.53 |
| 34 | i | 1404 | U | O4'-C1' | 13.50 | 1.59 | 1.41 |
| 34 | i | 1455 | G | C2'-C1' | -13.48 | 1.38 | 1.53 |
| 34 | i | 1805 | C | O4'-C1' | 13.48 | 1.59 | 1.41 |
| 34 | i | 1471 | G | C2'-C1' | -13.47 | 1.38 | 1.53 |
| 34 | i | 568 | C | O4'-C1' | 13.46 | 1.59 | 1.41 |
| 34 | i | 1577 | C | C2'-C1' | -13.45 | 1.38 | 1.53 |
| 34 | i | 1666 | G | O4'-C1' | 13.45 | 1.59 | 1.41 |
| 34 | i | 1777 | C | O4'-C1' | 13.39 | 1.59 | 1.41 |
| 34 | i | 858 | A | O4'-C1' | 13.39 | 1.59 | 1.41 |
| 34 | i | 402 | G | O4'-C1' | 13.39 | 1.59 | 1.41 |
| 34 | i | 728 | U | O4'-C1' | 13.39 | 1.59 | 1.41 |
| 34 | i | 980 | C | C2'-C1' | -13.38 | 1.38 | 1.53 |
| 34 | i | 174 | C | O4'-C1' | 13.36 | 1.59 | 1.41 |
| 34 | i | 548 | G | C2'-C1' | -13.36 | 1.38 | 1.53 |
| 34 | i | 510 | A | C2'-C1' | -13.35 | 1.38 | 1.53 |
| 34 | i | 1623 | C | C2'-C1' | -13.34 | 1.38 | 1.53 |
| 34 | i | 1091 | U | C2'-C1' | -13.34 | 1.38 | 1.53 |
| 34 | i | 986 | A | O4'-C1' | 13.31 | 1.58 | 1.41 |
| 34 | i | 54 | A | O4'-C1' | 13.29 | 1.58 | 1.41 |
| 34 | i | 1267 | C | O4'-C1' | 13.29 | 1.58 | 1.41 |
| 34 | i | 1847 | C | O4'-C1' | 13.29 | 1.58 | 1.41 |
| 34 | i | 1433 | C | C2'-C1' | -13.27 | 1.38 | 1.53 |
| 34 | i | 1074 | C | C2'-C1' | -13.27 | 1.38 | 1.53 |
| 34 | i | 538 | C | C2'-C1' | -13.27 | 1.38 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 1128 | C | C2'-C1' | -13.27 | 1.38 | 1.53 |
| 34 | i | 1270 | G | C2'-C1' | -13.26 | 1.38 | 1.53 |
| 34 | i | 1063 | C | O4'-C1' | 13.26 | 1.58 | 1.41 |
| 34 | i | 1406 | C | C2'-C1' | -13.24 | 1.38 | 1.53 |
| 34 | i | 1639 | C | C2'-C1' | -13.21 | 1.38 | 1.53 |
| 34 | i | 144 | U | C2'-C1' | -13.21 | 1.38 | 1.53 |
| 34 | i | 1232 | G | O4'-C1' | -13.20 | 1.24 | 1.41 |
| 34 | i | 1257 | C | O4'-C1' | 13.17 | 1.58 | 1.41 |
| 34 | i | 826 | A | O4'-C1' | -13.15 | 1.24 | 1.41 |
| 34 | i | 1583 | A | C2'-C1' | -13.13 | 1.39 | 1.53 |
| 34 | i | 287 | U | O4'-C1' | 13.12 | 1.58 | 1.41 |
| 34 | i | 1447 | G | O4'-C1' | 13.10 | 1.58 | 1.41 |
| 34 | i | 1690 | A | O4'-C1' | 13.10 | 1.58 | 1.41 |
| 34 | i | 1715 | U | C2'-C1' | 13.04 | 1.67 | 1.53 |
| 34 | i | 565 | A | O4'-C1' | 13.04 | 1.58 | 1.41 |
| 34 | i | 1122 | G | C2'-C1' | -13.04 | 1.39 | 1.53 |
| 34 | i | 1600 | G | C2'-C1' | -13.02 | 1.39 | 1.53 |
| 34 | i | 1015 | C | O4'-C1' | 13.01 | 1.58 | 1.41 |
| 34 | i | 1683 | C | O4'-C1' | 13.00 | 1.58 | 1.41 |
| 34 | i | 1075 | C | O4'-C1' | 12.99 | 1.58 | 1.41 |
| 34 | i | 1515 | G | C2'-C1' | -12.95 | 1.39 | 1.53 |
| 34 | i | 542 | G | C2'-C1' | -12.95 | 1.39 | 1.53 |
| 34 | i | 1771 | G | C2'-C1' | -12.92 | 1.39 | 1.53 |
| 34 | i | 1542 | C | O4'-C1' | 12.91 | 1.58 | 1.41 |
| 34 | i | 985 | C | O4'-C1' | 12.87 | 1.58 | 1.41 |
| 34 | i | 1546 | U | C2'-C1' | -12.87 | 1.39 | 1.53 |
| 34 | i | 274 | G | C2'-C1' | -12.87 | 1.39 | 1.53 |
| 34 | i | 1539 | C | O4'-C1' | 12.81 | 1.58 | 1.41 |
| 34 | i | 687 | G | O4'-C1' | 12.80 | 1.58 | 1.41 |
| 34 | i | 1837 | G | C2'-C1' | -12.80 | 1.39 | 1.53 |
| 34 | i | 1390 | G | C2'-C1' | -12.80 | 1.39 | 1.53 |
| 34 | i | 726 | C | C2'-C1' | -12.78 | 1.39 | 1.53 |
| 34 | i | 1087 | C | O4'-C1' | 12.78 | 1.58 | 1.41 |
| 34 | i | 973 | C | O4'-C1' | 12.77 | 1.58 | 1.41 |
| 34 | i | 646 | G | C2'-C1' | -12.77 | 1.39 | 1.53 |
| 34 | i | 1563 | C | O4'-C1' | 12.73 | 1.58 | 1.41 |
| 34 | i | 1792 | C | C2'-C1' | -12.72 | 1.39 | 1.53 |
| 34 | i | 1856 | G | O4'-C1' | 12.71 | 1.58 | 1.41 |
| 34 | i | 1160 | G | C2'-C1' | -12.69 | 1.39 | 1.53 |
| 34 | i | 981 | G | C2'-C1' | -12.69 | 1.39 | 1.53 |
| 34 | i | 1786 | G | C2'-C1' | -12.67 | 1.39 | 1.53 |
| 34 | i | 731 | C | O4'-C1' | 12.66 | 1.58 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 282 | G | C2'-C1' | -12.66 | 1.39 | 1.53 |
| 34 | i | 484 | C | O4'-C1' | 12.66 | 1.58 | 1.41 |
| 34 | i | 1113 | C | O4'-C1' | -12.65 | 1.25 | 1.41 |
| 34 | i | 1259 | U | O4'-C1' | 12.62 | 1.58 | 1.41 |
| 34 | i | 324 | C | O4'-C1' | 12.62 | 1.58 | 1.41 |
| 34 | i | 80 | G | O4'-C1' | 12.62 | 1.58 | 1.41 |
| 34 | i | 798 | A | C2'-C1' | -12.61 | 1.39 | 1.53 |
| 34 | i | 539 | C | O4'-C1' | 12.60 | 1.58 | 1.41 |
| 34 | i | 193 | C | O4'-C1' | 12.59 | 1.58 | 1.41 |
| 34 | i | 788 | C | O4'-C1' | 12.59 | 1.58 | 1.41 |
| 34 | i | 853 | U | C2'-C1' | -12.59 | 1.39 | 1.53 |
| 34 | i | 1451 | A | O4'-C1' | 12.59 | 1.58 | 1.41 |
| 34 | i | 1677 | C | O4'-C1' | 12.58 | 1.58 | 1.41 |
| 34 | i | 546 | U | C2'-C1' | -12.57 | 1.39 | 1.53 |
| 34 | i | 1376 | C | C2'-C1' | -12.56 | 1.39 | 1.53 |
| 34 | i | 907 | C | C2'-C1' | -12.55 | 1.39 | 1.53 |
| 34 | i | 482 | C | O4'-C1' | 12.55 | 1.57 | 1.41 |
| 34 | i | 1079 | A | C2'-C1' | -12.53 | 1.39 | 1.53 |
| 34 | i | 1711 | C | O4'-C1' | 12.51 | 1.57 | 1.41 |
| 34 | i | 1326 | G | C2'-C1' | -12.51 | 1.39 | 1.53 |
| 34 | i | 741 | C | C2'-C1' | -12.50 | 1.39 | 1.53 |
| 34 | i | 1165 | G | C2'-C1' | -12.47 | 1.39 | 1.53 |
| 34 | i | 1632 | A | C2'-C1' | 12.46 | 1.67 | 1.53 |
| 34 | i | 1300 | U | C2'-C1' | -12.45 | 1.39 | 1.53 |
| 34 | i | 155 | G | C2'-C1' | -12.44 | 1.39 | 1.53 |
| 34 | i | 1436 | C | C2'-C1' | -12.44 | 1.39 | 1.53 |
| 34 | i | 744 | C | O4'-C1' | 12.39 | 1.57 | 1.41 |
| 34 | i | 1063 | C | C2'-C1' | -12.39 | 1.39 | 1.53 |
| 34 | i | 48 | C | O4'-C1' | 12.39 | 1.57 | 1.41 |
| 34 | i | 622 | C | C2'-C1' | -12.38 | 1.39 | 1.53 |
| 34 | i | 650 | C | O4'-C1' | 12.37 | 1.57 | 1.41 |
| 34 | i | 1579 | G | C2'-C1' | -12.36 | 1.39 | 1.53 |
| 34 | i | 1002 | C | C2'-C1' | -12.36 | 1.39 | 1.53 |
| 34 | i | 1262 | C | C2'-C1' | -12.35 | 1.39 | 1.53 |
| 34 | i | 1322 | U | O4'-C1' | 12.33 | 1.57 | 1.41 |
| 34 | i | 1312 | C | C2'-C1' | -12.33 | 1.39 | 1.53 |
| 34 | i | 64 | A | O4'-C1' | -12.30 | 1.25 | 1.41 |
| 34 | i | 1003 | C | C2'-C1' | -12.30 | 1.39 | 1.53 |
| 34 | i | 34 | U | C2'-C1' | -12.27 | 1.39 | 1.53 |
| 34 | i | 611 | C | C2'-C1' | -12.26 | 1.39 | 1.53 |
| 34 | i | 1261 | A | C2'-C1' | -12.25 | 1.39 | 1.53 |
| 34 | i | 522 | C | O4'-C1' | 12.23 | 1.57 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 369 | C | C2'-C1' | -12.23 | 1.39 | 1.53 |
| 34 | i | 1734 | C | O4'-C1' | 12.23 | 1.57 | 1.41 |
| 34 | i | 1338 | U | O4'-C1' | 12.22 | 1.57 | 1.41 |
| 34 | i | 1262 | C | O4'-C1' | 12.20 | 1.57 | 1.41 |
| 32 | f | 152 | LYS | C-O | -12.18 | 1.00 | 1.23 |
| 13 | M | 132 | LYS | C-OXT | -12.15 | 1.00 | 1.23 |
| 34 | i | 623 | C | O4'-C1' | 12.15 | 1.57 | 1.41 |
| 14 | N | 151 | ALA | C-OXT | -12.15 | 1.00 | 1.23 |
| 34 | i | 1737 | C | C2'-C1' | -12.15 | 1.40 | 1.53 |
| 34 | i | 62 | G | O4'-C1' | 12.14 | 1.57 | 1.41 |
| 34 | i | 1542 | C | C2'-C1' | -12.14 | 1.40 | 1.53 |
| 34 | i | 869 | G | C2'-C1' | -12.14 | 1.40 | 1.53 |
| 34 | i | 638 | A | C2'-C1' | -12.13 | 1.40 | 1.53 |
| 20 | T | 144 | LYS | C-O | -12.13 | 1.00 | 1.23 |
| 13 | M | 132 | LYS | C-O | -12.12 | 1.00 | 1.23 |
| 3 | C | 263 | THR | C-O | -12.12 | 1.00 | 1.23 |
| 23 | W | 130 | PHE | C-OXT | -12.12 | 1.00 | 1.23 |
| 28 | b | 84 | HIS | C-OXT | -12.11 | 1.00 | 1.23 |
| 24 | X | 142 | ARG | C-O | -12.10 | 1.00 | 1.23 |
| 8 | H | 194 | LEU | C-O | -12.08 | 1.00 | 1.23 |
| 14 | N | 151 | ALA | C-O | -12.08 | 1.00 | 1.23 |
| 34 | i | 1116 | U | C2'-C1' | -12.08 | 1.40 | 1.53 |
| 31 | e | 133 | SER | C-O | -12.08 | 1.00 | 1.23 |
| 34 | i | 1801 | C | O4'-C1' | 12.07 | 1.57 | 1.41 |
| 34 | i | 1532 | A | O4'-C1' | 12.07 | 1.57 | 1.41 |
| 34 | i | 1404 | U | C2'-C1' | -12.07 | 1.40 | 1.53 |
| 34 | i | 598 | C | O4'-C1' | 12.06 | 1.57 | 1.41 |
| 34 | i | 583 | C | O4'-C1' | 12.06 | 1.57 | 1.41 |
| 5 | E | 263 | GLY | C-OXT | -12.05 | 1.00 | 1.23 |
| 6 | F | 204 | ARG | C-OXT | -12.05 | 1.00 | 1.23 |
| 31 | e | 133 | SER | C-OXT | -12.04 | 1.00 | 1.23 |
| 30 | d | 56 | ASP | C-O | -12.03 | 1.00 | 1.23 |
| 34 | i | 970 | C | C2'-C1' | -12.03 | 1.40 | 1.53 |
| 34 | i | 1222 | G | O4'-C1' | 12.03 | 1.57 | 1.41 |
| 34 | i | 1066 | A | C2'-C1' | -12.02 | 1.40 | 1.53 |
| 6 | F | 204 | ARG | C-O | -12.01 | 1.00 | 1.23 |
| 11 | K | 98 | ARG | C-O | -12.00 | 1.00 | 1.23 |
| 23 | W | 130 | PHE | C-O | -12.00 | 1.00 | 1.23 |
| 29 | c | 68 | LEU | C-O | -12.00 | 1.00 | 1.23 |
| 30 | d | 56 | ASP | C-OXT | -12.00 | 1.00 | 1.23 |
| 34 | i | 299 | G | O4'-C1' | 11.99 | 1.57 | 1.41 |
| 1 | A | 209 | GLU | C-O | -11.99 | 1.00 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 12 | L | 158 | PHE | C-OXT | -11.99 | 1.00 | 1.23 |
| 34 | i | 612 | C | O4'-C1' | 11.99 | 1.57 | 1.41 |
| 4 | D | 227 | LYS | C-O | -11.98 | 1.00 | 1.23 |
| 12 | L | 158 | PHE | C-O | -11.98 | 1.00 | 1.23 |
| 34 | i | 1548 | C | O4'-C1' | -11.97 | 1.26 | 1.41 |
| 34 | i | 465 | C | O4'-C1' | 11.97 | 1.57 | 1.41 |
| 33 | g | 314 | ILE | C-O | -11.95 | 1.00 | 1.23 |
| 8 | H | 194 | LEU | C-OXT | -11.94 | 1.00 | 1.23 |
| 10 | J | 146 | SER | C-N | 11.92 | 1.61 | 1.34 |
| 34 | i | 971 | G | C2'-C1' | -11.92 | 1.40 | 1.53 |
| 34 | i | 1009 | U | C2'-C1' | -11.91 | 1.40 | 1.53 |
| 34 | i | 56 | G | C2'-C1' | -11.91 | 1.40 | 1.53 |
| 34 | i | 1788 | C | O4'-C1' | 11.91 | 1.57 | 1.41 |
| 34 | i | 276 | U | O4'-C1' | 11.90 | 1.57 | 1.41 |
| 34 | i | 553 | G | O4'-C1' | 11.90 | 1.57 | 1.41 |
| 28 | b | 84 | HIS | C-O | -11.89 | 1.00 | 1.23 |
| 34 | i | 302 | C | O4'-C1' | 11.89 | 1.57 | 1.41 |
| 34 | i | 1573 | U | C2'-C1' | 11.88 | 1.66 | 1.53 |
| 34 | i | 1114 | C | C2'-C1' | 11.87 | 1.66 | 1.53 |
| 34 | i | 1524 | C | C2'-C1' | -11.86 | 1.40 | 1.53 |
| 34 | i | 18 | C | O4'-C1' | 11.84 | 1.57 | 1.41 |
| 34 | i | 664 | C | C2'-C1' | -11.82 | 1.40 | 1.53 |
| 34 | i | 67 | C | C2'-C1' | 11.81 | 1.66 | 1.53 |
| 34 | i | 1060 | C | O4'-C1' | 11.80 | 1.56 | 1.41 |
| 34 | i | 906 | G | C2'-C1' | -11.80 | 1.40 | 1.53 |
| 34 | i | 727 | G | C2'-C1' | -11.80 | 1.40 | 1.53 |
| 34 | i | 1650 | C | O4'-C1' | 11.80 | 1.56 | 1.41 |
| 34 | i | 907 | C | O4'-C1' | 11.79 | 1.56 | 1.41 |
| 34 | i | 667 | G | C2'-C1' | -11.77 | 1.40 | 1.53 |
| 34 | i | 1628 | A | O4'-C1' | 11.77 | 1.56 | 1.41 |
| 34 | i | 318 | U | C2'-C1' | -11.75 | 1.40 | 1.53 |
| 34 | i | 1428 | U | O4'-C1' | 11.74 | 1.56 | 1.41 |
| 34 | i | 569 | C | O4'-C1' | 11.73 | 1.56 | 1.41 |
| 34 | i | 670 | G | C2'-C1' | -11.73 | 1.40 | 1.53 |
| 34 | i | 539 | C | C2'-C1' | -11.69 | 1.40 | 1.53 |
| 34 | i | 1260 | C | C2'-C1' | -11.68 | 1.40 | 1.53 |
| 34 | i | 396 | U | C2'-C1' | -11.68 | 1.40 | 1.53 |
| 34 | i | 639 | U | C2'-C1' | -11.68 | 1.40 | 1.53 |
| 34 | i | 589 | A | C2'-C1' | -11.67 | 1.40 | 1.53 |
| 34 | i | 833 | A | C2'-C1' | -11.67 | 1.40 | 1.53 |
| 34 | i | 1387 | C | O4'-C1' | 11.67 | 1.56 | 1.41 |
| 34 | i | 864 | G | O4'-C1' | 11.66 | 1.56 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 325 | G | O4'-C1' | -11.66 | 1.26 | 1.41 |
| 34 | i | 1698 | C | O4'-C1' | 11.62 | 1.56 | 1.41 |
| 34 | i | 606 | A | O4'-C1' | 11.60 | 1.56 | 1.41 |
| 34 | i | 1537 | C | O4'-C1' | 11.58 | 1.56 | 1.41 |
| 19 | S | 141 | ARG | C-N | 11.58 | 1.60 | 1.34 |
| 34 | i | 549 | G | C2'-C1' | -11.58 | 1.40 | 1.53 |
| 34 | i | 545 | A | O4'-C1' | 11.57 | 1.56 | 1.41 |
| 34 | i | 1181 | C | O4'-C1' | 11.57 | 1.56 | 1.41 |
| 34 | i | 947 | C | C2'-C1' | -11.55 | 1.40 | 1.53 |
| 34 | i | 1195 | A | C2'-C1' | -11.55 | 1.40 | 1.53 |
| 34 | i | 1074 | C | O4'-C1' | 11.54 | 1.56 | 1.41 |
| 34 | i | 407 | C | O4'-C1' | 11.53 | 1.56 | 1.41 |
| 34 | i | 668 | U | C2'-C1' | -11.52 | 1.40 | 1.53 |
| 34 | i | 976 | A | C2'-C1' | -11.50 | 1.40 | 1.53 |
| 34 | i | 805 | A | C2'-C1' | -11.50 | 1.40 | 1.53 |
| 34 | i | 471 | C | C2'-C1' | -11.50 | 1.40 | 1.53 |
| 34 | i | 1114 | C | O4'-C1' | -11.49 | 1.26 | 1.41 |
| 34 | i | 436 | G | O4'-C1' | 11.48 | 1.56 | 1.41 |
| 34 | i | 1732 | G | O4'-C1' | 11.47 | 1.56 | 1.41 |
| 34 | i | 559 | A | C2'-C1' | -11.45 | 1.40 | 1.53 |
| 34 | i | 851 | G | C2'-C1' | -11.44 | 1.40 | 1.53 |
| 34 | i | 622 | C | O4'-C1' | 11.44 | 1.56 | 1.41 |
| 34 | i | 887 | G | O4'-C1' | 11.41 | 1.56 | 1.41 |
| 34 | i | 436 | G | C2'-C1' | -11.40 | 1.40 | 1.53 |
| 34 | i | 521 | A | O4'-C1' | 11.40 | 1.56 | 1.41 |
| 34 | i | 1025 | G | C2'-C1' | -11.40 | 1.40 | 1.53 |
| 34 | i | 500 | G | C2'-C1' | -11.40 | 1.40 | 1.53 |
| 34 | i | 288 | A | C2'-C1' | -11.38 | 1.40 | 1.53 |
| 34 | i | 1323 | G | C2'-C1' | -11.38 | 1.40 | 1.53 |
| 25 | Y | 86 | GLU | C-N | 11.35 | 1.55 | 1.34 |
| 34 | i | 48 | C | C2'-C1' | -11.34 | 1.40 | 1.53 |
| 34 | i | 682 | G | C2'-C1' | -11.34 | 1.40 | 1.53 |
| 34 | i | 452 | C | C2'-C1' | -11.33 | 1.40 | 1.53 |
| 34 | i | 1101 | G | C2'-C1' | -11.33 | 1.40 | 1.53 |
| 34 | i | 1124 | C | O4'-C1' | 11.33 | 1.56 | 1.41 |
| 34 | i | 360 | G | C2'-C1' | -11.30 | 1.41 | 1.53 |
| 34 | i | 323 | G | C2'-C1' | -11.30 | 1.41 | 1.53 |
| 34 | i | 395 | G | C2'-C1' | -11.28 | 1.41 | 1.53 |
| 34 | i | 1653 | G | C2'-C1' | -11.27 | 1.41 | 1.53 |
| 34 | i | 1775 | A | C2'-C1' | -11.27 | 1.41 | 1.53 |
| 34 | i | 900 | A | O4'-C1' | 11.24 | 1.56 | 1.41 |
| 34 | i | 736 | C | O4'-C1' | 11.24 | 1.56 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 1669 | G | O4'-C1' | 11.22 | 1.56 | 1.41 |
| 34 | i | 936 | U | C2'-C1' | -11.22 | 1.41 | 1.53 |
| 34 | i | 414 | C | O4'-C1' | 11.21 | 1.56 | 1.41 |
| 34 | i | 635 | C | O4'-C1' | 11.20 | 1.56 | 1.41 |
| 23 | W | 2 | VAL | C-N | 11.20 | 1.59 | 1.34 |
| 7 | G | 131 | ARG | CG-CD | 11.20 | 1.79 | 1.51 |
| 34 | i | 1792 | C | O4'-C1' | 11.18 | 1.56 | 1.41 |
| 34 | i | 1448 | A | O4'-C1' | 11.17 | 1.56 | 1.41 |
| 34 | i | 335 | U | C2'-C1' | -11.14 | 1.41 | 1.53 |
| 34 | i | 938 | G | C2'-C1' | -11.14 | 1.41 | 1.53 |
| 34 | i | 1044 | G | O4'-C1' | 11.14 | 1.56 | 1.41 |
| 34 | i | 1202 | G | C2'-C1' | -11.14 | 1.41 | 1.53 |
| 34 | i | 964 | U | O4'-C1' | 11.13 | 1.56 | 1.41 |
| 34 | i | 84 | A | O4'-C1' | 11.12 | 1.56 | 1.41 |
| 34 | i | 839 | C | O4'-C1' | 11.11 | 1.56 | 1.41 |
| 34 | i | 1220 | G | C2'-C1' | -11.09 | 1.41 | 1.53 |
| 34 | i | 1238 | U | C2'-C1' | -11.09 | 1.41 | 1.53 |
| 34 | i | 1568 | G | C2'-C1' | -11.09 | 1.41 | 1.53 |
| 34 | i | 77 | A | C2'-C1' | 11.09 | 1.65 | 1.53 |
| 34 | i | 1015 | C | C2'-C1' | -11.08 | 1.41 | 1.53 |
| 34 | i | 1585 | C | O4'-C1' | 11.07 | 1.56 | 1.41 |
| 7 | G | 131 | ARG | C-N | 11.07 | 1.59 | 1.34 |
| 34 | i | 347 | C | C2'-C1' | -11.06 | 1.41 | 1.53 |
| 34 | i | 479 | A | O4'-C1' | 11.05 | 1.56 | 1.41 |
| 34 | i | 871 | A | O4'-C1' | 11.04 | 1.56 | 1.41 |
| 34 | i | 402 | G | C2'-C1' | -11.04 | 1.41 | 1.53 |
| 34 | i | 691 | G | C2'-C1' | -11.00 | 1.41 | 1.53 |
| 34 | i | 1813 | A | C2'-C1' | -11.00 | 1.41 | 1.53 |
| 34 | i | 901 | C | O4'-C1' | 10.99 | 1.55 | 1.41 |
| 34 | i | 1226 | C | O4'-C1' | 10.98 | 1.55 | 1.41 |
| 34 | i | 1603 | U | O4'-C1' | 10.98 | 1.55 | 1.41 |
| 34 | i | 1289 | A | C2'-C1' | -10.98 | 1.41 | 1.53 |
| 34 | i | 4 | C | O4'-C1' | 10.97 | 1.55 | 1.41 |
| 18 | R | 1 | MET | C-N | -10.96 | 1.13 | 1.33 |
| 34 | i | 664 | C | O4'-C1' | 10.95 | 1.55 | 1.41 |
| 34 | i | 1120 | C | C2'-C1' | -10.94 | 1.41 | 1.53 |
| 34 | i | 582 | C | O4'-C1' | -10.92 | 1.27 | 1.41 |
| 34 | i | 1176 | C | O4'-C1' | 10.90 | 1.55 | 1.41 |
| 34 | i | 547 | U | C2'-C1' | -10.89 | 1.41 | 1.53 |
| 34 | i | 462 | C | O4'-C1' | 10.88 | 1.55 | 1.41 |
| 34 | i | 870 | G | C2'-C1' | -10.87 | 1.41 | 1.53 |
| 34 | i | 1716 | U | C2'-C1' | 10.87 | 1.65 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 1369 | C | O4'-C1' | 10.86 | 1.55 | 1.41 |
| 34 | i | 812 | A | O4'-C1' | 10.84 | 1.55 | 1.41 |
| 34 | i | 432 | C | O4'-C1' | 10.83 | 1.55 | 1.41 |
| 34 | i | 414 | C | C2'-C1' | -10.83 | 1.41 | 1.53 |
| 34 | i | 1834 | U | C2'-C1' | -10.82 | 1.41 | 1.53 |
| 34 | i | 839 | C | C2'-C1' | -10.82 | 1.41 | 1.53 |
| 34 | i | 1403 | U | C2'-C1' | -10.80 | 1.41 | 1.53 |
| 34 | i | 1400 | U | C2'-C1' | -10.79 | 1.41 | 1.53 |
| 34 | i | 975 | C | O4'-C1' | 10.78 | 1.55 | 1.41 |
| 34 | i | 633 | A | O4'-C1' | 10.77 | 1.55 | 1.41 |
| 34 | i | 1159 | C | O4'-C1' | 10.76 | 1.55 | 1.41 |
| 34 | i | 1257 | C | C2'-C1' | -10.76 | 1.41 | 1.53 |
| 34 | i | 916 | A | C2'-C1' | -10.76 | 1.41 | 1.53 |
| 34 | i | 483 | A | C2'-C1' | -10.75 | 1.41 | 1.53 |
| 34 | i | 1208 | G | C2'-C1' | -10.75 | 1.41 | 1.53 |
| 34 | i | 1527 | C | C2'-C1' | -10.75 | 1.41 | 1.53 |
| 34 | i | 1209 | C | O4'-C1' | 10.74 | 1.55 | 1.41 |
| 34 | i | 640 | A | O4'-C1' | 10.74 | 1.55 | 1.41 |
| 34 | i | 488 | C | O4'-C1' | 10.74 | 1.55 | 1.41 |
| 34 | i | 1301 | C | C2'-C1' | -10.74 | 1.41 | 1.53 |
| 34 | i | 308 | C | O4'-C1' | 10.73 | 1.55 | 1.41 |
| 34 | i | 1547 | G | C2'-C1' | 10.73 | 1.65 | 1.53 |
| 34 | i | 1807 | A | C2'-C1' | -10.71 | 1.41 | 1.53 |
| 34 | i | 327 | C | C2'-C1' | -10.71 | 1.41 | 1.53 |
| 34 | i | 487 | C | O4'-C1' | 10.71 | 1.55 | 1.41 |
| 34 | i | 1050 | G | C2'-C1' | -10.68 | 1.41 | 1.53 |
| 34 | i | 1200 | A | O4'-C1' | 10.68 | 1.55 | 1.41 |
| 34 | i | 1207 | G | C2'-C1' | -10.66 | 1.41 | 1.53 |
| 34 | i | 1048 | A | O4'-C1' | 10.66 | 1.55 | 1.41 |
| 34 | i | 1578 | C | O4'-C1' | 10.66 | 1.55 | 1.41 |
| 34 | i | 1481 | U | C2'-C1' | -10.65 | 1.41 | 1.53 |
| 34 | i | 1496 | G | O4'-C1' | 10.65 | 1.55 | 1.41 |
| 34 | i | 352 | C | O4'-C1' | 10.64 | 1.55 | 1.41 |
| 34 | i | 1684 | C | C2'-C1' | -10.63 | 1.41 | 1.53 |
| 34 | i | 1481 | U | O4'-C1' | 10.63 | 1.55 | 1.41 |
| 34 | i | 143 | U | O4'-C1' | 10.63 | 1.55 | 1.41 |
| 34 | i | 1708 | C | O4'-C1' | 10.62 | 1.55 | 1.41 |
| 19 | S | 54 | LYS | N-CA | 10.61 | 1.67 | 1.46 |
| 34 | i | 286 | C | C2'-C1' | -10.61 | 1.41 | 1.53 |
| 34 | i | 1729 | G | C2'-C1' | -10.61 | 1.41 | 1.53 |
| 34 | i | 875 | C | C2'-C1' | -10.60 | 1.41 | 1.53 |
| 34 | i | 868 | A | O4'-C1' | -10.59 | 1.27 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 416 | A | O4'-C1' | 10.58 | 1.55 | 1.41 |
| 34 | i | 1258 | C | O4'-C1' | 10.57 | 1.55 | 1.41 |
| 34 | i | 1752 | G | C2'-C1' | -10.56 | 1.41 | 1.53 |
| 9 | I | 43 | ILE | CA-C | -10.56 | 1.25 | 1.52 |
| 34 | i | 1259 | U | C2'-C1' | -10.55 | 1.41 | 1.53 |
| 34 | i | 547 | U | O4'-C1' | 10.54 | 1.55 | 1.41 |
| 34 | i | 449 | C | O4'-C1' | 10.53 | 1.55 | 1.41 |
| 34 | i | 50 | A | C2'-C1' | -10.53 | 1.41 | 1.53 |
| 34 | i | 605 | C | C2'-C1' | -10.51 | 1.41 | 1.53 |
| 34 | i | 507 | C | C2'-C1' | -10.50 | 1.41 | 1.53 |
| 34 | i | 316 | C | O4'-C1' | 10.50 | 1.55 | 1.41 |
| 34 | i | 1280 | A | O4'-C1' | 10.50 | 1.55 | 1.41 |
| 34 | i | 984 | C | C2'-C1' | -10.49 | 1.41 | 1.53 |
| 34 | i | 16 | G | C2'-C1' | -10.49 | 1.41 | 1.53 |
| 19 | S | 40 | TYR | C-N | -10.48 | 1.09 | 1.34 |
| 34 | i | 933 | C | O4'-C1' | 10.47 | 1.55 | 1.41 |
| 34 | i | 241 | A | O4'-C1' | 10.47 | 1.55 | 1.41 |
| 34 | i | 355 | C | O4'-C1' | 10.46 | 1.55 | 1.41 |
| 34 | i | 529 | C | O4'-C1' | 10.46 | 1.55 | 1.41 |
| 34 | i | 480 | C | O4'-C1' | 10.46 | 1.55 | 1.41 |
| 34 | i | 1755 | U | O4'-C1' | 10.46 | 1.55 | 1.41 |
| 34 | i | 1128 | C | O4'-C1' | 10.45 | 1.55 | 1.41 |
| 34 | i | 385 | G | C2'-C1' | -10.44 | 1.41 | 1.53 |
| 34 | i | 54 | A | C2'-C1' | -10.44 | 1.41 | 1.53 |
| 34 | i | 1578 | C | C2'-C1' | -10.44 | 1.41 | 1.53 |
| 34 | i | 1624 | C | C2'-C1' | -10.44 | 1.41 | 1.53 |
| 34 | i | 825 | C | O4'-C1' | 10.44 | 1.55 | 1.41 |
| 34 | i | 178 | C | C2'-C1' | -10.42 | 1.41 | 1.53 |
| 34 | i | 1398 | A | O4'-C1' | 10.41 | 1.55 | 1.41 |
| 34 | i | 1778 | G | O4'-C1' | 10.41 | 1.55 | 1.41 |
| 34 | i | 1700 | C | O4'-C1' | 10.40 | 1.55 | 1.41 |
| 34 | i | 170 | A | O4'-C1' | -10.40 | 1.28 | 1.41 |
| 34 | i | 1105 | C | O4'-C1' | -10.40 | 1.28 | 1.41 |
| 34 | i | 1617 | U | C2'-C1' | -10.40 | 1.42 | 1.53 |
| 34 | i | 1375 | A | C2'-C1' | -10.39 | 1.42 | 1.53 |
| 34 | i | 560 | C | O4'-C1' | 10.39 | 1.55 | 1.41 |
| 34 | i | 558 | C | O4'-C1' | 10.37 | 1.55 | 1.41 |
| 34 | i | 230 | C | O4'-C1' | 10.36 | 1.55 | 1.41 |
| 34 | i | 1309 | A | C2'-C1' | -10.34 | 1.42 | 1.53 |
| 34 | i | 1324 | G | C2'-C1' | -10.32 | 1.42 | 1.53 |
| 34 | i | 1682 | C | O4'-C1' | 10.31 | 1.55 | 1.41 |
| 34 | i | 1230 | C | C2'-C1' | -10.31 | 1.42 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 1576 | C | O4'-C1' | 10.31 | 1.55 | 1.41 |
| 34 | i | 1682 | C | C2'-C1' | -10.31 | 1.42 | 1.53 |
| 34 | i | 1272 | A | O4'-C1' | 10.27 | 1.55 | 1.41 |
| 34 | i | 75 | G | C2'-C1' | -10.27 | 1.42 | 1.53 |
| 34 | i | 729 | C | O4'-C1' | 10.27 | 1.54 | 1.41 |
| 34 | i | 410 | G | C2'-C1' | -10.26 | 1.42 | 1.53 |
| 34 | i | 1410 | A | C2'-C1' | -10.25 | 1.42 | 1.53 |
| 34 | i | 382 | A | O4'-C1' | 10.25 | 1.54 | 1.41 |
| 34 | i | 1486 | G | C2'-C1' | -10.25 | 1.42 | 1.53 |
| 34 | i | 1783 | G | O4'-C1' | 10.24 | 1.54 | 1.41 |
| 34 | i | 79 | A | C2'-C1' | 10.23 | 1.64 | 1.53 |
| 34 | i | 1835 | C | O4'-C1' | 10.23 | 1.54 | 1.41 |
| 34 | i | 1165 | G | O4'-C1' | 10.23 | 1.54 | 1.41 |
| 34 | i | 52 | G | C2'-C1' | -10.22 | 1.42 | 1.53 |
| 34 | i | 84 | A | C2'-C1' | -10.22 | 1.42 | 1.53 |
| 34 | i | 1411 | C | C2'-C1' | -10.21 | 1.42 | 1.53 |
| 34 | i | 653 | C | C2'-C1' | -10.20 | 1.42 | 1.53 |
| 34 | i | 315 | C | C2'-C1' | 10.20 | 1.64 | 1.53 |
| 34 | i | 352 | C | C2'-C1' | -10.19 | 1.42 | 1.53 |
| 34 | i | 313 | C | O4'-C1' | 10.18 | 1.54 | 1.41 |
| 34 | i | 1651 | G | C2'-C1' | -10.18 | 1.42 | 1.53 |
| 34 | i | 977 | A | O4'-C1' | 10.17 | 1.54 | 1.41 |
| 34 | i | 683 | G | C2'-C1' | -10.16 | 1.42 | 1.53 |
| 34 | i | 1573 | U | O4'-C1' | -10.16 | 1.28 | 1.41 |
| 34 | i | 1766 | C | C2'-C1' | -10.14 | 1.42 | 1.53 |
| 34 | i | 1271 | G | C2'-C1' | -10.14 | 1.42 | 1.53 |
| 34 | i | 209 | C | O4'-C1' | 10.12 | 1.54 | 1.41 |
| 34 | i | 1827 | C | O4'-C1' | 10.12 | 1.54 | 1.41 |
| 34 | i | 563 | U | C2'-C1' | -10.09 | 1.42 | 1.53 |
| 34 | i | 1071 | C | C2'-C1' | -10.09 | 1.42 | 1.53 |
| 34 | i | 823 | A | C2'-C1' | -10.09 | 1.42 | 1.53 |
| 34 | i | 1076 | A | O4'-C1' | -10.08 | 1.28 | 1.41 |
| 34 | i | 76 | U | O4'-C1' | 10.07 | 1.54 | 1.41 |
| 34 | i | 1139 | A | C2'-C1' | -10.06 | 1.42 | 1.53 |
| 34 | i | 1181 | C | C2'-C1' | -10.06 | 1.42 | 1.53 |
| 34 | i | 428 | G | C2'-C1' | 10.05 | 1.64 | 1.53 |
| 34 | i | 588 | G | C2'-C1' | -10.05 | 1.42 | 1.53 |
| 34 | i | 1133 | U | O4'-C1' | 10.05 | 1.54 | 1.41 |
| 34 | i | 82 | G | C2'-C1' | 10.04 | 1.64 | 1.53 |
| 34 | i | 1312 | C | O4'-C1' | 10.04 | 1.54 | 1.41 |
| 34 | i | 486 | C | O4'-C1' | 10.03 | 1.54 | 1.41 |
| 34 | i | 1096 | A | O4'-C1' | 10.03 | 1.54 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34 | i | 120 | U | C2'-C1' | -10.02 | 1.42 | 1.53 |
| 34 | i | 809 | A | O4'-C1' | 10.01 | 1.54 | 1.41 |
| 34 | i | 1098 | G | C2'-C1' | -10.00 | 1.42 | 1.53 |
| 34 | i | 85 | A | C2'-C1' | -10.00 | 1.42 | 1.53 |
| 34 | i | 1359 | C | O4'-C1' | 9.99 | 1.54 | 1.41 |
| 34 | i | 1377 | G | O4'-C1' | -9.99 | 1.28 | 1.41 |
| 34 | i | 1467 | C | C2'-C1' | -9.97 | 1.42 | 1.53 |
| 34 | i | 1316 | G | O4'-C1' | -9.97 | 1.28 | 1.41 |
| 34 | i | 1504 | A | C2'-C1' | 9.97 | 1.64 | 1.53 |
| 34 | i | 1600 | G | O4'-C1' | 9.96 | 1.54 | 1.41 |
| 34 | i | 142 | C | O4'-C1' | -9.96 | 1.28 | 1.41 |
| 34 | i | 66 | G | O4'-C1' | 9.96 | 1.54 | 1.41 |
| 34 | i | 1585 | C | C2'-C1' | -9.94 | 1.42 | 1.53 |
| 34 | i | 111 | A | O4'-C1' | -9.93 | 1.28 | 1.41 |
| 34 | i | 193 | C | C2'-C1' | -9.93 | 1.42 | 1.53 |
| 34 | i | 1819 | A | C2'-C1' | 9.93 | 1.64 | 1.53 |
| 34 | i | 1678 | C | O4'-C1' | 9.92 | 1.54 | 1.41 |
| 34 | i | 1787 | A | O4'-C1' | 9.92 | 1.54 | 1.41 |
| 34 | i | 437 | A | C2'-C1' | 9.91 | 1.64 | 1.53 |
| 34 | i | 533 | C | O4'-C1' | 9.91 | 1.54 | 1.41 |
| 34 | i | 1779 | C | C2'-C1' | 9.90 | 1.64 | 1.53 |
| 34 | i | 1055 | G | C2'-C1' | -9.90 | 1.42 | 1.53 |
| 34 | i | 1006 | G | O4'-C1' | -9.90 | 1.28 | 1.41 |
| 34 | i | 1209 | C | C2'-C1' | -9.89 | 1.42 | 1.53 |
| 34 | i | 1822 | C | O4'-C1' | 9.89 | 1.54 | 1.41 |
| 34 | i | 149 | A | O4'-C1' | 9.87 | 1.54 | 1.41 |
| 34 | i | 392 | C | O4'-C1' | 9.87 | 1.54 | 1.41 |
| 34 | i | 946 | C | O4'-C1' | 9.86 | 1.54 | 1.41 |
| 34 | i | 1503 | G | C2'-C1' | -9.86 | 1.42 | 1.53 |
| 34 | i | 1329 | U | C2'-C1' | 9.86 | 1.64 | 1.53 |
| 34 | i | 1740 | A | C2'-C1' | 9.86 | 1.64 | 1.53 |
| 34 | i | 1559 | C | O4'-C1' | 9.85 | 1.54 | 1.41 |
| 34 | i | 956 | U | O4'-C1' | 9.85 | 1.54 | 1.41 |
| 34 | i | 564 | A | C2'-C1' | -9.84 | 1.42 | 1.53 |
| 34 | i | 311 | C | C2'-C1' | -9.84 | 1.42 | 1.53 |
| 34 | i | 1594 | U | C2'-C1' | 9.82 | 1.64 | 1.53 |
| 34 | i | 1432 | C | C2'-C1' | -9.82 | 1.42 | 1.53 |
| 34 | i | 645 | A | C2'-C1' | -9.82 | 1.42 | 1.53 |
| 34 | i | 96 | C | O4'-C1' | 9.81 | 1.54 | 1.41 |
| 34 | i | 487 | C | C2'-C1' | -9.81 | 1.42 | 1.53 |
| 34 | i | 1338 | U | C2'-C1' | -9.80 | 1.42 | 1.53 |
| 34 | i | 359 | C | C2'-C1' | -9.80 | 1.42 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 855 | G | C2'-C1' | -9.79 | 1.42 | 1.53 |
| 34 | i | 932 | G | C2'-C1' | -9.79 | 1.42 | 1.53 |
| 34 | i | 298 | G | O4'-C1' | -9.79 | 1.28 | 1.41 |
| 34 | i | 1029 | G | C2'-C1' | -9.78 | 1.42 | 1.53 |
| 34 | i | 1428 | U | C2'-C1' | -9.76 | 1.42 | 1.53 |
| 34 | i | 1201 | C | C2'-C1' | -9.75 | 1.42 | 1.53 |
| 34 | i | 654 | A | C2'-C1' | -9.74 | 1.42 | 1.53 |
| 34 | i | 560 | C | C2'-C1' | -9.74 | 1.42 | 1.53 |
| 34 | i | 1462 | G | C2'-C1' | -9.73 | 1.42 | 1.53 |
| 34 | i | 1204 | A | C2'-C1' | 9.72 | 1.64 | 1.53 |
| 34 | i | 544 | A | C2'-C1' | -9.71 | 1.42 | 1.53 |
| 34 | i | 1320 | G | C2'-C1' | -9.70 | 1.42 | 1.53 |
| 34 | i | 1784 | A | C2'-C1' | -9.70 | 1.42 | 1.53 |
| 34 | i | 481 | C | C2'-C1' | -9.68 | 1.42 | 1.53 |
| 34 | i | 67 | C | O4'-C1' | -9.67 | 1.29 | 1.41 |
| 34 | i | 888 | U | C2'-C1' | -9.67 | 1.42 | 1.53 |
| 34 | i | 31 | U | C2'-C1' | 9.65 | 1.64 | 1.53 |
| 34 | i | 419 | C | O4'-C1' | 9.65 | 1.54 | 1.41 |
| 34 | i | 1120 | C | O4'-C1' | 9.64 | 1.54 | 1.41 |
| 34 | i | 1707 | A | C2'-C1' | -9.63 | 1.42 | 1.53 |
| 34 | i | 1808 | G | C2'-C1' | -9.63 | 1.42 | 1.53 |
| 34 | i | 1031 | A | C2'-C1' | -9.63 | 1.42 | 1.53 |
| 34 | i | 1099 | C | C2'-C1' | -9.62 | 1.42 | 1.53 |
| 34 | i | 1337 | C | O4'-C1' | 9.62 | 1.54 | 1.41 |
| 34 | i | 88 | G | C2'-C1' | -9.61 | 1.42 | 1.53 |
| 34 | i | 1296 | U | O4'-C1' | -9.60 | 1.29 | 1.41 |
| 34 | i | 507 | C | O4'-C1' | 9.60 | 1.54 | 1.41 |
| 34 | i | 829 | C | C2'-C1' | -9.59 | 1.42 | 1.53 |
| 34 | i | 1669 | G | C2'-C1' | -9.58 | 1.42 | 1.53 |
| 34 | i | 1464 | C | O4'-C1' | 9.58 | 1.54 | 1.41 |
| 34 | i | 150 | A | O4'-C1' | 9.57 | 1.54 | 1.41 |
| 34 | i | 166 | A | C2'-C1' | -9.56 | 1.42 | 1.53 |
| 34 | i | 675 | A | C2'-C1' | -9.56 | 1.42 | 1.53 |
| 34 | i | 657 | U | O4'-C1' | 9.55 | 1.54 | 1.41 |
| 34 | i | 448 | A | O4'-C1' | 9.55 | 1.54 | 1.41 |
| 34 | i | 445 | A | O4'-C1' | 9.54 | 1.54 | 1.41 |
| 34 | i | 1572 | G | O4'-C1' | 9.54 | 1.54 | 1.41 |
| 34 | i | 13 | C | C2'-C1' | -9.53 | 1.42 | 1.53 |
| 34 | i | 511 | A | C2'-C1' | -9.53 | 1.42 | 1.53 |
| 34 | i | 1437 | U | C2'-C1' | 9.52 | 1.63 | 1.53 |
| 34 | i | 1339 | U | O4'-C1' | 9.52 | 1.54 | 1.41 |
| 34 | i | 799 | C | C2'-C1' | -9.52 | 1.42 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1742 | C | O3'-P | -9.52 | 1.49 | 1.61 |
| 34 | i | 173 | A | O4'-C1' | 9.50 | 1.54 | 1.41 |
| 34 | i | 212 | G | O4'-C1' | 9.50 | 1.53 | 1.41 |
| 34 | i | 1536 | G | C2'-C1' | -9.50 | 1.43 | 1.53 |
| 19 | S | 6 | PRO | CA-C | 9.48 | 1.71 | 1.52 |
| 34 | i | 298 | G | C2'-C1' | 9.47 | 1.63 | 1.53 |
| 34 | i | 980 | C | O4'-C1' | 9.46 | 1.53 | 1.41 |
| 10 | J | 35 | TYR | CD1-CE1 | -9.46 | 1.25 | 1.39 |
| 34 | i | 1211 | C | C2'-C1' | 9.45 | 1.63 | 1.53 |
| 34 | i | 311 | C | O4'-C1' | 9.45 | 1.53 | 1.41 |
| 34 | i | 743 | U | O4'-C1' | 9.44 | 1.53 | 1.41 |
| 34 | i | 1790 | G | C2'-C1' | -9.43 | 1.43 | 1.53 |
| 34 | i | 1440 | U | C2'-C1' | -9.42 | 1.43 | 1.53 |
| 34 | i | 1365 | A | C2'-C1' | -9.41 | 1.43 | 1.53 |
| 34 | i | 1101 | G | O4'-C1' | 9.40 | 1.53 | 1.41 |
| 34 | i | 1112 | C | O4'-C1' | -9.40 | 1.29 | 1.41 |
| 34 | i | 285 | U | O4'-C1' | 9.40 | 1.53 | 1.41 |
| 34 | i | 1025 | G | O4'-C1' | 9.40 | 1.53 | 1.41 |
| 34 | i | 1713 | G | C2'-C1' | -9.40 | 1.43 | 1.53 |
| 34 | i | 884 | U | O4'-C1' | 9.39 | 1.53 | 1.41 |
| 34 | i | 726 | C | O4'-C1' | 9.38 | 1.53 | 1.41 |
| 34 | i | 1328 | A | O4'-C1' | 9.37 | 1.53 | 1.41 |
| 34 | i | 1735 | C | O4'-C1' | 9.36 | 1.53 | 1.41 |
| 34 | i | 1781 | G | C2'-C1' | -9.36 | 1.43 | 1.53 |
| 34 | i | 1251 | G | O4'-C1' | 9.36 | 1.53 | 1.41 |
| 34 | i | 1301 | C | O4'-C1' | 9.36 | 1.53 | 1.41 |
| 34 | i | 1534 | U | C2'-C1' | 9.35 | 1.63 | 1.53 |
| 34 | i | 1118 | A | C2'-C1' | 9.35 | 1.63 | 1.53 |
| 34 | i | 614 | C | O4'-C1' | 9.34 | 1.53 | 1.41 |
| 34 | i | 457 | G | O4'-C1' | 9.33 | 1.53 | 1.41 |
| 34 | i | 1029 | G | O4'-C1' | 9.32 | 1.53 | 1.41 |
| 34 | i | 440 | C | C2'-C1' | 9.32 | 1.63 | 1.53 |
| 34 | i | 1548 | C | C2'-C1' | 9.32 | 1.63 | 1.53 |
| 34 | i | 53 | C | O4'-C1' | 9.32 | 1.53 | 1.41 |
| 34 | i | 1618 | A | C2'-C1' | 9.31 | 1.63 | 1.53 |
| 34 | i | 1861 | U | C2'-C1' | 9.31 | 1.63 | 1.53 |
| 34 | i | 927 | C | O4'-C1' | 9.30 | 1.53 | 1.41 |
| 34 | i | 332 | C | O4'-C1' | 9.30 | 1.53 | 1.41 |
| 34 | i | 234 | C | C2'-C1' | 9.30 | 1.63 | 1.53 |
| 34 | i | 790 | A | O4'-C1' | 9.29 | 1.53 | 1.41 |
| 34 | i | 1849 | G | C2'-C1' | -9.29 | 1.43 | 1.53 |
| 34 | i | 1744 | G | C2'-C1' | -9.29 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1335 | U | P-O5' | -9.28 | 1.50 | 1.59 |
| 34 | i | 1402 | G | C2'-C1' | -9.27 | 1.43 | 1.53 |
| 34 | i | 1622 | C | O4'-C1' | 9.27 | 1.53 | 1.41 |
| 34 | i | 678 | U | O4'-C1' | -9.26 | 1.29 | 1.41 |
| 19 | S | 40 | TYR | CA-C | -9.25 | 1.28 | 1.52 |
| 34 | i | 367 | G | C2'-C1' | -9.25 | 1.43 | 1.53 |
| 34 | i | 1557 | C | O4'-C1' | 9.25 | 1.53 | 1.41 |
| 34 | i | 1460 | C | O4'-C1' | 9.23 | 1.53 | 1.41 |
| 34 | i | 1729 | G | O4'-C1' | 9.22 | 1.53 | 1.41 |
| 34 | i | 944 | C | O4'-C1' | 9.21 | 1.53 | 1.41 |
| 34 | i | 618 | A | O4'-C1' | -9.19 | 1.29 | 1.41 |
| 4 | D | 96 | LEU | C-N | 9.17 | 1.55 | 1.34 |
| 34 | i | 1177 | A | C2'-C1' | -9.16 | 1.43 | 1.53 |
| 34 | i | 49 | C | C2'-C1' | -9.15 | 1.43 | 1.53 |
| 34 | i | 405 | A | C2'-C1' | 9.15 | 1.63 | 1.53 |
| 34 | i | 1477 | G | C2'-C1' | -9.14 | 1.43 | 1.53 |
| 34 | i | 650 | C | C2'-C1' | -9.14 | 1.43 | 1.53 |
| 34 | i | 666 | C | O4'-C1' | 9.13 | 1.53 | 1.41 |
| 34 | i | 1049 | C | O4'-C1' | 9.13 | 1.53 | 1.41 |
| 34 | i | 1275 | C | C2'-C1' | 9.13 | 1.63 | 1.53 |
| 34 | i | 42 | A | C2'-C1' | -9.12 | 1.43 | 1.53 |
| 34 | i | 939 | U | O4'-C1' | 9.12 | 1.53 | 1.41 |
| 34 | i | 827 | G | C2'-C1' | -9.12 | 1.43 | 1.53 |
| 3 | C | 47 | PRO | N-CD | 9.10 | 1.60 | 1.47 |
| 34 | i | 481 | C | O4'-C1' | 9.09 | 1.53 | 1.41 |
| 2 | B | 155 | TYR | CB-CG | -9.09 | 1.38 | 1.51 |
| 34 | i | 1607 | G | C2'-C1' | 9.09 | 1.63 | 1.53 |
| 34 | i | 895 | U | O4'-C1' | 9.08 | 1.53 | 1.41 |
| 34 | i | 804 | A | O4'-C1' | 9.08 | 1.53 | 1.41 |
| 34 | i | 1850 | C | O4'-C1' | 9.07 | 1.53 | 1.41 |
| 34 | i | 171 | A | O4'-C1' | -9.06 | 1.29 | 1.41 |
| 34 | i | 1385 | C | C2'-C1' | -9.05 | 1.43 | 1.53 |
| 34 | i | 1028 | C | C2'-C1' | -9.04 | 1.43 | 1.53 |
| 34 | i | 1647 | G | C2'-C1' | -9.03 | 1.43 | 1.53 |
| 34 | i | 1341 | G | O4'-C1' | 9.02 | 1.53 | 1.41 |
| 34 | i | 1565 | G | O4'-C1' | -9.02 | 1.29 | 1.41 |
| 34 | i | 666 | C | C2'-C1' | -9.02 | 1.43 | 1.53 |
| 27 | a | 10 | ARG | CD-NE | 9.00 | 1.61 | 1.46 |
| 34 | i | 1288 | C | C2'-C1' | -8.99 | 1.43 | 1.53 |
| 8 | H | 109 | ARG | CA-CB | -8.98 | 1.34 | 1.53 |
| 34 | i | 373 | G | O4'-C1' | 8.97 | 1.53 | 1.41 |
| 34 | i | 1646 | A | C2'-C1' | 8.97 | 1.63 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 211 | U | O4'-C1' | 8.97 | 1.53 | 1.41 |
| 34 | i | 1040 | G | C2'-C1' | -8.97 | 1.43 | 1.53 |
| 34 | i | 972 | G | C2'-C1' | -8.96 | 1.43 | 1.53 |
| 34 | i | 1018 | U | O4'-C1' | 8.95 | 1.53 | 1.41 |
| 34 | i | 1559 | C | C2'-C1' | -8.95 | 1.43 | 1.53 |
| 34 | i | 1533 | C | O4'-C1' | 8.94 | 1.53 | 1.41 |
| 34 | i | 1780 | U | O4'-C1' | 8.94 | 1.53 | 1.41 |
| 34 | i | 683 | G | O4'-C1' | 8.92 | 1.53 | 1.41 |
| 34 | i | 204 | G | C2'-C1' | 8.92 | 1.63 | 1.53 |
| 34 | i | 69 | C | O4'-C1' | 8.91 | 1.53 | 1.41 |
| 34 | i | 1054 | A | O4'-C1' | 8.91 | 1.53 | 1.41 |
| 34 | i | 41 | G | O4'-C1' | 8.90 | 1.53 | 1.41 |
| 34 | i | 97 | U | O4'-C1' | 8.89 | 1.53 | 1.41 |
| 34 | i | 1829 | A | O4'-C1' | 8.89 | 1.53 | 1.41 |
| 34 | i | 1370 | C | O4'-C1' | 8.89 | 1.53 | 1.41 |
| 34 | i | 653 | C | O4'-C1' | 8.88 | 1.53 | 1.41 |
| 34 | i | 432 | C | C2'-C1' | -8.87 | 1.43 | 1.53 |
| 34 | i | 1478 | C | O4'-C1' | 8.87 | 1.53 | 1.41 |
| 34 | i | 813 | G | C2'-C1' | -8.86 | 1.43 | 1.53 |
| 34 | i | 1336 | U | C2'-C1' | 8.86 | 1.63 | 1.53 |
| 34 | i | 178 | C | O4'-C1' | 8.86 | 1.53 | 1.41 |
| 34 | i | 1813 | A | O4'-C1' | 8.86 | 1.53 | 1.41 |
| 34 | i | 220 | C | O4'-C1' | 8.85 | 1.53 | 1.41 |
| 34 | i | 1791 | U | O4'-C1' | 8.85 | 1.53 | 1.41 |
| 34 | i | 936 | U | O4'-C1' | 8.85 | 1.53 | 1.41 |
| 34 | i | 1104 | G | O4'-C1' | -8.84 | 1.30 | 1.41 |
| 34 | i | 1385 | C | O4'-C1' | 8.84 | 1.53 | 1.41 |
| 34 | i | 1571 | G | O4'-C1' | 8.84 | 1.53 | 1.41 |
| 34 | i | 106 | C | O4'-C1' | 8.82 | 1.53 | 1.41 |
| 7 | G | 36 | VAL | CB-CG1 | -8.82 | 1.34 | 1.52 |
| 34 | i | 1039 | G | C2'-C1' | -8.82 | 1.43 | 1.53 |
| 34 | i | 1407 | G | O4'-C1' | 8.82 | 1.53 | 1.41 |
| 34 | i | 69 | C | C2'-C1' | -8.82 | 1.43 | 1.53 |
| 34 | i | 1225 | G | C2'-C1' | -8.82 | 1.43 | 1.53 |
| 34 | i | 26 | U | O4'-C1' | 8.81 | 1.53 | 1.41 |
| 27 | a | 97 | PRO | C-N | 8.80 | 1.50 | 1.34 |
| 34 | i | 194 | C | O4'-C1' | 8.80 | 1.53 | 1.41 |
| 34 | i | 189 | G | O4'-C1' | 8.80 | 1.53 | 1.41 |
| 34 | i | 900 | A | C2'-C1' | -8.80 | 1.43 | 1.53 |
| 34 | i | 510 | A | O4'-C1' | 8.79 | 1.53 | 1.41 |
| 34 | i | 939 | U | C2'-C1' | -8.78 | 1.43 | 1.53 |
| 34 | i | 1706 | U | C2'-C1' | -8.76 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 380 | C | O4'-C1' | 8.76 | 1.53 | 1.41 |
| 34 | i | 1678 | C | C2'-C1' | -8.75 | 1.43 | 1.53 |
| 34 | i | 540 | C | O4'-C1' | 8.75 | 1.53 | 1.41 |
| 34 | i | 1456 | C | O4'-C1' | 8.74 | 1.53 | 1.41 |
| 34 | i | 1822 | C | C2'-C1' | -8.73 | 1.43 | 1.53 |
| 34 | i | 989 | G | C2'-C1' | -8.73 | 1.43 | 1.53 |
| 34 | i | 575 | C | O4'-C1' | 8.72 | 1.52 | 1.41 |
| 34 | i | 1440 | U | O4'-C1' | 8.72 | 1.52 | 1.41 |
| 34 | i | 170 | A | C2'-C1' | -8.72 | 1.43 | 1.53 |
| 34 | i | 1158 | C | O4'-C1' | 8.71 | 1.52 | 1.41 |
| 34 | i | 688 | U | C2'-C1' | -8.71 | 1.43 | 1.53 |
| 34 | i | 1218 | G | C2'-C1' | -8.70 | 1.43 | 1.53 |
| 34 | i | 853 | U | O4'-C1' | 8.70 | 1.52 | 1.41 |
| 19 | S | 54 | LYS | CA-C | 8.70 | 1.75 | 1.52 |
| 34 | i | 883 | U | O4'-C1' | -8.70 | 1.30 | 1.41 |
| 34 | i | 1176 | C | C2'-C1' | -8.69 | 1.43 | 1.53 |
| 34 | i | 1085 | G | C2'-C1' | -8.69 | 1.43 | 1.53 |
| 34 | i | 824 | G | O4'-C1' | -8.68 | 1.30 | 1.41 |
| 34 | i | 1560 | C | O4'-C1' | 8.68 | 1.52 | 1.41 |
| 34 | i | 17 | C | O4'-C1' | 8.68 | 1.52 | 1.41 |
| 34 | i | 677 | C | C2'-C1' | -8.68 | 1.43 | 1.53 |
| 34 | i | 1434 | A | O4'-C1' | 8.67 | 1.52 | 1.41 |
| 34 | i | 1465 | A | O4'-C1' | 8.67 | 1.52 | 1.41 |
| 34 | i | 292 | A | C2'-C1' | 8.66 | 1.62 | 1.53 |
| 34 | i | 1692 | A | C2'-C1' | 8.66 | 1.62 | 1.53 |
| 34 | i | 844 | U | O4'-C1' | 8.65 | 1.52 | 1.41 |
| 34 | i | 807 | A | C2'-C1' | -8.65 | 1.43 | 1.53 |
| 34 | i | 324 | C | C2'-C1' | -8.64 | 1.43 | 1.53 |
| 34 | i | 235 | C | O4'-C1' | 8.64 | 1.52 | 1.41 |
| 34 | i | 574 | A | C2'-C1' | -8.63 | 1.43 | 1.53 |
| 34 | i | 1221 | U | O4'-C1' | 8.62 | 1.52 | 1.41 |
| 34 | i | 107 | A | C2'-C1' | 8.61 | 1.62 | 1.53 |
| 34 | i | 537 | G | C2'-C1' | -8.60 | 1.43 | 1.53 |
| 34 | i | 1142 | C | O4'-C1' | 8.60 | 1.52 | 1.41 |
| 34 | i | 543 | U | O4'-C1' | 8.60 | 1.52 | 1.41 |
| 34 | i | 1185 | A | O4'-C1' | 8.59 | 1.52 | 1.41 |
| 34 | i | 30 | C | O4'-C1' | 8.59 | 1.52 | 1.41 |
| 34 | i | 1775 | A | O4'-C1' | 8.59 | 1.52 | 1.41 |
| 34 | i | 1221 | U | C2'-C1' | -8.54 | 1.44 | 1.53 |
| 34 | i | 1825 | A | O4'-C1' | 8.54 | 1.52 | 1.41 |
| 34 | i | 649 | G | O4'-C1' | -8.54 | 1.30 | 1.41 |
| 34 | i | 593 | C | O4'-C1' | 8.54 | 1.52 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1267 | C | C2'-C1' | -8.53 | 1.44 | 1.53 |
| 34 | i | 1200 | A | C2'-C1' | -8.53 | 1.44 | 1.53 |
| 34 | i | 1331 | G | C2'-C1' | -8.53 | 1.44 | 1.53 |
| 34 | i | 1068 | U | C2'-C1' | 8.52 | 1.62 | 1.53 |
| 34 | i | 1138 | G | C2'-C1' | 8.52 | 1.62 | 1.53 |
| 34 | i | 1414 | C | C2'-C1' | -8.52 | 1.44 | 1.53 |
| 34 | i | 50 | A | O4'-C1' | 8.51 | 1.52 | 1.41 |
| 34 | i | 1490 | U | C2'-C1' | 8.51 | 1.62 | 1.53 |
| 34 | i | 376 | C | C2'-C1' | -8.51 | 1.44 | 1.53 |
| 34 | i | 443 | C | O4'-C1' | 8.51 | 1.52 | 1.41 |
| 34 | i | 1345 | G | O4'-C1' | 8.49 | 1.52 | 1.41 |
| 34 | i | 1532 | A | C2'-C1' | 8.49 | 1.62 | 1.53 |
| 34 | i | 33 | G | C2'-C1' | -8.49 | 1.44 | 1.53 |
| 34 | i | 53 | C | C2'-C1' | 8.49 | 1.62 | 1.53 |
| 34 | i | 1624 | C | O4'-C1' | 8.49 | 1.52 | 1.41 |
| 34 | i | 168 | C | C2'-C1' | -8.48 | 1.44 | 1.53 |
| 34 | i | 361 | A | C2'-C1' | -8.48 | 1.44 | 1.53 |
| 34 | i | 1807 | A | O4'-C1' | 8.48 | 1.52 | 1.41 |
| 34 | i | 670 | G | O4'-C1' | 8.48 | 1.52 | 1.41 |
| 34 | i | 453 | C | O4'-C1' | 8.47 | 1.52 | 1.41 |
| 34 | i | 1495 | U | C2'-C1' | -8.46 | 1.44 | 1.53 |
| 34 | i | 1223 | G | O4'-C1' | 8.46 | 1.52 | 1.41 |
| 34 | i | 1168 | U | C2'-C1' | 8.46 | 1.62 | 1.53 |
| 4 | D | 4 | GLN | N-CA | -8.45 | 1.29 | 1.46 |
| 34 | i | 1672 | U | C2'-C1' | 8.44 | 1.62 | 1.53 |
| 34 | i | 1212 | C | O4'-C1' | 8.44 | 1.52 | 1.41 |
| 34 | i | 409 | G | O4'-C1' | 8.44 | 1.52 | 1.41 |
| 34 | i | 441 | G | C2'-C1' | -8.44 | 1.44 | 1.53 |
| 34 | i | 1476 | A | O4'-C1' | 8.43 | 1.52 | 1.41 |
| 34 | i | 1527 | C | O4'-C1' | 8.43 | 1.52 | 1.41 |
| 34 | i | 923 | C | O4'-C1' | 8.43 | 1.52 | 1.41 |
| 34 | i | 1611 | U | O4'-C1' | 8.42 | 1.52 | 1.41 |
| 34 | i | 661 | A | C2'-C1' | -8.42 | 1.44 | 1.53 |
| 34 | i | 1264 | C | O4'-C1' | 8.42 | 1.52 | 1.41 |
| 34 | i | 147 | A | C2'-C1' | 8.42 | 1.62 | 1.53 |
| 34 | i | 148 | U | C2'-C1' | 8.41 | 1.62 | 1.53 |
| 34 | i | 990 | C | C2'-C1' | -8.41 | 1.44 | 1.53 |
| 34 | i | 18 | C | C2'-C1' | -8.40 | 1.44 | 1.53 |
| 34 | i | 236 | C | O4'-C1' | 8.39 | 1.52 | 1.41 |
| 34 | i | 462 | C | C2'-C1' | -8.39 | 1.44 | 1.53 |
| 34 | i | 1079 | A | O4'-C1' | 8.39 | 1.52 | 1.41 |
| 10 | J | 164 | PRO | C-N | 8.39 | 1.53 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 165 | G | C2'-C1' | 8.38 | 1.62 | 1.53 |
| 34 | i | 159 | A | O4'-C1' | 8.37 | 1.52 | 1.41 |
| 34 | i | 1019 | A | C2'-C1' | 8.37 | 1.62 | 1.53 |
| 34 | i | 1367 | U | O4'-C1' | 8.36 | 1.52 | 1.41 |
| 34 | i | 1304 | U | O4'-C1' | -8.36 | 1.30 | 1.41 |
| 34 | i | 354 | A | C2'-C1' | -8.36 | 1.44 | 1.53 |
| 34 | i | 1292 | U | C2'-C1' | -8.36 | 1.44 | 1.53 |
| 34 | i | 965 | U | O4'-C1' | 8.35 | 1.52 | 1.41 |
| 34 | i | 1630 | C | O4'-C1' | 8.35 | 1.52 | 1.41 |
| 34 | i | 348 | C | O4'-C1' | 8.34 | 1.52 | 1.41 |
| 34 | i | 736 | C | C2'-C1' | -8.34 | 1.44 | 1.53 |
| 34 | i | 596 | G | O4'-C1' | -8.33 | 1.30 | 1.41 |
| 34 | i | 1325 | U | O4'-C1' | 8.32 | 1.52 | 1.41 |
| 34 | i | 465 | C | C2'-C1' | -8.32 | 1.44 | 1.53 |
| 34 | i | 937 | C | O4'-C1' | 8.32 | 1.52 | 1.41 |
| 34 | i | 1785 | A | O4'-C1' | 8.31 | 1.52 | 1.41 |
| 34 | i | 1569 | C | C2'-C1' | -8.31 | 1.44 | 1.53 |
| 34 | i | 557 | C | O4'-C1' | 8.31 | 1.52 | 1.41 |
| 34 | i | 908 | C | O4'-C1' | 8.31 | 1.52 | 1.41 |
| 34 | i | 625 | G | O4'-C1' | 8.30 | 1.52 | 1.41 |
| 34 | i | 1840 | G | C2'-C1' | -8.30 | 1.44 | 1.53 |
| 34 | i | 1252 | G | O4'-C1' | 8.30 | 1.52 | 1.41 |
| 34 | i | 1861 | U | O4'-C1' | -8.30 | 1.30 | 1.41 |
| 34 | i | 902 | U | O4'-C1' | 8.29 | 1.52 | 1.41 |
| 34 | i | 176 | U | O4'-C1' | 8.29 | 1.52 | 1.41 |
| 34 | i | 625 | G | C2'-C1' | -8.29 | 1.44 | 1.53 |
| 34 | i | 941 | U | C2'-C1' | -8.29 | 1.44 | 1.53 |
| 34 | i | 1401 | A | C2'-C1' | -8.29 | 1.44 | 1.53 |
| 34 | i | 1661 | C | O4'-C1' | 8.29 | 1.52 | 1.41 |
| 34 | i | 528 | U | O4'-C1' | 8.28 | 1.52 | 1.41 |
| 34 | i | 875 | C | O4'-C1' | 8.28 | 1.52 | 1.41 |
| 34 | i | 1046 | A | C2'-C1' | -8.27 | 1.44 | 1.53 |
| 34 | i | 72 | C | C2'-C1' | 8.27 | 1.62 | 1.53 |
| 34 | i | 832 | G | C2'-C1' | 8.26 | 1.62 | 1.53 |
| 34 | i | 187 | C | C2'-C1' | -8.26 | 1.44 | 1.53 |
| 34 | i | 1487 | G | C2'-C1' | -8.25 | 1.44 | 1.53 |
| 34 | i | 1295 | A | C2'-C1' | 8.25 | 1.62 | 1.53 |
| 34 | i | 1309 | A | O4'-C1' | 8.25 | 1.52 | 1.41 |
| 34 | i | 1304 | U | C2'-C1' | 8.24 | 1.62 | 1.53 |
| 34 | i | 955 | G | C2'-C1' | -8.23 | 1.44 | 1.53 |
| 34 | i | 313 | C | C2'-C1' | -8.23 | 1.44 | 1.53 |
| 34 | i | 607 | G | C2'-C1' | -8.23 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1679 | C | O4'-C1' | 8.21 | 1.52 | 1.41 |
| 34 | i | 1577 | C | O4'-C1' | 8.21 | 1.52 | 1.41 |
| 34 | i | 164 | A | O4'-C1' | 8.21 | 1.52 | 1.41 |
| 34 | i | 918 | A | C2'-C1' | 8.21 | 1.62 | 1.53 |
| 34 | i | 824 | G | C2'-C1' | -8.21 | 1.44 | 1.53 |
| 34 | i | 1663 | U | P-O5' | -8.21 | 1.51 | 1.59 |
| 34 | i | 1183 | G | O4'-C1' | 8.19 | 1.52 | 1.41 |
| 34 | i | 1558 | G | C2'-C1' | -8.19 | 1.44 | 1.53 |
| 34 | i | 1261 | A | O4'-C1' | 8.18 | 1.52 | 1.41 |
| 34 | i | 741 | C | O3'-P | -8.18 | 1.51 | 1.61 |
| 3 | C | 193 | PRO | N-CD | 8.17 | 1.59 | 1.47 |
| 34 | i | 1075 | C | C2'-C1' | -8.17 | 1.44 | 1.53 |
| 34 | i | 40 | A | C2'-C1' | 8.17 | 1.62 | 1.53 |
| 34 | i | 676 | U | C2'-C1' | 8.16 | 1.62 | 1.53 |
| 34 | i | 1140 | A | O4'-C1' | 8.16 | 1.52 | 1.41 |
| 34 | i | 1059 | C | C2'-C1' | -8.15 | 1.44 | 1.53 |
| 34 | i | 618 | A | C2'-C1' | 8.15 | 1.62 | 1.53 |
| 34 | i | 1086 | C | O4'-C1' | 8.13 | 1.52 | 1.41 |
| 34 | i | 303 | G | C2'-C1' | 8.12 | 1.62 | 1.53 |
| 34 | i | 1699 | C | C2'-C1' | -8.12 | 1.44 | 1.53 |
| 34 | i | 739 | U | O4'-C1' | 8.11 | 1.52 | 1.41 |
| 34 | i | 302 | C | C2'-C1' | -8.11 | 1.44 | 1.53 |
| 34 | i | 1390 | G | O4'-C1' | 8.11 | 1.52 | 1.41 |
| 34 | i | 1107 | U | O4'-C1' | 8.10 | 1.52 | 1.41 |
| 34 | i | 1480 | A | O4'-C1' | 8.10 | 1.52 | 1.41 |
| 34 | i | 1794 | A | O4'-C1' | 8.09 | 1.52 | 1.41 |
| 34 | i | 943 | G | C2'-C1' | -8.09 | 1.44 | 1.53 |
| 34 | i | 959 | A | O4'-C1' | -8.08 | 1.31 | 1.41 |
| 34 | i | 219 | U | O4'-C1' | 8.08 | 1.52 | 1.41 |
| 34 | i | 630 | A | O4'-C1' | 8.07 | 1.52 | 1.41 |
| 34 | i | 1001 | G | C2'-C1' | -8.07 | 1.44 | 1.53 |
| 34 | i | 727 | G | O4'-C1' | 8.06 | 1.52 | 1.41 |
| 34 | i | 1824 | U | O4'-C1' | 8.06 | 1.52 | 1.41 |
| 34 | i | 336 | C | O4'-C1' | 8.06 | 1.52 | 1.41 |
| 34 | i | 1028 | C | O4'-C1' | 8.06 | 1.52 | 1.41 |
| 34 | i | 1733 | C | C2'-C1' | -8.06 | 1.44 | 1.53 |
| 34 | i | 1201 | C | O4'-C1' | 8.04 | 1.52 | 1.41 |
| 34 | i | 152 | U | C2'-C1' | -8.04 | 1.44 | 1.53 |
| 34 | i | 1623 | C | O4'-C1' | 8.04 | 1.52 | 1.41 |
| 19 | S | 95 | TYR | CD1-CE1 | -8.04 | 1.27 | 1.39 |
| 20 | T | 4 | VAL | C-N | 8.04 | 1.52 | 1.34 |
| 34 | i | 26 | U | C2'-C1' | -8.04 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 7 | G | 36 | VAL | CA-CB | -8.03 | 1.37 | 1.54 |
| 34 | i | 1394 | G | C2'-C1' | -8.03 | 1.44 | 1.53 |
| 34 | i | 537 | G | O4'-C1' | 8.03 | 1.52 | 1.41 |
| 34 | i | 369 | C | O4'-C1' | 8.03 | 1.52 | 1.41 |
| 34 | i | 317 | G | O4'-C1' | -8.02 | 1.31 | 1.41 |
| 34 | i | 1102 | C | C2'-C1' | 8.02 | 1.62 | 1.53 |
| 34 | i | 835 | C | C2'-C1' | -8.02 | 1.44 | 1.53 |
| 34 | i | 1425 | G | O3'-P | -8.02 | 1.51 | 1.61 |
| 34 | i | 1800 | A | C2'-C1' | -8.01 | 1.44 | 1.53 |
| 34 | i | 536 | G | O4'-C1' | 8.01 | 1.52 | 1.41 |
| 34 | i | 57 | U | C2'-C1' | 8.01 | 1.62 | 1.53 |
| 34 | i | 1579 | G | O4'-C1' | 8.00 | 1.52 | 1.41 |
| 34 | i | 1604 | C | O4'-C1' | 8.00 | 1.52 | 1.41 |
| 18 | R | 89 | SER | CA-C | 7.99 | 1.73 | 1.52 |
| 34 | i | 1450 | A | O4'-C1' | 7.99 | 1.52 | 1.41 |
| 34 | i | 1446 | G | C2'-C1' | -7.98 | 1.44 | 1.53 |
| 34 | i | 1705 | C | O4'-C1' | 7.98 | 1.52 | 1.41 |
| 34 | i | 624 | A | O4'-C1' | 7.97 | 1.52 | 1.41 |
| 34 | i | 1327 | C | O4'-C1' | 7.96 | 1.52 | 1.41 |
| 34 | i | 86 | C | C2'-C1' | -7.96 | 1.44 | 1.53 |
| 34 | i | 988 | A | O4'-C1' | 7.96 | 1.51 | 1.41 |
| 34 | i | 1652 | G | C2'-C1' | -7.96 | 1.44 | 1.53 |
| 34 | i | 1482 | A | P-O5' | -7.95 | 1.51 | 1.59 |
| 34 | i | 37 | C | C2'-C1' | -7.95 | 1.44 | 1.53 |
| 34 | i | 1447 | G | C2'-C1' | -7.94 | 1.44 | 1.53 |
| 34 | i | 599 | U | O4'-C1' | 7.94 | 1.51 | 1.41 |
| 34 | i | 1386 | U | C2'-C1' | -7.94 | 1.44 | 1.53 |
| 34 | i | 1535 | G | C2'-C1' | -7.94 | 1.44 | 1.53 |
| 34 | i | 863 | G | O4'-C1' | 7.93 | 1.51 | 1.41 |
| 34 | i | 1150 | U | O4'-C1' | -7.93 | 1.31 | 1.41 |
| 34 | i | 1279 | C | C2'-C1' | -7.92 | 1.44 | 1.53 |
| 34 | i | 1522 | C | O4'-C1' | 7.92 | 1.51 | 1.41 |
| 34 | i | 1061 | G | C2'-C1' | -7.92 | 1.44 | 1.53 |
| 34 | i | 1857 | A | C2'-C1' | 7.92 | 1.62 | 1.53 |
| 34 | i | 1537 | C | C2'-C1' | -7.92 | 1.44 | 1.53 |
| 34 | i | 1321 | G | O4'-C1' | 7.91 | 1.51 | 1.41 |
| 34 | i | 492 | C | O4'-C1' | 7.91 | 1.51 | 1.41 |
| 34 | i | 486 | C | C2'-C1' | -7.90 | 1.44 | 1.53 |
| 34 | i | 1126 | G | O4'-C1' | -7.90 | 1.31 | 1.41 |
| 34 | i | 969 | C | O4'-C1' | 7.90 | 1.51 | 1.41 |
| 34 | i | 275 | C | O4'-C1' | 7.88 | 1.51 | 1.41 |
| 34 | i | 930 | G | C2'-C1' | -7.88 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 463 | A | O4'-C1' | 7.88 | 1.51 | 1.41 |
| 34 | i | 1818 | A | O4'-C1' | -7.88 | 1.31 | 1.41 |
| 7 | G | 131 | ARG | N-CA | -7.87 | 1.30 | 1.46 |
| 34 | i | 338 | A | C2'-C1' | -7.86 | 1.44 | 1.53 |
| 34 | i | 948 | G | C2'-C1' | -7.86 | 1.44 | 1.53 |
| 34 | i | 1480 | A | C2'-C1' | -7.86 | 1.44 | 1.53 |
| 34 | i | 1796 | C | O4'-C1' | 7.85 | 1.51 | 1.41 |
| 34 | i | 337 | G | O4'-C1' | 7.85 | 1.51 | 1.41 |
| 34 | i | 953 | A | C2'-C1' | -7.83 | 1.44 | 1.53 |
| 34 | i | 876 | G | C2'-C1' | 7.83 | 1.61 | 1.53 |
| 34 | i | 119 | U | C2'-C1' | -7.83 | 1.44 | 1.53 |
| 34 | i | 1385 | C | P-O5' | -7.82 | 1.51 | 1.59 |
| 34 | i | 226 | A | C2'-C1' | -7.81 | 1.44 | 1.53 |
| 34 | i | 557 | C | C2'-C1' | -7.81 | 1.44 | 1.53 |
| 34 | i | 171 | A | C2'-C1' | 7.80 | 1.61 | 1.53 |
| 34 | i | 399 | C | O4'-C1' | 7.78 | 1.51 | 1.41 |
| 34 | i | 521 | A | O3'-P | -7.78 | 1.51 | 1.61 |
| 34 | i | 566 | A | C2'-C1' | -7.77 | 1.44 | 1.53 |
| 34 | i | 190 | A | O4'-C1' | 7.77 | 1.51 | 1.41 |
| 34 | i | 880 | C | O4'-C1' | 7.77 | 1.51 | 1.41 |
| 34 | i | 1687 | U | C2'-C1' | -7.77 | 1.44 | 1.53 |
| 34 | i | 924 | G | C2'-C1' | -7.76 | 1.44 | 1.53 |
| 34 | i | 1403 | U | O4'-C1' | 7.76 | 1.51 | 1.41 |
| 34 | i | 447 | C | O4'-C1' | 7.76 | 1.51 | 1.41 |
| 34 | i | 1071 | C | O4'-C1' | 7.76 | 1.51 | 1.41 |
| 34 | i | 1592 | C | C2'-C1' | -7.75 | 1.44 | 1.53 |
| 34 | i | 37 | C | O4'-C1' | 7.75 | 1.51 | 1.41 |
| 34 | i | 342 | U | O4'-C1' | 7.74 | 1.51 | 1.41 |
| 34 | i | 544 | A | O4'-C1' | -7.74 | 1.31 | 1.41 |
| 34 | i | 829 | C | O4'-C1' | 7.74 | 1.51 | 1.41 |
| 34 | i | 685 | G | C1'-N9 | -7.73 | 1.36 | 1.46 |
| 34 | i | 1027 | A | O4'-C1' | 7.73 | 1.51 | 1.41 |
| 34 | i | 60 | A | O4'-C1' | -7.73 | 1.31 | 1.41 |
| 34 | i | 200 | U | C2'-C1' | -7.72 | 1.44 | 1.53 |
| 34 | i | 368 | U | C2'-C1' | -7.72 | 1.44 | 1.53 |
| 34 | i | 189 | G | C2'-C1' | -7.72 | 1.44 | 1.53 |
| 34 | i | 29 | G | C2'-C1' | -7.71 | 1.44 | 1.53 |
| 34 | i | 938 | G | O4'-C1' | 7.71 | 1.51 | 1.41 |
| 34 | i | 1332 | C | O4'-C1' | 7.71 | 1.51 | 1.41 |
| 34 | i | 563 | U | O4'-C1' | 7.70 | 1.51 | 1.41 |
| 34 | i | 604 | G | C1'-N9 | -7.70 | 1.36 | 1.46 |
| 10 | J | 35 | TYR | CD2-CE2 | -7.70 | 1.27 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 449 | C | C2'-C1' | -7.69 | 1.44 | 1.53 |
| 7 | G | 130 | PRO | C-N | -7.69 | 1.16 | 1.34 |
| 34 | i | 820 | C | O4'-C1' | 7.68 | 1.51 | 1.41 |
| 34 | i | 452 | C | O4'-C1' | 7.67 | 1.51 | 1.41 |
| 34 | i | 1123 | C | O4'-C1' | 7.67 | 1.51 | 1.41 |
| 34 | i | 38 | A | C2'-C1' | 7.67 | 1.61 | 1.53 |
| 34 | i | 846 | C | O4'-C1' | 7.67 | 1.51 | 1.41 |
| 34 | i | 864 | G | C2'-C1' | -7.66 | 1.45 | 1.53 |
| 34 | i | 846 | C | C2'-C1' | -7.66 | 1.45 | 1.53 |
| 34 | i | 874 | G | C2'-C1' | -7.66 | 1.45 | 1.53 |
| 34 | i | 1384 | A | O4'-C1' | 7.65 | 1.51 | 1.41 |
| 34 | i | 1664 | G | C2'-C1' | -7.65 | 1.45 | 1.53 |
| 34 | i | 49 | C | O4'-C1' | 7.64 | 1.51 | 1.41 |
| 34 | i | 1313 | U | O4'-C1' | 7.64 | 1.51 | 1.41 |
| 34 | i | 1045 | A | O4'-C1' | -7.64 | 1.31 | 1.41 |
| 34 | i | 1343 | U | O4'-C1' | 7.64 | 1.51 | 1.41 |
| 34 | i | 399 | C | C2'-C1' | -7.62 | 1.45 | 1.53 |
| 34 | i | 1444 | A | C2'-C1' | -7.62 | 1.45 | 1.53 |
| 34 | i | 1382 | A | O4'-C1' | 7.61 | 1.51 | 1.41 |
| 34 | i | 1245 | C | O4'-C1' | 7.60 | 1.51 | 1.41 |
| 34 | i | 725 | C | O4'-C1' | 7.60 | 1.51 | 1.41 |
| 34 | i | 1006 | G | C2'-C1' | 7.60 | 1.61 | 1.53 |
| 34 | i | 1823 | G | O4'-C1' | 7.60 | 1.51 | 1.41 |
| 34 | i | 1799 | G | O4'-C1' | 7.59 | 1.51 | 1.41 |
| 34 | i | 1633 | G | O4'-C1' | 7.58 | 1.51 | 1.41 |
| 34 | i | 271 | G | O3'-P | -7.58 | 1.52 | 1.61 |
| 19 | S | 82 | TRP | CA-CB | -7.57 | 1.37 | 1.53 |
| 34 | i | 1041 | U | O4'-C1' | 7.57 | 1.51 | 1.41 |
| 34 | i | 1292 | U | O4'-C1' | 7.57 | 1.51 | 1.41 |
| 34 | i | 689 | G | C1'-N9 | -7.56 | 1.36 | 1.46 |
| 34 | i | 1423 | C | C2'-C1' | 7.56 | 1.61 | 1.53 |
| 34 | i | 211 | U | O3'-P | -7.55 | 1.52 | 1.61 |
| 34 | i | 194 | C | C2'-C1' | -7.55 | 1.45 | 1.53 |
| 34 | i | 518 | A | O4'-C1' | 7.55 | 1.51 | 1.41 |
| 34 | i | 386 | U | O4'-C1' | 7.55 | 1.51 | 1.41 |
| 34 | i | 1398 | A | C2'-C1' | -7.54 | 1.45 | 1.53 |
| 34 | i | 485 | U | C2'-C1' | -7.54 | 1.45 | 1.53 |
| 34 | i | 1392 | A | C2'-C1' | 7.54 | 1.61 | 1.53 |
| 34 | i | 343 | C | O4'-C1' | 7.54 | 1.51 | 1.41 |
| 34 | i | 360 | G | O4'-C1' | 7.54 | 1.51 | 1.41 |
| 10 | J | 164 | PRO | N-CA | -7.53 | 1.34 | 1.47 |
| 34 | i | 1493 | G | O4'-C1' | 7.53 | 1.51 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1568 | G | O4'-C1' | 7.53 | 1.51 | 1.41 |
| 34 | i | 460 | G | C2'-C1' | -7.52 | 1.45 | 1.53 |
| 34 | i | 355 | C | C2'-C1' | -7.52 | 1.45 | 1.53 |
| 34 | i | 1465 | A | C2'-C1' | -7.52 | 1.45 | 1.53 |
| 34 | i | 95 | G | C2'-C1' | -7.51 | 1.45 | 1.53 |
| 34 | i | 202 | U | C2'-C1' | -7.51 | 1.45 | 1.53 |
| 34 | i | 1187 | C | O4'-C1' | 7.51 | 1.51 | 1.41 |
| 34 | i | 442 | G | O4'-C1' | 7.50 | 1.51 | 1.41 |
| 34 | i | 1145 | A | C2'-C1' | -7.50 | 1.45 | 1.53 |
| 34 | i | 1260 | C | O4'-C1' | 7.48 | 1.51 | 1.41 |
| 34 | i | 1123 | C | C2'-C1' | -7.48 | 1.45 | 1.53 |
| 34 | i | 1814 | G | C2'-C1' | -7.48 | 1.45 | 1.53 |
| 34 | i | 840 | U | O4'-C1' | 7.48 | 1.51 | 1.41 |
| 34 | i | 151 | C | P-O5' | -7.48 | 1.52 | 1.59 |
| 34 | i | 872 | C | O4'-C1' | 7.47 | 1.51 | 1.41 |
| 34 | i | 656 | U | O4'-C1' | 7.46 | 1.51 | 1.41 |
| 34 | i | 1138 | G | O4'-C1' | -7.46 | 1.31 | 1.41 |
| 34 | i | 859 | U | O4'-C1' | 7.46 | 1.51 | 1.41 |
| 34 | i | 818 | U | O4'-C1' | 7.46 | 1.51 | 1.41 |
| 34 | i | 1423 | C | O4'-C1' | 7.46 | 1.51 | 1.41 |
| 34 | i | 1850 | C | C2'-C1' | -7.46 | 1.45 | 1.53 |
| 7 | G | 170 | ARG | CA-CB | 7.46 | 1.70 | 1.53 |
| 34 | i | 1299 | C | O4'-C1' | -7.45 | 1.31 | 1.41 |
| 34 | i | 278 | U | O4'-C1' | 7.45 | 1.51 | 1.41 |
| 34 | i | 1137 | G | O4'-C1' | -7.45 | 1.31 | 1.41 |
| 34 | i | 1839 | A | C2'-C1' | -7.45 | 1.45 | 1.53 |
| 34 | i | 1638 | U | O4'-C1' | 7.45 | 1.51 | 1.41 |
| 34 | i | 1758 | G | C5'-C4' | 7.45 | 1.60 | 1.51 |
| 34 | i | 1626 | U | C2'-C1' | -7.44 | 1.45 | 1.53 |
| 34 | i | 223 | A | O4'-C1' | 7.43 | 1.51 | 1.41 |
| 34 | i | 1778 | G | C2'-C1' | -7.42 | 1.45 | 1.53 |
| 34 | i | 488 | C | C2'-C1' | -7.42 | 1.45 | 1.53 |
| 34 | i | 347 | C | O4'-C1' | 7.42 | 1.51 | 1.41 |
| 34 | i | 933 | C | C2'-C1' | -7.42 | 1.45 | 1.53 |
| 34 | i | 428 | G | O4'-C1' | -7.41 | 1.32 | 1.41 |
| 34 | i | 686 | G | C2'-C1' | -7.41 | 1.45 | 1.53 |
| 34 | i | 3 | C | C2'-C1' | 7.40 | 1.61 | 1.53 |
| 34 | i | 1151 | U | O4'-C1' | 7.40 | 1.51 | 1.41 |
| 34 | i | 377 | C | C2'-C1' | -7.40 | 1.45 | 1.53 |
| 34 | i | 493 | C | O4'-C1' | 7.40 | 1.51 | 1.41 |
| 34 | i | 1340 | A | O4'-C1' | 7.40 | 1.51 | 1.41 |
| 34 | i | 1676 | U | C2'-C1' | -7.39 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1808 | G | O4'-C1' | 7.39 | 1.51 | 1.41 |
| 34 | i | 86 | C | O4'-C1' | 7.39 | 1.51 | 1.41 |
| 34 | i | 1434 | A | C2'-C1' | 7.39 | 1.61 | 1.53 |
| 34 | i | 1345 | G | C2'-C1' | -7.39 | 1.45 | 1.53 |
| 34 | i | 820 | C | C2'-C1' | -7.38 | 1.45 | 1.53 |
| 34 | i | 845 | A | O4'-C1' | 7.38 | 1.51 | 1.41 |
| 34 | i | 1186 | A | O4'-C1' | 7.38 | 1.51 | 1.41 |
| 34 | i | 1835 | C | C2'-C1' | -7.38 | 1.45 | 1.53 |
| 34 | i | 515 | A | C2'-C1' | -7.38 | 1.45 | 1.53 |
| 34 | i | 1045 | A | C2'-C1' | 7.37 | 1.61 | 1.53 |
| 34 | i | 120 | U | O4'-C1' | 7.36 | 1.51 | 1.41 |
| 34 | i | 1091 | U | O4'-C1' | 7.35 | 1.51 | 1.41 |
| 34 | i | 225 | C | O3'-P | -7.35 | 1.52 | 1.61 |
| 34 | i | 1008 | A | C2'-C1' | -7.34 | 1.45 | 1.53 |
| 34 | i | 1363 | U | O4'-C1' | 7.34 | 1.51 | 1.41 |
| 16 | P | 122 | THR | CA-CB | 7.34 | 1.72 | 1.53 |
| 34 | i | 743 | U | O3'-P | -7.33 | 1.52 | 1.61 |
| 34 | i | 982 | G | C2'-C1' | -7.33 | 1.45 | 1.53 |
| 34 | i | 514 | U | O4'-C1' | 7.33 | 1.51 | 1.41 |
| 34 | i | 621 | U | C2'-C1' | -7.33 | 1.45 | 1.53 |
| 34 | i | 1668 | U | C2'-C1' | -7.31 | 1.45 | 1.53 |
| 34 | i | 1059 | C | O4'-C1' | 7.31 | 1.51 | 1.41 |
| 34 | i | 1798 | U | O4'-C1' | 7.31 | 1.51 | 1.41 |
| 34 | i | 213 | C | O4'-C1' | 7.30 | 1.51 | 1.41 |
| 9 | I | 3 | ILE | CA-CB | -7.29 | 1.38 | 1.54 |
| 34 | i | 404 | A | C2'-C1' | 7.28 | 1.61 | 1.53 |
| 34 | i | 85 | A | O4'-C1' | 7.27 | 1.51 | 1.41 |
| 34 | i | 456 | G | C4'-C3' | 7.27 | 1.61 | 1.53 |
| 34 | i | 798 | A | O4'-C1' | 7.27 | 1.51 | 1.41 |
| 34 | i | 1472 | A | C2'-C1' | 7.27 | 1.61 | 1.53 |
| 34 | i | 1489 | C | C2'-C1' | 7.27 | 1.61 | 1.53 |
| 34 | i | 216 | U | O4'-C1' | 7.26 | 1.51 | 1.41 |
| 14 | N | 137 | PRO | N-CD | 7.26 | 1.58 | 1.47 |
| 34 | i | 596 | G | C2'-C1' | -7.25 | 1.45 | 1.53 |
| 34 | i | 516 | A | C2'-C1' | -7.25 | 1.45 | 1.53 |
| 34 | i | 1741 | U | O3'-P | 7.24 | 1.69 | 1.61 |
| 34 | i | 1096 | A | C2'-C1' | -7.24 | 1.45 | 1.53 |
| 6 | F | 108 | PRO | N-CD | 7.24 | 1.57 | 1.47 |
| 34 | i | 652 | G | O4'-C1' | 7.23 | 1.51 | 1.41 |
| 34 | i | 361 | A | O4'-C1' | 7.22 | 1.51 | 1.41 |
| 34 | i | 35 | C | C2'-C1' | -7.21 | 1.45 | 1.53 |
| 34 | i | 1460 | C | C2'-C1' | -7.21 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10 | J | 91 | LYS | C-O | -7.21 | 1.09 | 1.23 |
| 34 | i | 1424 | G | C2'-C1' | 7.21 | 1.61 | 1.53 |
| 34 | i | 86 | C | P-O5' | -7.21 | 1.52 | 1.59 |
| 34 | i | 327 | C | O4'-C1' | 7.21 | 1.51 | 1.41 |
| 34 | i | 856 | G | O4'-C1' | 7.21 | 1.51 | 1.41 |
| 34 | i | 42 | A | O4'-C1' | 7.20 | 1.51 | 1.41 |
| 25 | Y | 91 | LEU | C-N | 7.20 | 1.50 | 1.34 |
| 34 | i | 576 | G | O4'-C1' | 7.20 | 1.51 | 1.41 |
| 34 | i | 6 | G | C2'-C1' | -7.18 | 1.45 | 1.53 |
| 34 | i | 632 | U | C2'-C1' | -7.18 | 1.45 | 1.53 |
| 34 | i | 660 | A | O4'-C1' | -7.18 | 1.32 | 1.41 |
| 34 | i | 1259 | U | C5'-C4' | 7.18 | 1.59 | 1.51 |
| 34 | i | 485 | U | O4'-C1' | 7.17 | 1.50 | 1.41 |
| 34 | i | 937 | C | C2'-C1' | -7.16 | 1.45 | 1.53 |
| 34 | i | 470 | G | C2'-C1' | -7.16 | 1.45 | 1.53 |
| 34 | i | 897 | G | C2'-C1' | -7.16 | 1.45 | 1.53 |
| 34 | i | 1223 | G | C2'-C1' | -7.15 | 1.45 | 1.53 |
| 34 | i | 1387 | C | C2'-C1' | -7.15 | 1.45 | 1.53 |
| 34 | i | 871 | A | C2'-C1' | -7.15 | 1.45 | 1.53 |
| 34 | i | 1256 | A | C2'-C1' | -7.13 | 1.45 | 1.53 |
| 7 | G | 131 | ARG | CB-CG | 7.13 | 1.71 | 1.52 |
| 34 | i | 1293 | U | C2'-C1' | 7.12 | 1.61 | 1.53 |
| 34 | i | 619 | A | C2'-C1' | 7.12 | 1.61 | 1.53 |
| 34 | i | 916 | A | O4'-C1' | 7.11 | 1.50 | 1.41 |
| 34 | i | 74 | G | O4'-C1' | 7.11 | 1.50 | 1.41 |
| 34 | i | 1033 | G | C2'-C1' | -7.11 | 1.45 | 1.53 |
| 34 | i | 1405 | A | O4'-C1' | 7.11 | 1.50 | 1.41 |
| 34 | i | 960 | A | C2'-C1' | 7.10 | 1.61 | 1.53 |
| 34 | i | 1528 | A | C2'-C1' | -7.09 | 1.45 | 1.53 |
| 34 | i | 1419 | C | C2'-C1' | -7.09 | 1.45 | 1.53 |
| 34 | i | 988 | A | C2'-C1' | -7.09 | 1.45 | 1.53 |
| 34 | i | 959 | A | C2'-C1' | -7.08 | 1.45 | 1.53 |
| 34 | i | 489 | G | C2'-C1' | -7.07 | 1.45 | 1.53 |
| 8 | H | 111 | LYS | CA-C | -7.06 | 1.34 | 1.52 |
| 24 | X | 24 | ASP | CA-C | -7.06 | 1.34 | 1.52 |
| 34 | i | 81 | U | O4'-C1' | 7.05 | 1.50 | 1.41 |
| 34 | i | 632 | U | O4'-C1' | 7.05 | 1.50 | 1.41 |
| 34 | i | 1255 | A | O4'-C1' | -7.05 | 1.32 | 1.41 |
| 34 | i | 104 | A | O4'-C1' | 7.04 | 1.50 | 1.41 |
| 34 | i | 390 | C | C2'-C1' | -7.03 | 1.45 | 1.53 |
| 34 | i | 1211 | C | O4'-C1' | 7.03 | 1.50 | 1.41 |
| 34 | i | 59 | U | C2'-C1' | 7.03 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1174 | U | C2'-C1' | -7.02 | 1.45 | 1.53 |
| 34 | i | 1355 | U | C2'-C1' | 7.02 | 1.61 | 1.53 |
| 34 | i | 880 | C | C2'-C1' | -7.01 | 1.45 | 1.53 |
| 34 | i | 674 | G | C2'-C1' | -7.01 | 1.45 | 1.53 |
| 34 | i | 818 | U | C2'-C1' | -7.00 | 1.45 | 1.53 |
| 34 | i | 1717 | G | O4'-C1' | 7.00 | 1.50 | 1.41 |
| 34 | i | 1843 | G | C2'-C1' | -7.00 | 1.45 | 1.53 |
| 34 | i | 1583 | A | O4'-C1' | 7.00 | 1.50 | 1.41 |
| 34 | i | 1125 | G | C2'-C1' | -6.99 | 1.45 | 1.53 |
| 34 | i | 655 | G | C2'-C1' | -6.98 | 1.45 | 1.53 |
| 34 | i | 1044 | G | C5'-C4' | 6.98 | 1.59 | 1.51 |
| 34 | i | 601 | G | O4'-C1' | 6.97 | 1.50 | 1.41 |
| 34 | i | 742 | C | C2'-C1' | -6.97 | 1.45 | 1.53 |
| 10 | J | 35 | TYR | CE1-CZ | -6.97 | 1.29 | 1.38 |
| 34 | i | 118 | C | O4'-C1' | 6.97 | 1.50 | 1.41 |
| 34 | i | 903 | G | O4'-C1' | 6.96 | 1.50 | 1.41 |
| 34 | i | 876 | G | O4'-C1' | -6.96 | 1.32 | 1.41 |
| 34 | i | 418 | U | C2'-C1' | 6.96 | 1.61 | 1.53 |
| 3 | C | 93 | LYS | C-N | -6.96 | 1.18 | 1.34 |
| 34 | i | 811 | U | O4'-C1' | 6.96 | 1.50 | 1.41 |
| 34 | i | 1039 | G | O4'-C1' | 6.95 | 1.50 | 1.41 |
| 34 | i | 1054 | A | C2'-C1' | -6.95 | 1.45 | 1.53 |
| 34 | i | 172 | U | O4'-C1' | 6.94 | 1.50 | 1.41 |
| 34 | i | 1395 | C | O4'-C1' | 6.94 | 1.50 | 1.41 |
| 34 | i | 1519 | G | O4'-C1' | -6.94 | 1.32 | 1.41 |
| 34 | i | 464 | G | C2'-C1' | -6.94 | 1.45 | 1.53 |
| 34 | i | 860 | A | C2'-C1' | -6.94 | 1.45 | 1.53 |
| 34 | i | 899 | A | O4'-C1' | -6.94 | 1.32 | 1.41 |
| 34 | i | 1250 | C | O4'-C1' | 6.94 | 1.50 | 1.41 |
| 34 | i | 823 | A | O4'-C1' | 6.93 | 1.50 | 1.41 |
| 34 | i | 609 | A | C2'-C1' | 6.93 | 1.60 | 1.53 |
| 34 | i | 735 | C | C2'-C1' | -6.93 | 1.45 | 1.53 |
| 34 | i | 231 | C | C2'-C1' | -6.92 | 1.45 | 1.53 |
| 34 | i | 264 | U | O3'-P | -6.92 | 1.52 | 1.61 |
| 34 | i | 1021 | U | C2'-C1' | 6.92 | 1.60 | 1.53 |
| 34 | i | 382 | A | C2'-C1' | -6.92 | 1.45 | 1.53 |
| 34 | i | 1283 | A | C2'-C1' | 6.91 | 1.60 | 1.53 |
| 34 | i | 1043 | C | C2'-C1' | -6.91 | 1.45 | 1.53 |
| 2 | B | 133 | TYR | CB-CG | -6.90 | 1.41 | 1.51 |
| 34 | i | 46 | A | C2'-C1' | -6.89 | 1.45 | 1.53 |
| 34 | i | 1782 | A | O4'-C1' | 6.89 | 1.50 | 1.41 |
| 34 | i | 1784 | A | O4'-C1' | 6.89 | 1.50 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1654 | U | O3'-P | -6.89 | 1.52 | 1.61 |
| 34 | i | 1805 | C | C2'-C1' | -6.89 | 1.45 | 1.53 |
| 34 | i | 65 | C | C2'-C1' | 6.88 | 1.60 | 1.53 |
| 34 | i | 1621 | C | O4'-C1' | 6.88 | 1.50 | 1.41 |
| 34 | i | 1032 | A | C2'-C1' | -6.88 | 1.45 | 1.53 |
| 34 | i | 668 | U | O4'-C1' | 6.87 | 1.50 | 1.41 |
| 34 | i | 983 | A | O4'-C1' | 6.87 | 1.50 | 1.41 |
| 34 | i | 325 | G | C2'-C1' | 6.86 | 1.60 | 1.53 |
| 35 | j | 23 | G | C1'-N9 | -6.86 | 1.37 | 1.46 |
| 34 | i | 1452 | G | O4'-C1' | 6.86 | 1.50 | 1.41 |
| 34 | i | 597 | U | C2'-C1' | -6.85 | 1.45 | 1.53 |
| 34 | i | 1244 | U | C2'-C1' | -6.85 | 1.45 | 1.53 |
| 34 | i | 1681 | G | C2'-C1' | -6.85 | 1.45 | 1.53 |
| 34 | i | 1696 | C | O4'-C1' | 6.85 | 1.50 | 1.41 |
| 34 | i | 1538 | U | P-O5' | -6.84 | 1.52 | 1.59 |
| 24 | X | 128 | VAL | CA-CB | -6.84 | 1.40 | 1.54 |
| 34 | i | 1175 | G | C2'-C1' | -6.84 | 1.45 | 1.53 |
| 34 | i | 1723 | U | O4'-C1' | 6.83 | 1.50 | 1.41 |
| 34 | i | 1303 | U | C2'-C1' | 6.83 | 1.60 | 1.53 |
| 34 | i | 896 | C | O4'-C1' | 6.83 | 1.50 | 1.41 |
| 24 | X | 126 | ALA | CA-CB | -6.82 | 1.38 | 1.52 |
| 34 | i | 1836 | C | C2'-C1' | -6.82 | 1.45 | 1.53 |
| 34 | i | 969 | C | C5'-C4' | 6.82 | 1.59 | 1.51 |
| 34 | i | 1670 | A | O4'-C1' | -6.82 | 1.32 | 1.41 |
| 34 | i | 435 | A | O4'-C1' | 6.81 | 1.50 | 1.41 |
| 34 | i | 1842 | U | C2'-C1' | -6.81 | 1.45 | 1.53 |
| 34 | i | 1144 | A | C2'-C1' | 6.80 | 1.60 | 1.53 |
| 34 | i | 348 | C | C2'-C1' | -6.80 | 1.45 | 1.53 |
| 34 | i | 1018 | U | O3'-P | -6.80 | 1.52 | 1.61 |
| 34 | i | 1149 | C | O4'-C1' | -6.79 | 1.32 | 1.41 |
| 34 | i | 1525 | U | O4'-C1' | 6.79 | 1.50 | 1.41 |
| 34 | i | 1031 | A | O4'-C1' | 6.79 | 1.50 | 1.41 |
| 34 | i | 314 | U | O4'-C1' | -6.78 | 1.32 | 1.41 |
| 34 | i | 1072 | G | C2'-C1' | -6.77 | 1.46 | 1.53 |
| 34 | i | 147 | A | O4'-C1' | -6.77 | 1.32 | 1.41 |
| 34 | i | 118 | C | C2'-C1' | -6.76 | 1.46 | 1.53 |
| 34 | i | 470 | G | O4'-C1' | 6.76 | 1.50 | 1.41 |
| 34 | i | 1378 | A | O4'-C1' | 6.76 | 1.50 | 1.41 |
| 34 | i | 513 | A | O4'-C1' | 6.76 | 1.50 | 1.41 |
| 34 | i | 941 | U | O4'-C1' | 6.75 | 1.50 | 1.41 |
| 34 | i | 438 | A | C2'-C1' | 6.75 | 1.60 | 1.53 |
| 34 | i | 628 | C | O4'-C1' | 6.74 | 1.50 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 19 | S | 95 | TYR | CE1-CZ | -6.73 | 1.29 | 1.38 |
| 34 | i | 1691 | C | C2'-C1' | -6.73 | 1.46 | 1.53 |
| 34 | i | 1734 | C | C2'-C1' | -6.73 | 1.46 | 1.53 |
| 34 | i | 556 | U | C2'-C1' | 6.72 | 1.60 | 1.53 |
| 34 | i | 434 | G | O4'-C1' | -6.72 | 1.32 | 1.41 |
| 34 | i | 397 | G | C2'-C1' | 6.72 | 1.60 | 1.53 |
| 34 | i | 320 | G | C2'-C1' | -6.71 | 1.46 | 1.53 |
| 34 | i | 663 | G | P-O5' | -6.71 | 1.53 | 1.59 |
| 34 | i | 699 | C | C5'-C4' | 6.71 | 1.59 | 1.51 |
| 34 | i | 1842 | U | O4'-C1' | 6.71 | 1.50 | 1.41 |
| 34 | i | 1707 | A | O4'-C1' | 6.70 | 1.50 | 1.41 |
| 34 | i | 1051 | A | C5'-C4' | 6.70 | 1.59 | 1.51 |
| 34 | i | 504 | U | C2'-C1' | -6.70 | 1.46 | 1.53 |
| 34 | i | 812 | A | C2'-C1' | -6.69 | 1.46 | 1.53 |
| 34 | i | 1203 | G | O4'-C1' | 6.68 | 1.50 | 1.41 |
| 34 | i | 1836 | C | O4'-C1' | 6.68 | 1.50 | 1.41 |
| 34 | i | 1514 | U | C2'-C1' | 6.67 | 1.60 | 1.53 |
| 34 | i | 996 | C | O4'-C1' | 6.67 | 1.50 | 1.41 |
| 10 | J | 163 | SER | C-N | -6.66 | 1.21 | 1.34 |
| 34 | i | 1035 | C | O4'-C1' | 6.66 | 1.50 | 1.41 |
| 34 | i | 913 | U | C2'-C1' | 6.66 | 1.60 | 1.53 |
| 34 | i | 14 | C | O4'-C1' | 6.65 | 1.50 | 1.41 |
| 34 | i | 165 | G | O4'-C1' | -6.65 | 1.33 | 1.41 |
| 34 | i | 1051 | A | O4'-C1' | 6.65 | 1.50 | 1.41 |
| 34 | i | 1634 | G | O4'-C1' | 6.65 | 1.50 | 1.41 |
| 34 | i | 1743 | G | C2'-C1' | -6.65 | 1.46 | 1.53 |
| 19 | S | 95 | TYR | CD2-CE2 | -6.64 | 1.29 | 1.39 |
| 34 | i | 388 | A | O4'-C1' | 6.64 | 1.50 | 1.41 |
| 34 | i | 1810 | G | C2'-C1' | -6.64 | 1.46 | 1.53 |
| 34 | i | 1735 | C | C2'-C1' | -6.63 | 1.46 | 1.53 |
| 34 | i | 338 | A | O4'-C1' | 6.63 | 1.50 | 1.41 |
| 34 | i | 946 | C | C2'-C1' | -6.62 | 1.46 | 1.53 |
| 34 | i | 1232 | G | C3'-C2' | 6.62 | 1.60 | 1.52 |
| 34 | i | 273 | G | O4'-C1' | 6.61 | 1.50 | 1.41 |
| 34 | i | 411 | G | O3'-P | -6.61 | 1.53 | 1.61 |
| 34 | i | 1391 | C | O4'-C1' | 6.61 | 1.50 | 1.41 |
| 7 | G | 157 | VAL | CA-CB | -6.61 | 1.40 | 1.54 |
| 34 | i | 103 | A | O4'-C1' | -6.61 | 1.33 | 1.41 |
| 34 | i | 494 | G | C2'-C1' | -6.60 | 1.46 | 1.53 |
| 34 | i | 1414 | C | O4'-C1' | -6.60 | 1.33 | 1.41 |
| 34 | i | 1731 | G | C2'-C1' | -6.60 | 1.46 | 1.53 |
| 34 | i | 1712 | C | O4'-C1' | 6.59 | 1.50 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 467 | G | C2'-C1' | -6.59 | 1.46 | 1.53 |
| 34 | i | 1479 | A | C2'-C1' | 6.57 | 1.60 | 1.53 |
| 34 | i | 1797 | U | O4'-C1' | 6.57 | 1.50 | 1.41 |
| 34 | i | 733 | G | C2'-C1' | 6.57 | 1.60 | 1.53 |
| 34 | i | 1499 | C | O4'-C1' | 6.57 | 1.50 | 1.41 |
| 34 | i | 101 | U | C2'-C1' | 6.56 | 1.60 | 1.53 |
| 34 | i | 9 | U | O4'-C1' | 6.56 | 1.50 | 1.41 |
| 34 | i | 227 | A | O4'-C1' | 6.55 | 1.50 | 1.41 |
| 34 | i | 1737 | C | O4'-C1' | 6.55 | 1.50 | 1.41 |
| 34 | i | 442 | G | C2'-C1' | -6.54 | 1.46 | 1.53 |
| 34 | i | 1667 | U | C2'-C1' | -6.54 | 1.46 | 1.53 |
| 34 | i | 1234 | U | C2'-C1' | -6.54 | 1.46 | 1.53 |
| 34 | i | 1626 | U | O4'-C1' | 6.54 | 1.50 | 1.41 |
| 34 | i | 100 | U | O4'-C1' | 6.53 | 1.50 | 1.41 |
| 34 | i | 1121 | C | O4'-C1' | 6.53 | 1.50 | 1.41 |
| 34 | i | 205 | G | O4'-C1' | 6.52 | 1.50 | 1.41 |
| 34 | i | 300 | G | C2'-C1' | -6.52 | 1.46 | 1.53 |
| 34 | i | 30 | C | C2'-C1' | -6.52 | 1.46 | 1.53 |
| 3 | C | 72 | PRO | N-CD | 6.51 | 1.56 | 1.47 |
| 34 | i | 806 | A | O4'-C1' | 6.51 | 1.50 | 1.41 |
| 34 | i | 795 | U | C2'-C1' | -6.50 | 1.46 | 1.53 |
| 34 | i | 1061 | G | O4'-C1' | 6.49 | 1.50 | 1.41 |
| 34 | i | 201 | G | C2'-C1' | 6.48 | 1.60 | 1.53 |
| 34 | i | 637 | U | O4'-C1' | 6.48 | 1.50 | 1.41 |
| 34 | i | 928 | G | C2'-C1' | -6.48 | 1.46 | 1.53 |
| 34 | i | 965 | U | C2'-C1' | -6.48 | 1.46 | 1.53 |
| 34 | i | 958 | A | C2'-C1' | 6.48 | 1.60 | 1.53 |
| 34 | i | 471 | C | O4'-C1' | 6.48 | 1.50 | 1.41 |
| 34 | i | 1243 | C | O4'-C1' | 6.47 | 1.50 | 1.41 |
| 34 | i | 892 | U | O4'-C1' | 6.47 | 1.50 | 1.41 |
| 34 | i | 1702 | U | C2'-C1' | -6.46 | 1.46 | 1.53 |
| 34 | i | 1392 | A | O4'-C1' | -6.46 | 1.33 | 1.41 |
| 9 | I | 8 | TRP | CD2-CE3 | -6.45 | 1.30 | 1.40 |
| 34 | i | 920 | G | P-O5' | -6.45 | 1.53 | 1.59 |
| 34 | i | 1463 | C | O4'-C1' | 6.45 | 1.50 | 1.41 |
| 34 | i | 1797 | U | C2'-C1' | -6.45 | 1.46 | 1.53 |
| 34 | i | 1030 | A | C2'-C1' | 6.45 | 1.60 | 1.53 |
| 34 | i | 799 | C | O4'-C1' | 6.44 | 1.50 | 1.41 |
| 34 | i | 826 | A | C2'-C1' | 6.43 | 1.60 | 1.53 |
| 34 | i | 1603 | U | C2'-C1' | -6.43 | 1.46 | 1.53 |
| 34 | i | 458 | A | C2'-C1' | -6.42 | 1.46 | 1.53 |
| 34 | i | 421 | G | C2'-C1' | -6.41 | 1.46 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1569 | C | O4'-C1' | 6.41 | 1.50 | 1.41 |
| 34 | i | 160 | U | O4'-C1' | 6.40 | 1.50 | 1.41 |
| 34 | i | 627 | U | C2'-C1' | 6.40 | 1.60 | 1.53 |
| 34 | i | 1090 | C | C2'-C1' | -6.39 | 1.46 | 1.53 |
| 34 | i | 1610 | U | O4'-C1' | 6.39 | 1.50 | 1.41 |
| 34 | i | 1121 | C | C2'-C1' | -6.39 | 1.46 | 1.53 |
| 34 | i | 1278 | A | O4'-C1' | 6.39 | 1.50 | 1.41 |
| 34 | i | 1173 | U | O4'-C1' | 6.38 | 1.50 | 1.41 |
| 34 | i | 1840 | G | O4'-C1' | 6.37 | 1.50 | 1.41 |
| 34 | i | 1311 | U | C5'-C4' | 6.36 | 1.58 | 1.51 |
| 34 | i | 370 | G | O4'-C1' | -6.36 | 1.33 | 1.41 |
| 34 | i | 639 | U | O4'-C1' | 6.36 | 1.50 | 1.41 |
| 7 | G | 156 | TYR | CB-CG | -6.35 | 1.42 | 1.51 |
| 34 | i | 94 | G | O4'-C1' | 6.35 | 1.50 | 1.41 |
| 34 | i | 290 | A | C2'-C1' | 6.35 | 1.60 | 1.53 |
| 34 | i | 406 | U | C2'-C1' | 6.35 | 1.60 | 1.53 |
| 34 | i | 1615 | A | O4'-C1' | -6.35 | 1.33 | 1.41 |
| 34 | i | 1799 | G | C2'-C1' | -6.35 | 1.46 | 1.53 |
| 34 | i | 389 | C | C2'-C1' | -6.35 | 1.46 | 1.53 |
| 34 | i | 997 | A | C2'-C1' | 6.34 | 1.60 | 1.53 |
| 34 | i | 1103 | G | C2'-C1' | -6.34 | 1.46 | 1.53 |
| 34 | i | 1622 | C | C2'-C1' | -6.34 | 1.46 | 1.53 |
| 34 | i | 1334 | G | O4'-C1' | 6.33 | 1.49 | 1.41 |
| 34 | i | 1032 | A | C5'-C4' | 6.33 | 1.58 | 1.51 |
| 34 | i | 1102 | C | O4'-C1' | 6.33 | 1.49 | 1.41 |
| 34 | i | 139 | C | C2'-C1' | 6.33 | 1.60 | 1.53 |
| 34 | i | 1138 | G | P-O5' | -6.33 | 1.53 | 1.59 |
| 10 | J | 101 | LYS | N-CA | 6.32 | 1.58 | 1.46 |
| 34 | i | 1256 | A | O3'-P | -6.32 | 1.53 | 1.61 |
| 34 | i | 408 | A | O4'-C1' | 6.32 | 1.49 | 1.41 |
| 34 | i | 1215 | C | O4'-C1' | 6.32 | 1.49 | 1.41 |
| 34 | i | 1233 | C | P-O5' | -6.32 | 1.53 | 1.59 |
| 34 | i | 962 | U | C2'-C1' | -6.31 | 1.46 | 1.53 |
| 4 | D | 20 | GLU | CG-CD | 6.30 | 1.61 | 1.51 |
| 34 | i | 1047 | G | C2'-C1' | -6.30 | 1.46 | 1.53 |
| 34 | i | 1444 | A | O4'-C1' | 6.30 | 1.49 | 1.41 |
| 34 | i | 528 | U | C2'-C1' | -6.30 | 1.46 | 1.53 |
| 34 | i | 567 | U | O4'-C1' | 6.30 | 1.49 | 1.41 |
| 34 | i | 1042 | U | O4'-C1' | 6.30 | 1.49 | 1.41 |
| 34 | i | 461 | G | O4'-C1' | -6.29 | 1.33 | 1.41 |
| 7 | G | 170 | ARG | CA-C | -6.28 | 1.36 | 1.52 |
| 5 | E | 150 | PRO | N-CD | 6.28 | 1.56 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17 | Q | 145 | TYR | CD2-CE2 | -6.28 | 1.29 | 1.39 |
| 34 | i | 1584 | A | C2'-C1' | 6.28 | 1.60 | 1.53 |
| 34 | i | 879 | U | C5'-C4' | 6.27 | 1.58 | 1.51 |
| 34 | i | 1753 | G | C2'-C1' | -6.27 | 1.46 | 1.53 |
| 26 | Z | 104 | ARG | CD-NE | -6.27 | 1.35 | 1.46 |
| 34 | i | 404 | A | O4'-C1' | 6.27 | 1.49 | 1.41 |
| 34 | i | 1426 | C | P-O5' | -6.26 | 1.53 | 1.59 |
| 34 | i | 665 | U | O4'-C1' | 6.26 | 1.49 | 1.41 |
| 34 | i | 898 | G | C2'-C1' | -6.26 | 1.46 | 1.53 |
| 34 | i | 954 | G | O4'-C1' | -6.26 | 1.33 | 1.41 |
| 34 | i | 793 | C | O3'-P | -6.26 | 1.53 | 1.61 |
| 34 | i | 1280 | A | C2'-C1' | -6.26 | 1.46 | 1.53 |
| 34 | i | 273 | G | C2'-C1' | -6.25 | 1.46 | 1.53 |
| 18 | R | 89 | SER | C-N | 6.25 | 1.48 | 1.34 |
| 34 | i | 220 | C | C2'-C1' | -6.25 | 1.46 | 1.53 |
| 34 | i | 1628 | A | C2'-C1' | -6.25 | 1.46 | 1.53 |
| 34 | i | 1684 | C | O4'-C1' | 6.25 | 1.49 | 1.41 |
| 34 | i | 1426 | C | C2'-C1' | 6.24 | 1.60 | 1.53 |
| 34 | i | 1476 | A | C2'-C1' | -6.24 | 1.46 | 1.53 |
| 10 | J | 144 | ILE | CA-CB | -6.24 | 1.40 | 1.54 |
| 34 | i | 656 | U | O3'-P | -6.24 | 1.53 | 1.61 |
| 34 | i | 1097 | U | C2'-C1' | -6.24 | 1.46 | 1.53 |
| 34 | i | 974 | G | C2'-C1' | -6.23 | 1.46 | 1.53 |
| 34 | i | 678 | U | C2'-C1' | 6.22 | 1.60 | 1.53 |
| 34 | i | 1167 | G | C2'-C1' | 6.22 | 1.60 | 1.53 |
| 34 | i | 1167 | G | C5'-C4' | 6.22 | 1.58 | 1.51 |
| 34 | i | 889 | U | C2'-C1' | 6.22 | 1.60 | 1.53 |
| 34 | i | 364 | G | C2'-C1' | -6.21 | 1.46 | 1.53 |
| 34 | i | 33 | G | O4'-C1' | 6.21 | 1.49 | 1.41 |
| 34 | i | 1402 | G | O4'-C1' | 6.21 | 1.49 | 1.41 |
| 34 | i | 583 | C | C2'-C1' | -6.21 | 1.46 | 1.53 |
| 34 | i | 601 | G | C2'-C1' | -6.20 | 1.46 | 1.53 |
| 34 | i | 969 | C | C2'-C1' | -6.20 | 1.46 | 1.53 |
| 34 | i | 469 | C | O4'-C1' | 6.19 | 1.49 | 1.41 |
| 34 | i | 477 | U | C4'-C3' | 6.19 | 1.59 | 1.53 |
| 34 | i | 1085 | G | O4'-C1' | 6.19 | 1.49 | 1.41 |
| 35 | j | 49 | A | C1'-N9 | -6.18 | 1.38 | 1.46 |
| 17 | Q | 145 | TYR | CD1-CE1 | -6.18 | 1.30 | 1.39 |
| 34 | i | 337 | G | C2'-C1' | -6.18 | 1.46 | 1.53 |
| 34 | i | 1657 | U | O4'-C1' | 6.16 | 1.49 | 1.41 |
| 24 | X | 116 | PRO | CA-C | 6.16 | 1.65 | 1.52 |
| 34 | i | 1415 | C | O4'-C1' | 6.16 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3 | C | 195 | PRO | N-CD | 6.16 | 1.56 | 1.47 |
| 34 | i | 1093 | G | O4'-C1' | -6.15 | 1.33 | 1.41 |
| 34 | i | 1852 | G | C2'-C1' | -6.15 | 1.46 | 1.53 |
| 34 | i | 356 | U | O4'-C1' | 6.14 | 1.49 | 1.41 |
| 34 | i | 335 | U | O4'-C1' | 6.14 | 1.49 | 1.41 |
| 34 | i | 1119 | C | C5'-C4' | 6.14 | 1.58 | 1.51 |
| 34 | i | 494 | G | C3'-C2' | -6.13 | 1.46 | 1.52 |
| 34 | i | 806 | A | C2'-C1' | -6.13 | 1.46 | 1.53 |
| 27 | a | 10 | ARG | NE-CZ | 6.13 | 1.41 | 1.33 |
| 34 | i | 1078 | A | O4'-C1' | 6.13 | 1.49 | 1.41 |
| 34 | i | 945 | G | C2'-C1' | -6.13 | 1.46 | 1.53 |
| 34 | i | 1791 | U | P-O5' | -6.12 | 1.53 | 1.59 |
| 34 | i | 994 | A | C2'-C1' | 6.12 | 1.60 | 1.53 |
| 34 | i | 1700 | C | C2'-C1' | -6.12 | 1.46 | 1.53 |
| 34 | i | 1652 | G | C4'-C3' | 6.11 | 1.59 | 1.53 |
| 34 | i | 1284 | U | C5'-C4' | 6.11 | 1.58 | 1.51 |
| 34 | i | 930 | G | O4'-C1' | 6.10 | 1.49 | 1.41 |
| 34 | i | 349 | U | C2'-C1' | -6.10 | 1.46 | 1.53 |
| 34 | i | 1373 | U | C2'-C1' | -6.10 | 1.46 | 1.53 |
| 34 | i | 867 | U | O4'-C1' | -6.09 | 1.33 | 1.41 |
| 34 | i | 627 | U | C5'-C4' | 6.09 | 1.58 | 1.51 |
| 34 | i | 1515 | G | C4'-C3' | 6.09 | 1.59 | 1.53 |
| 34 | i | 1740 | A | O4'-C1' | -6.09 | 1.33 | 1.41 |
| 34 | i | 1800 | A | O4'-C1' | 6.08 | 1.49 | 1.41 |
| 34 | i | 1739 | G | C2'-C1' | 6.08 | 1.60 | 1.53 |
| 34 | i | 1804 | U | O4'-C1' | 6.08 | 1.49 | 1.41 |
| 18 | R | 111 | PHE | CB-CG | -6.08 | 1.41 | 1.51 |
| 6 | F | 45 | TYR | CB-CG | -6.07 | 1.42 | 1.51 |
| 34 | i | 472 | G | C2'-C1' | -6.07 | 1.46 | 1.53 |
| 34 | i | 370 | G | P-O5' | -6.07 | 1.53 | 1.59 |
| 34 | i | 1650 | C | C2'-C1' | -6.07 | 1.46 | 1.53 |
| 34 | i | 1132 | U | O4'-C1' | 6.06 | 1.49 | 1.41 |
| 34 | i | 1397 | A | C2'-C1' | 6.06 | 1.60 | 1.53 |
| 34 | i | 934 | A | C2'-C1' | -6.06 | 1.46 | 1.53 |
| 7 | G | 36 | VAL | CB-CG2 | -6.05 | 1.40 | 1.52 |
| 34 | i | 396 | U | O4'-C1' | 6.05 | 1.49 | 1.41 |
| 34 | i | 1032 | A | O4'-C1' | 6.05 | 1.49 | 1.41 |
| 34 | i | 629 | C | C2'-C1' | -6.05 | 1.46 | 1.53 |
| 34 | i | 170 | A | O3'-P | -6.05 | 1.53 | 1.61 |
| 34 | i | 155 | G | O4'-C1' | 6.05 | 1.49 | 1.41 |
| 34 | i | 449 | C | C5'-C4' | 6.05 | 1.58 | 1.51 |
| 34 | i | 1066 | A | O4'-C1' | 6.04 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1641 | C | C4'-O4' | -6.04 | 1.37 | 1.45 |
| 18 | R | 86 | PRO | N-CD | 6.03 | 1.56 | 1.47 |
| 34 | i | 8 | U | C2'-C1' | 6.03 | 1.59 | 1.53 |
| 34 | i | 342 | U | C4'-C3' | -6.02 | 1.46 | 1.53 |
| 34 | i | 1016 | A | C5'-C4' | 6.02 | 1.58 | 1.51 |
| 34 | i | 1427 | G | O4'-C1' | 6.02 | 1.49 | 1.41 |
| 34 | i | 301 | C | C2'-C1' | 6.01 | 1.59 | 1.53 |
| 34 | i | 1774 | G | O4'-C1' | 6.01 | 1.49 | 1.41 |
| 34 | i | 891 | G | C2'-C1' | -6.01 | 1.46 | 1.53 |
| 34 | i | 214 | A | C2'-C1' | -6.00 | 1.46 | 1.53 |
| 34 | i | 1777 | C | C2'-C1' | -6.00 | 1.46 | 1.53 |
| 34 | i | 391 | A | C2'-C1' | 6.00 | 1.59 | 1.53 |
| 34 | i | 1564 | A | C2'-C1' | 6.00 | 1.59 | 1.53 |
| 34 | i | 1332 | C | P-O5' | -6.00 | 1.53 | 1.59 |
| 34 | i | 155 | G | P-O5' | -5.99 | 1.53 | 1.59 |
| 8 | H | 111 | LYS | N-CA | 5.98 | 1.58 | 1.46 |
| 34 | i | 1264 | C | C2'-C1' | -5.98 | 1.46 | 1.53 |
| 34 | i | 1037 | G | O4'-C1' | 5.98 | 1.49 | 1.41 |
| 34 | i | 529 | C | C2'-C1' | -5.97 | 1.46 | 1.53 |
| 34 | i | 1710 | A | O4'-C1' | 5.96 | 1.49 | 1.41 |
| 35 | j | 59 | A | C1'-N9 | -5.96 | 1.38 | 1.46 |
| 34 | i | 106 | C | C2'-C1' | -5.96 | 1.46 | 1.53 |
| 34 | i | 656 | U | C2'-C1' | 5.96 | 1.59 | 1.53 |
| 34 | i | 175 | A | O4'-C1' | 5.96 | 1.49 | 1.41 |
| 34 | i | 83 | A | C2'-C1' | -5.96 | 1.46 | 1.53 |
| 34 | i | 593 | C | C2'-C1' | -5.96 | 1.46 | 1.53 |
| 34 | i | 649 | G | C2'-C1' | 5.96 | 1.59 | 1.53 |
| 34 | i | 1172 | G | O4'-C1' | 5.96 | 1.49 | 1.41 |
| 34 | i | 343 | C | O3'-P | -5.95 | 1.54 | 1.61 |
| 34 | i | 1502 | A | O4'-C1' | 5.95 | 1.49 | 1.41 |
| 34 | i | 210 | G | C2'-C1' | 5.94 | 1.59 | 1.53 |
| 34 | i | 318 | U | O4'-C1' | 5.94 | 1.49 | 1.41 |
| 34 | i | 1652 | G | P-O5' | -5.94 | 1.53 | 1.59 |
| 34 | i | 795 | U | C3'-C2' | 5.93 | 1.59 | 1.52 |
| 34 | i | 797 | U | P-O5' | -5.93 | 1.53 | 1.59 |
| 7 | G | 131 | ARG | C-O | -5.93 | 1.12 | 1.23 |
| 34 | i | 146 | G | C3'-O3' | 5.93 | 1.50 | 1.42 |
| 34 | i | 1296 | U | C2'-C1' | 5.92 | 1.59 | 1.53 |
| 34 | i | 1311 | U | O4'-C1' | -5.92 | 1.33 | 1.41 |
| 32 | f | 85 | TYR | CE2-CZ | -5.92 | 1.30 | 1.38 |
| 34 | i | 351 | U | C2'-C1' | 5.92 | 1.59 | 1.53 |
| 34 | i | 2 | A | O4'-C1' | 5.92 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10 | J | 188 | GLY | CA-C | 5.92 | 1.61 | 1.51 |
| 34 | i | 1667 | U | P-O5' | -5.91 | 1.53 | 1.59 |
| 34 | i | 742 | C | C5'-C4' | 5.91 | 1.58 | 1.51 |
| 34 | i | 1582 | G | O4'-C1' | -5.91 | 1.33 | 1.41 |
| 34 | i | 1845 | A | C2'-C1' | 5.91 | 1.59 | 1.53 |
| 34 | i | 602 | U | C2'-C1' | -5.91 | 1.46 | 1.53 |
| 34 | i | 1633 | G | C2'-C1' | -5.90 | 1.46 | 1.53 |
| 34 | i | 68 | A | O4'-C1' | 5.90 | 1.49 | 1.41 |
| 34 | i | 1776 | G | C2'-C1' | -5.90 | 1.46 | 1.53 |
| 34 | i | 54 | A | C5'-C4' | 5.89 | 1.58 | 1.51 |
| 34 | i | 1604 | C | P-O5' | -5.89 | 1.53 | 1.59 |
| 34 | i | 1680 | U | C5'-C4' | 5.89 | 1.58 | 1.51 |
| 34 | i | 805 | A | O4'-C1' | 5.89 | 1.49 | 1.41 |
| 34 | i | 1730 | A | O4'-C1' | 5.88 | 1.49 | 1.41 |
| 34 | i | 1830 | G | C2'-C1' | -5.88 | 1.46 | 1.53 |
| 10 | J | 187 | ALA | CA-C | 5.88 | 1.68 | 1.52 |
| 34 | i | 282 | G | O4'-C1' | 5.88 | 1.49 | 1.41 |
| 34 | i | 825 | C | O3'-P | -5.87 | 1.54 | 1.61 |
| 23 | W | 129 | PHE | CB-CG | -5.87 | 1.41 | 1.51 |
| 34 | i | 804 | A | O3'-P | -5.87 | 1.54 | 1.61 |
| 34 | i | 231 | C | O4'-C1' | 5.87 | 1.49 | 1.41 |
| 34 | i | 1591 | U | O4'-C1' | 5.86 | 1.49 | 1.41 |
| 5 | E | 130 | PHE | CB-CG | -5.86 | 1.41 | 1.51 |
| 34 | i | 545 | A | C2'-C1' | -5.86 | 1.47 | 1.53 |
| 24 | X | 23 | HIS | N-CA | -5.85 | 1.34 | 1.46 |
| 34 | i | 1415 | C | O3'-P | -5.85 | 1.54 | 1.61 |
| 34 | i | 990 | C | O4'-C1' | 5.85 | 1.49 | 1.41 |
| 34 | i | 408 | A | C5'-C4' | 5.85 | 1.58 | 1.51 |
| 4 | D | 4 | GLN | C-N | -5.84 | 1.20 | 1.34 |
| 34 | i | 279 | G | C2'-C1' | 5.84 | 1.59 | 1.53 |
| 34 | i | 819 | U | O4'-C1' | -5.84 | 1.34 | 1.41 |
| 34 | i | 1639 | C | O4'-C1' | 5.83 | 1.49 | 1.41 |
| 34 | i | 366 | A | C2'-C1' | -5.83 | 1.47 | 1.53 |
| 34 | i | 1324 | G | O4'-C1' | 5.83 | 1.49 | 1.41 |
| 34 | i | 439 | A | C5'-C4' | 5.83 | 1.58 | 1.51 |
| 34 | i | 566 | A | O4'-C1' | 5.82 | 1.49 | 1.41 |
| 34 | i | 565 | A | C2'-C1' | -5.80 | 1.47 | 1.53 |
| 34 | i | 743 | U | C2'-C1' | -5.79 | 1.47 | 1.53 |
| 34 | i | 1523 | G | O4'-C1' | -5.79 | 1.34 | 1.41 |
| 34 | i | 1577 | C | C5'-C4' | 5.78 | 1.58 | 1.51 |
| 34 | i | 1048 | A | O3'-P | -5.78 | 1.54 | 1.61 |
| 34 | i | 1015 | C | C4'-C3' | 5.77 | 1.59 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1412 | C | C2'-C1' | -5.77 | 1.47 | 1.53 |
| 34 | i | 1394 | G | O4'-C1' | 5.77 | 1.49 | 1.41 |
| 34 | i | 1402 | G | C5'-C4' | 5.77 | 1.58 | 1.51 |
| 34 | i | 1821 | U | O4'-C1' | 5.77 | 1.49 | 1.41 |
| 34 | i | 834 | G | C2'-C1' | -5.77 | 1.47 | 1.53 |
| 34 | i | 1161 | G | C2'-C1' | 5.77 | 1.59 | 1.53 |
| 34 | i | 1310 | U | O4'-C1' | -5.76 | 1.34 | 1.41 |
| 34 | i | 285 | U | C2'-C1' | -5.76 | 1.47 | 1.53 |
| 34 | i | 1040 | G | O4'-C1' | 5.76 | 1.49 | 1.41 |
| 34 | i | 1567 | C | C2'-C1' | -5.76 | 1.47 | 1.53 |
| 34 | i | 883 | U | C5'-C4' | 5.76 | 1.58 | 1.51 |
| 34 | i | 1845 | A | O4'-C1' | 5.75 | 1.49 | 1.41 |
| 34 | i | 415 | G | P-O5' | -5.75 | 1.53 | 1.59 |
| 34 | i | 647 | U | O4'-C1' | 5.75 | 1.49 | 1.41 |
| 34 | i | 1567 | C | O4'-C1' | 5.75 | 1.49 | 1.41 |
| 31 | e | 77 | HIS | C-N | 5.75 | 1.43 | 1.33 |
| 34 | i | 211 | U | C2'-C1' | -5.74 | 1.47 | 1.53 |
| 34 | i | 1014 | U | O4'-C1' | 5.74 | 1.49 | 1.41 |
| 34 | i | 1473 | U | O4'-C1' | 5.74 | 1.49 | 1.41 |
| 34 | i | 654 | A | O4'-C1' | 5.73 | 1.49 | 1.41 |
| 34 | i | 589 | A | O4'-C1' | 5.73 | 1.49 | 1.41 |
| 34 | i | 1073 | A | O4'-C1' | 5.72 | 1.49 | 1.41 |
| 34 | i | 854 | A | O4'-C1' | 5.72 | 1.49 | 1.41 |
| 34 | i | 1232 | G | C2'-C1' | -5.71 | 1.47 | 1.53 |
| 34 | i | 1038 | A | O4'-C1' | 5.71 | 1.49 | 1.41 |
| 34 | i | 307 | G | C2'-C1' | -5.70 | 1.47 | 1.53 |
| 34 | i | 914 | U | O4'-C1' | 5.70 | 1.49 | 1.41 |
| 34 | i | 1414 | C | O3'-P | -5.70 | 1.54 | 1.61 |
| 34 | i | 317 | G | C5'-C4' | 5.70 | 1.58 | 1.51 |
| 34 | i | 1026 | A | C2'-C1' | 5.70 | 1.59 | 1.53 |
| 34 | i | 1599 | G | C3'-C2' | -5.70 | 1.46 | 1.52 |
| 34 | i | 319 | G | C2'-C1' | -5.70 | 1.47 | 1.53 |
| 34 | i | 721 | C | P-O5' | 5.70 | 1.65 | 1.59 |
| 34 | i | 1647 | G | O4'-C1' | 5.70 | 1.49 | 1.41 |
| 10 | J | 188 | GLY | N-CA | 5.69 | 1.54 | 1.46 |
| 34 | i | 1658 | A | O4'-C1' | 5.69 | 1.49 | 1.41 |
| 34 | i | 1439 | C | O4'-C1' | 5.69 | 1.49 | 1.41 |
| 32 | f | 136 | PHE | CB-CG | -5.68 | 1.41 | 1.51 |
| 34 | i | 1335 | U | C2'-C1' | -5.68 | 1.47 | 1.53 |
| 34 | i | 1487 | G | O4'-C1' | 5.68 | 1.49 | 1.41 |
| 34 | i | 1809 | A | O4'-C1' | 5.68 | 1.49 | 1.41 |
| 34 | i | 1272 | A | P-O5' | -5.68 | 1.54 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8 | H | 67 | PRO | N-CD | 5.67 | 1.55 | 1.47 |
| 34 | i | 794 | G | O3'-P | -5.67 | 1.54 | 1.61 |
| 34 | i | 1712 | C | C2'-C1' | -5.67 | 1.47 | 1.53 |
| 34 | i | 98 | C | O4'-C1' | 5.67 | 1.49 | 1.41 |
| 34 | i | 1556 | A | O4'-C1' | 5.67 | 1.49 | 1.41 |
| 34 | i | 410 | G | O4'-C1' | -5.67 | 1.34 | 1.41 |
| 34 | i | 562 | U | C2'-C1' | 5.67 | 1.59 | 1.53 |
| 34 | i | 1618 | A | O4'-C1' | -5.67 | 1.34 | 1.41 |
| 11 | K | 40 | VAL | CB-CG1 | -5.66 | 1.41 | 1.52 |
| 34 | i | 1725 | U | O4'-C1' | 5.66 | 1.49 | 1.41 |
| 34 | i | 97 | U | C2'-C1' | -5.65 | 1.47 | 1.53 |
| 34 | i | 457 | G | C2'-C1' | -5.65 | 1.47 | 1.53 |
| 34 | i | 1356 | U | C2'-C1' | -5.65 | 1.47 | 1.53 |
| 34 | i | 1662 | U | C2'-C1' | -5.65 | 1.47 | 1.53 |
| 34 | i | 1760 | C | C4'-C3' | 5.65 | 1.59 | 1.53 |
| 9 | I | 6 | ASP | N-CA | -5.65 | 1.35 | 1.46 |
| 34 | i | 1246 | A | C2'-C1' | 5.65 | 1.59 | 1.53 |
| 34 | i | 1711 | C | C2'-C1' | -5.65 | 1.47 | 1.53 |
| 34 | i | 644 | A | O4'-C1' | 5.65 | 1.49 | 1.41 |
| 32 | f | 148 | TYR | CD1-CE1 | -5.64 | 1.30 | 1.39 |
| 34 | i | 911 | G | O4'-C1' | -5.64 | 1.34 | 1.41 |
| 34 | i | 1862 | U | C4'-C3' | 5.64 | 1.59 | 1.53 |
| 34 | i | 306 | C | O4'-C1' | 5.64 | 1.49 | 1.41 |
| 34 | i | 1419 | C | C5'-C4' | 5.64 | 1.58 | 1.51 |
| 34 | i | 1799 | G | C5'-C4' | 5.63 | 1.58 | 1.51 |
| 34 | i | 1641 | C | C5'-C4' | 5.63 | 1.58 | 1.51 |
| 34 | i | 1544 | U | O4'-C1' | 5.62 | 1.49 | 1.41 |
| 34 | i | 36 | U | O4'-C1' | 5.62 | 1.49 | 1.41 |
| 17 | Q | 145 | TYR | CB-CG | -5.62 | 1.43 | 1.51 |
| 34 | i | 224 | U | C5'-C4' | 5.62 | 1.58 | 1.51 |
| 34 | i | 1696 | C | C5'-C4' | 5.61 | 1.58 | 1.51 |
| 34 | i | 18 | C | O3'-P | -5.61 | 1.54 | 1.61 |
| 34 | i | 189 | G | C3'-C2' | -5.61 | 1.46 | 1.52 |
| 34 | i | 1821 | U | C2'-C1' | -5.61 | 1.47 | 1.53 |
| 34 | i | 497 | G | C5'-C4' | 5.61 | 1.58 | 1.51 |
| 31 | e | 97 | GLU | CG-CD | -5.60 | 1.43 | 1.51 |
| 34 | i | 1218 | G | O4'-C1' | 5.60 | 1.49 | 1.41 |
| 34 | i | 1727 | G | C2'-C1' | -5.60 | 1.47 | 1.53 |
| 34 | i | 314 | U | O3'-P | -5.60 | 1.54 | 1.61 |
| 34 | i | 336 | C | P-O5' | -5.60 | 1.54 | 1.59 |
| 34 | i | 93 | U | C2'-C1' | 5.59 | 1.59 | 1.53 |
| 34 | i | 99 | A | P-O5' | -5.59 | 1.54 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1702 | U | O4'-C1' | 5.59 | 1.49 | 1.41 |
| 34 | i | 817 | G | O3'-P | -5.59 | 1.54 | 1.61 |
| 12 | L | 102 | PHE | C-O | 5.59 | 1.33 | 1.23 |
| 34 | i | 550 | A | C2'-C1' | -5.59 | 1.47 | 1.53 |
| 34 | i | 965 | U | C5'-C4' | 5.58 | 1.58 | 1.51 |
| 34 | i | 586 | U | C2'-C1' | -5.58 | 1.47 | 1.53 |
| 34 | i | 1248 | C | O4'-C1' | 5.58 | 1.49 | 1.41 |
| 10 | J | 187 | ALA | N-CA | 5.58 | 1.57 | 1.46 |
| 12 | L | 103 | GLU | CG-CD | 5.58 | 1.60 | 1.51 |
| 34 | i | 1370 | C | C2'-C1' | -5.58 | 1.47 | 1.53 |
| 34 | i | 1379 | A | O4'-C1' | 5.58 | 1.49 | 1.41 |
| 34 | i | 1789 | G | C2'-C1' | -5.57 | 1.47 | 1.53 |
| 34 | i | 472 | G | O4'-C1' | -5.57 | 1.34 | 1.41 |
| 18 | R | 42 | PRO | N-CD | 5.57 | 1.55 | 1.47 |
| 34 | i | 1764 | G | C5'-C4' | 5.57 | 1.58 | 1.51 |
| 34 | i | 1405 | A | C5'-C4' | 5.56 | 1.58 | 1.51 |
| 34 | i | 21 | U | C2'-C1' | 5.56 | 1.59 | 1.53 |
| 34 | i | 955 | G | O4'-C1' | 5.56 | 1.48 | 1.41 |
| 34 | i | 1609 | A | C2'-C1' | -5.56 | 1.47 | 1.53 |
| 34 | i | 1196 | A | C2'-C1' | -5.56 | 1.47 | 1.53 |
| 34 | i | 1382 | A | C5'-C4' | 5.56 | 1.58 | 1.51 |
| 34 | i | 312 | C | C2'-C1' | -5.55 | 1.47 | 1.53 |
| 34 | i | 669 | A | C2'-C1' | -5.55 | 1.47 | 1.53 |
| 34 | i | 221 | A | O4'-C1' | 5.55 | 1.48 | 1.41 |
| 34 | i | 402 | G | C5'-C4' | 5.55 | 1.58 | 1.51 |
| 34 | i | 430 | G | C2'-C1' | -5.55 | 1.47 | 1.53 |
| 34 | i | 1424 | G | O4'-C1' | -5.55 | 1.34 | 1.41 |
| 34 | i | 962 | U | O4'-C1' | 5.54 | 1.48 | 1.41 |
| 34 | i | 1833 | U | O3'-P | -5.54 | 1.54 | 1.61 |
| 34 | i | 308 | C | P-O5' | -5.54 | 1.54 | 1.59 |
| 34 | i | 374 | U | O4'-C1' | 5.54 | 1.48 | 1.41 |
| 34 | i | 1373 | U | O4'-C1' | 5.54 | 1.48 | 1.41 |
| 34 | i | 427 | G | C2'-C1' | -5.53 | 1.47 | 1.53 |
| 34 | i | 1372 | A | C3'-C2' | -5.53 | 1.46 | 1.52 |
| 34 | i | 1726 | A | O4'-C1' | 5.53 | 1.48 | 1.41 |
| 34 | i | 152 | U | C5'-C4' | 5.53 | 1.57 | 1.51 |
| 34 | i | 460 | G | O4'-C1' | 5.52 | 1.48 | 1.41 |
| 34 | i | 796 | U | P-O5' | -5.52 | 1.54 | 1.59 |
| 34 | i | 1418 | G | C2'-C1' | 5.52 | 1.59 | 1.53 |
| 34 | i | 1415 | C | C2'-C1' | 5.51 | 1.59 | 1.53 |
| 34 | i | 731 | C | C2'-C1' | -5.51 | 1.47 | 1.53 |
| 34 | i | 1445 | G | O4'-C1' | 5.51 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 112 | U | C5'-C4' | 5.51 | 1.57 | 1.51 |
| 34 | i | 272 | C | O3'-P | -5.50 | 1.54 | 1.61 |
| 34 | i | 77 | A | C4'-C3' | 5.50 | 1.59 | 1.53 |
| 34 | i | 1780 | U | C2'-C1' | -5.50 | 1.47 | 1.53 |
| 34 | i | 1375 | A | O4'-C1' | 5.49 | 1.48 | 1.41 |
| 34 | i | 910 | U | C2'-C1' | 5.49 | 1.59 | 1.53 |
| 34 | i | 45 | A | C2'-C1' | -5.49 | 1.47 | 1.53 |
| 34 | i | 94 | G | O3'-P | -5.49 | 1.54 | 1.61 |
| 34 | i | 401 | G | C2'-C1' | -5.49 | 1.47 | 1.53 |
| 34 | i | 469 | C | C2'-C1' | -5.49 | 1.47 | 1.53 |
| 34 | i | 1332 | C | C2'-C1' | -5.49 | 1.47 | 1.53 |
| 34 | i | 1673 | A | O4'-C1' | -5.49 | 1.34 | 1.41 |
| 34 | i | 1494 | A | C4'-C3' | -5.48 | 1.47 | 1.52 |
| 34 | i | 281 | U | O3'-P | -5.48 | 1.54 | 1.61 |
| 34 | i | 1819 | A | O4'-C1' | -5.48 | 1.34 | 1.41 |
| 34 | i | 34 | U | C5'-C4' | 5.48 | 1.57 | 1.51 |
| 34 | i | 325 | G | C4'-C3' | 5.48 | 1.59 | 1.53 |
| 34 | i | 1829 | A | C2'-C1' | -5.47 | 1.47 | 1.53 |
| 34 | i | 428 | G | O3'-P | -5.47 | 1.54 | 1.61 |
| 34 | i | 343 | C | P-O5' | -5.47 | 1.54 | 1.59 |
| 34 | i | 1366 | A | O4'-C1' | 5.46 | 1.48 | 1.41 |
| 11 | K | 89 | ILE | N-CA | -5.46 | 1.35 | 1.46 |
| 34 | i | 112 | U | O3'-P | -5.46 | 1.54 | 1.61 |
| 34 | i | 976 | A | O4'-C1' | 5.46 | 1.48 | 1.41 |
| 34 | i | 411 | G | C2'-C1' | -5.46 | 1.47 | 1.53 |
| 34 | i | 577 | A | C2'-C1' | -5.45 | 1.47 | 1.53 |
| 34 | i | 1412 | C | O3'-P | -5.45 | 1.54 | 1.61 |
| 34 | i | 395 | G | O4'-C1' | 5.45 | 1.48 | 1.41 |
| 34 | i | 1334 | G | P-O5' | -5.44 | 1.54 | 1.59 |
| 34 | i | 1462 | G | O3'-P | -5.44 | 1.54 | 1.61 |
| 34 | i | 266 | G | C5'-C4' | 5.44 | 1.57 | 1.51 |
| 34 | i | 1124 | C | O3'-P | -5.44 | 1.54 | 1.61 |
| 34 | i | 32 | U | C2'-C1' | 5.44 | 1.59 | 1.53 |
| 34 | i | 145 | G | O4'-C1' | 5.44 | 1.48 | 1.41 |
| 34 | i | 188 | U | O4'-C1' | 5.44 | 1.48 | 1.41 |
| 34 | i | 1637 | U | C2'-C1' | 5.44 | 1.59 | 1.53 |
| 34 | i | 1504 | A | O4'-C1' | -5.44 | 1.34 | 1.41 |
| 34 | i | 629 | C | O4'-C1' | 5.43 | 1.48 | 1.41 |
| 34 | i | 574 | A | O4'-C1' | 5.43 | 1.48 | 1.41 |
| 34 | i | 82 | G | O3'-P | -5.42 | 1.54 | 1.61 |
| 34 | i | 1564 | A | P-O5' | -5.42 | 1.54 | 1.59 |
| 34 | i | 520 | U | O3'-P | -5.42 | 1.54 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11 | K | 37 | ASP | CB-CG | 5.42 | 1.63 | 1.51 |
| 34 | i | 418 | U | O4'-C1' | -5.42 | 1.34 | 1.41 |
| 34 | i | 87 | U | O4'-C1' | 5.41 | 1.48 | 1.41 |
| 26 | Z | 104 | ARG | N-CA | -5.41 | 1.35 | 1.46 |
| 34 | i | 1302 | U | C2'-C1' | -5.41 | 1.47 | 1.53 |
| 34 | i | 390 | C | C5'-C4' | 5.41 | 1.57 | 1.51 |
| 34 | i | 585 | U | C2'-C1' | -5.41 | 1.47 | 1.53 |
| 34 | i | 1636 | A | O3'-P | -5.41 | 1.54 | 1.61 |
| 34 | i | 73 | C | O4'-C1' | 5.40 | 1.48 | 1.41 |
| 34 | i | 186 | G | O4'-C1' | 5.40 | 1.48 | 1.41 |
| 34 | i | 1076 | A | O3'-P | -5.40 | 1.54 | 1.61 |
| 34 | i | 1390 | G | C4'-O4' | 5.40 | 1.52 | 1.45 |
| 34 | i | 44 | U | C2'-C1' | -5.39 | 1.47 | 1.53 |
| 34 | i | 139 | C | O3'-P | -5.39 | 1.54 | 1.61 |
| 34 | i | 818 | U | C4'-C3' | 5.39 | 1.59 | 1.53 |
| 34 | i | 979 | A | O4'-C1' | 5.39 | 1.48 | 1.41 |
| 34 | i | 1395 | C | C2'-C1' | -5.39 | 1.47 | 1.53 |
| 34 | i | 1068 | U | O4'-C1' | 5.39 | 1.48 | 1.41 |
| 34 | i | 1657 | U | C2'-C1' | -5.39 | 1.47 | 1.53 |
| 34 | i | 1400 | U | C4'-C3' | 5.38 | 1.59 | 1.53 |
| 34 | i | 403 | G | C2'-C1' | -5.38 | 1.47 | 1.53 |
| 34 | i | 1172 | G | C2'-C1' | -5.38 | 1.47 | 1.53 |
| 34 | i | 517 | C | O4'-C1' | 5.38 | 1.48 | 1.41 |
| 34 | i | 1665 | C | O4'-C1' | 5.38 | 1.48 | 1.41 |
| 34 | i | 1130 | G | C2'-C1' | -5.37 | 1.47 | 1.53 |
| 34 | i | 1141 | A | C2'-C1' | 5.37 | 1.59 | 1.53 |
| 34 | i | 839 | C | O3'-P | -5.37 | 1.54 | 1.61 |
| 34 | i | 1812 | A | C5'-C4' | 5.37 | 1.57 | 1.51 |
| 2 | B | 155 | TYR | CD1-CE1 | -5.37 | 1.31 | 1.39 |
| 34 | i | 1529 | C | O4'-C1' | 5.36 | 1.48 | 1.41 |
| 34 | i | 1341 | G | C2'-C1' | -5.36 | 1.47 | 1.53 |
| 34 | i | 867 | U | C3'-O3' | 5.36 | 1.49 | 1.42 |
| 34 | i | 1718 | G | O4'-C1' | -5.36 | 1.34 | 1.41 |
| 34 | i | 1027 | A | C2'-C1' | -5.35 | 1.47 | 1.53 |
| 34 | i | 1064 | G | C2'-C1' | -5.35 | 1.47 | 1.53 |
| 34 | i | 1146 | A | C5'-C4' | 5.35 | 1.57 | 1.51 |
| 34 | i | 1009 | U | O4'-C1' | 5.35 | 1.48 | 1.41 |
| 34 | i | 1523 | G | P-O5' | -5.35 | 1.54 | 1.59 |
| 34 | i | 1365 | A | O4'-C1' | 5.35 | 1.48 | 1.41 |
| 9 | I | 8 | TRP | CB-CG | 5.34 | 1.59 | 1.50 |
| 34 | i | 346 | C | C2'-C1' | -5.34 | 1.47 | 1.53 |
| 34 | i | 573 | A | O4'-C1' | 5.34 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 626 | C | P-O5' | -5.34 | 1.54 | 1.59 |
| 34 | i | 216 | U | C5'-C4' | 5.33 | 1.57 | 1.51 |
| 34 | i | 288 | A | C5'-C4' | 5.33 | 1.57 | 1.51 |
| 34 | i | 387 | G | O4'-C1' | 5.32 | 1.48 | 1.41 |
| 34 | i | 978 | G | C2'-C1' | -5.32 | 1.47 | 1.53 |
| 34 | i | 643 | A | C2'-C1' | -5.32 | 1.47 | 1.53 |
| 34 | i | 942 | U | C2'-C1' | -5.32 | 1.47 | 1.53 |
| 12 | L | 20 | LYS | N-CA | -5.31 | 1.35 | 1.46 |
| 10 | J | 144 | ILE | C-N | 5.31 | 1.44 | 1.34 |
| 13 | M | 116 | LYS | N-CA | 5.31 | 1.56 | 1.46 |
| 3 | C | 182 | PRO | N-CD | 5.31 | 1.55 | 1.47 |
| 34 | i | 1056 | A | C2'-C1' | -5.30 | 1.47 | 1.53 |
| 34 | i | 241 | A | C2'-C1' | 5.30 | 1.59 | 1.53 |
| 34 | i | 281 | U | C2'-C1' | 5.30 | 1.59 | 1.53 |
| 7 | G | 180 | VAL | CA-CB | -5.30 | 1.43 | 1.54 |
| 34 | i | 1094 | C | O4'-C1' | 5.30 | 1.48 | 1.41 |
| 34 | i | 1680 | U | C2'-C1' | -5.29 | 1.47 | 1.53 |
| 34 | i | 1279 | C | O3'-P | -5.29 | 1.54 | 1.61 |
| 34 | i | 90 | G | O4'-C1' | 5.29 | 1.48 | 1.41 |
| 34 | i | 645 | A | C5'-C4' | 5.29 | 1.57 | 1.51 |
| 34 | i | 901 | C | C2'-C1' | -5.29 | 1.47 | 1.53 |
| 34 | i | 1523 | G | C5'-C4' | -5.29 | 1.45 | 1.51 |
| 34 | i | 1088 | G | O4'-C1' | 5.29 | 1.48 | 1.41 |
| 34 | i | 1148 | U | O4'-C1' | 5.29 | 1.48 | 1.41 |
| 34 | i | 1709 | U | O4'-C1' | 5.29 | 1.48 | 1.41 |
| 34 | i | 861 | A | C5'-C4' | 5.28 | 1.57 | 1.51 |
| 34 | i | 1416 | G | O4'-C1' | 5.28 | 1.48 | 1.41 |
| 7 | G | 169 | PRO | N-CD | 5.28 | 1.55 | 1.47 |
| 34 | i | 290 | A | C3'-C2' | -5.28 | 1.47 | 1.52 |
| 34 | i | 83 | A | O4'-C1' | 5.28 | 1.48 | 1.41 |
| 34 | i | 1704 | G | C2'-C1' | -5.28 | 1.47 | 1.53 |
| 8 | H | 111 | LYS | CA-CB | 5.28 | 1.65 | 1.53 |
| 34 | i | 1287 | A | C2'-C1' | 5.28 | 1.59 | 1.53 |
| 34 | i | 1847 | C | P-O5' | -5.28 | 1.54 | 1.59 |
| 34 | i | 553 | G | C5'-C4' | 5.27 | 1.57 | 1.51 |
| 34 | i | 1260 | C | O3'-P | -5.27 | 1.54 | 1.61 |
| 24 | X | 139 | GLU | CB-CG | 5.27 | 1.62 | 1.52 |
| 34 | i | 1708 | C | C2'-C1' | -5.27 | 1.47 | 1.53 |
| 34 | i | 267 | G | O3'-P | -5.27 | 1.54 | 1.61 |
| 34 | i | 1621 | C | C2'-C1' | -5.27 | 1.47 | 1.53 |
| 34 | i | 1311 | U | C2'-C1' | 5.27 | 1.59 | 1.53 |
| 6 | F | 130 | ARG | N-CA | 5.26 | 1.56 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 98 | C | C4'-C3' | 5.26 | 1.58 | 1.53 |
| 34 | i | 1344 | G | O3'-P | -5.26 | 1.54 | 1.61 |
| 34 | i | 801 | U | C2'-C1' | -5.25 | 1.47 | 1.53 |
| 34 | i | 1533 | C | O3'-P | -5.25 | 1.54 | 1.61 |
| 34 | i | 1795 | A | C5'-C4' | 5.25 | 1.57 | 1.51 |
| 27 | a | 97 | PRO | CA-C | 5.25 | 1.63 | 1.52 |
| 34 | i | 1119 | C | O4'-C1' | 5.25 | 1.48 | 1.41 |
| 34 | i | 1070 | C | O4'-C1' | 5.24 | 1.48 | 1.41 |
| 34 | i | 360 | G | C4'-C3' | 5.23 | 1.58 | 1.53 |
| 34 | i | 1563 | C | C5'-C4' | 5.23 | 1.57 | 1.51 |
| 34 | i | 394 | G | C5'-C4' | 5.23 | 1.57 | 1.51 |
| 34 | i | 1538 | U | O4'-C1' | 5.22 | 1.48 | 1.41 |
| 34 | i | 176 | U | P-O5' | -5.22 | 1.54 | 1.59 |
| 34 | i | 730 | C | O3'-P | -5.22 | 1.54 | 1.61 |
| 34 | i | 1339 | U | C2'-C1' | -5.22 | 1.47 | 1.53 |
| 34 | i | 1713 | G | P-O5' | -5.22 | 1.54 | 1.59 |
| 34 | i | 1543 | G | C4'-C3' | -5.21 | 1.47 | 1.52 |
| 34 | i | 217 | U | P-O5' | -5.21 | 1.54 | 1.59 |
| 34 | i | 1730 | A | C2'-C1' | -5.21 | 1.47 | 1.53 |
| 34 | i | 1649 | G | C2'-C1' | -5.21 | 1.47 | 1.53 |
| 35 | j | 53 | A | C1'-N9 | -5.21 | 1.39 | 1.46 |
| 34 | i | 1339 | U | O3'-P | -5.21 | 1.54 | 1.61 |
| 34 | i | 1858 | U | P-O5' | -5.21 | 1.54 | 1.59 |
| 35 | j | 19 | A | C1'-N9 | -5.21 | 1.39 | 1.46 |
| 18 | R | 89 | SER | N-CA | 5.20 | 1.56 | 1.46 |
| 34 | i | 1167 | G | O3'-P | -5.20 | 1.54 | 1.61 |
| 34 | i | 1609 | A | P-O5' | -5.20 | 1.54 | 1.59 |
| 34 | i | 1601 | G | O4'-C1' | -5.20 | 1.34 | 1.41 |
| 34 | i | 1503 | G | O3'-P | -5.20 | 1.54 | 1.61 |
| 34 | i | 1157 | U | C2'-C1' | 5.19 | 1.59 | 1.53 |
| 34 | i | 1363 | U | C2'-C1' | -5.19 | 1.47 | 1.53 |
| 34 | i | 1667 | U | O4'-C1' | 5.19 | 1.48 | 1.41 |
| 34 | i | 878 | U | C4'-C3' | 5.19 | 1.58 | 1.53 |
| 34 | i | 667 | G | O4'-C1' | 5.19 | 1.48 | 1.41 |
| 34 | i | 1439 | C | O3'-P | -5.19 | 1.54 | 1.61 |
| 11 | K | 35 | LEU | N-CA | -5.18 | 1.35 | 1.46 |
| 34 | i | 1848 | U | C2'-C1' | 5.18 | 1.59 | 1.53 |
| 34 | i | 917 | G | O4'-C1' | 5.18 | 1.48 | 1.41 |
| 34 | i | 1199 | G | O4'-C1' | 5.18 | 1.48 | 1.41 |
| 2 | B | 41 | ILE | N-CA | -5.18 | 1.35 | 1.46 |
| 24 | X | 115 | ILE | CA-C | -5.18 | 1.39 | 1.52 |
| 34 | i | 1638 | U | C2'-C1' | -5.18 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | N | 136 | PRO | N-CD | 5.18 | 1.55 | 1.47 |
| 34 | i | 659 | A | C2'-C1' | 5.18 | 1.59 | 1.53 |
| 34 | i | 1695 | C | O4'-C1' | 5.18 | 1.48 | 1.41 |
| 34 | i | 21 | U | O4'-C1' | 5.17 | 1.48 | 1.41 |
| 34 | i | 1761 | C | C4'-C3' | 5.17 | 1.58 | 1.53 |
| 34 | i | 951 | A | C5'-C4' | 5.17 | 1.57 | 1.51 |
| 34 | i | 687 | G | C2'-C1' | -5.17 | 1.47 | 1.53 |
| 34 | i | 1346 | U | O4'-C1' | 5.17 | 1.48 | 1.41 |
| 11 | K | 93 | THR | CA-C | 5.17 | 1.66 | 1.52 |
| 34 | i | 1264 | C | P-O5' | -5.17 | 1.54 | 1.59 |
| 34 | i | 542 | G | O4'-C1' | 5.16 | 1.48 | 1.41 |
| 34 | i | 619 | A | C5'-C4' | 5.16 | 1.57 | 1.51 |
| 10 | J | 89 | GLU | CG-CD | -5.16 | 1.44 | 1.51 |
| 34 | i | 1406 | C | C4'-O4' | -5.16 | 1.38 | 1.45 |
| 34 | i | 662 | A | C4'-C3' | 5.16 | 1.58 | 1.53 |
| 34 | i | 935 | U | C5'-C4' | 5.15 | 1.57 | 1.51 |
| 34 | i | 1695 | C | C2'-C1' | 5.15 | 1.59 | 1.53 |
| 34 | i | 1206 | G | O4'-C1' | -5.15 | 1.34 | 1.41 |
| 34 | i | 1235 | U | O3'-P | -5.15 | 1.54 | 1.61 |
| 34 | i | 1627 | G | O4'-C1' | -5.15 | 1.34 | 1.41 |
| 34 | i | 421 | G | C4'-C3' | -5.15 | 1.47 | 1.52 |
| 34 | i | 1540 | A | C2'-C1' | -5.15 | 1.47 | 1.53 |
| 34 | i | 1429 | C | O3'-P | 5.14 | 1.67 | 1.61 |
| 34 | i | 1776 | G | C5'-C4' | 5.14 | 1.57 | 1.51 |
| 34 | i | 1792 | C | C5'-C4' | 5.14 | 1.57 | 1.51 |
| 34 | i | 672 | U | P-O5' | -5.14 | 1.54 | 1.59 |
| 34 | i | 1391 | C | C5'-C4' | 5.14 | 1.57 | 1.51 |
| 34 | i | 1618 | A | C4'-C3' | -5.14 | 1.47 | 1.52 |
| 34 | i | 1808 | G | C5'-C4' | 5.14 | 1.57 | 1.51 |
| 34 | i | 78 | C | C3'-C2' | 5.13 | 1.58 | 1.52 |
| 34 | i | 1766 | C | C3'-C2' | -5.13 | 1.47 | 1.52 |
| 2 | B | 155 | TYR | CD2-CE2 | -5.13 | 1.31 | 1.39 |
| 34 | i | 1592 | C | C4'-O4' | -5.13 | 1.38 | 1.45 |
| 26 | Z | 104 | ARG | CG-CD | 5.13 | 1.64 | 1.51 |
| 34 | i | 1490 | U | O4'-C1' | -5.13 | 1.34 | 1.41 |
| 34 | i | 116 | U | O4'-C1' | 5.13 | 1.48 | 1.41 |
| 34 | i | 535 | A | C2'-C1' | 5.13 | 1.58 | 1.53 |
| 34 | i | 1177 | A | C5'-C4' | 5.13 | 1.57 | 1.51 |
| 34 | i | 853 | U | P-O5' | 5.12 | 1.64 | 1.59 |
| 34 | i | 102 | A | O3'-P | -5.12 | 1.55 | 1.61 |
| 34 | i | 95 | G | O4'-C1' | 5.12 | 1.48 | 1.41 |
| 5 | E | 31 | PRO | N-CD | 5.11 | 1.54 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34 | i | 1242 | A | C2'-C1' | -5.11 | 1.47 | 1.53 |
| 34 | i | 659 | A | O3'-P | -5.11 | 1.55 | 1.61 |
| 34 | i | 1364 | U | O4'-C1' | 5.11 | 1.48 | 1.41 |
| 34 | i | 1029 | G | O3'-P | -5.10 | 1.55 | 1.61 |
| 34 | i | 978 | G | C5'-C4' | 5.10 | 1.57 | 1.51 |
| 34 | i | 1417 | A | O4'-C1' | 5.10 | 1.48 | 1.41 |
| 34 | i | 1467 | C | P-O5' | -5.10 | 1.54 | 1.59 |
| 34 | i | 651 | U | C5'-C4' | 5.10 | 1.57 | 1.51 |
| 22 | V | 33 | PRO | N-CD | 5.09 | 1.54 | 1.47 |
| 34 | i | 790 | A | C2'-C1' | -5.09 | 1.47 | 1.53 |
| 34 | i | 1314 | G | C2'-C1' | -5.08 | 1.47 | 1.53 |
| 34 | i | 1344 | G | C2'-C1' | 5.08 | 1.58 | 1.53 |
| 34 | i | 1380 | C | O4'-C1' | 5.08 | 1.48 | 1.41 |
| 34 | i | 1768 | C | O4'-C1' | 5.08 | 1.48 | 1.41 |
| 34 | i | 151 | C | C2'-C1' | -5.08 | 1.47 | 1.53 |
| 34 | i | 543 | U | P-O5' | -5.08 | 1.54 | 1.59 |
| 34 | i | 1432 | C | O3'-P | -5.08 | 1.55 | 1.61 |
| 34 | i | 1546 | U | O3'-P | -5.08 | 1.55 | 1.61 |
| 34 | i | 1541 | G | O4'-C1' | -5.07 | 1.35 | 1.41 |
| 34 | i | 1846 | C | C2'-C1' | -5.07 | 1.47 | 1.53 |
| 34 | i | 1818 | A | C3'-C2' | 5.07 | 1.58 | 1.52 |
| 34 | i | 349 | U | C5'-C4' | 5.07 | 1.57 | 1.51 |
| 34 | i | 1358 | U | O4'-C1' | -5.07 | 1.35 | 1.41 |
| 34 | i | 1232 | G | C4'-C3' | -5.06 | 1.47 | 1.52 |
| 34 | i | 113 | G | C4'-C3' | 5.06 | 1.58 | 1.53 |
| 34 | i | 1689 | U | C5'-C4' | 5.06 | 1.57 | 1.51 |
| 34 | i | 910 | U | O4'-C1' | 5.06 | 1.48 | 1.41 |
| 34 | i | 1039 | G | C5'-C4' | 5.05 | 1.57 | 1.51 |
| 26 | Z | 104 | ARG | CB-CG | -5.05 | 1.39 | 1.52 |
| 34 | i | 1549 | C | O3'-P | -5.05 | 1.55 | 1.61 |
| 34 | i | 1328 | A | P-O5' | -5.05 | 1.54 | 1.59 |
| 34 | i | 1420 | G | C5'-C4' | 5.05 | 1.57 | 1.51 |
| 34 | i | 674 | G | C4'-C3' | 5.04 | 1.58 | 1.53 |
| 34 | i | 791 | A | O4'-C1' | 5.04 | 1.48 | 1.41 |
| 34 | i | 1775 | A | C5'-C4' | 5.04 | 1.57 | 1.51 |
| 1 | A | 200 | ASP | CA-C | -5.04 | 1.39 | 1.52 |
| 20 | T | 82 | ARG | CD-NE | 5.03 | 1.55 | 1.46 |
| 34 | i | 51 | U | P-O5' | -5.03 | 1.54 | 1.59 |
| 34 | i | 742 | C | O4'-C1' | 5.03 | 1.48 | 1.41 |
| 34 | i | 394 | G | O4'-C1' | -5.03 | 1.35 | 1.41 |
| 34 | i | 288 | A | O4'-C1' | 5.02 | 1.48 | 1.41 |
| 34 | i | 600 | G | P-O5' | -5.02 | 1.54 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | L | 152 | LYS | C-N | 5.02 | 1.45 | 1.34 |
| 34 | i | 597 | U | O4'-C1' | 5.02 | 1.48 | 1.41 |
| 34 | i | 683 | G | C4'-O4' | 5.02 | 1.52 | 1.45 |
| 34 | i | 1168 | U | O3'-P | -5.02 | 1.55 | 1.61 |
| 34 | i | 308 | C | C2'-C1' | -5.02 | 1.47 | 1.53 |
| 34 | i | 140 | U | C2'-C1' | -5.01 | 1.47 | 1.53 |
| 34 | i | 484 | C | C5'-C4' | 5.01 | 1.57 | 1.51 |
| 2 | B | 221 | PRO | N-CD | 5.01 | 1.54 | 1.47 |
| 34 | i | 1397 | A | C5'-C4' | 5.01 | 1.57 | 1.51 |
| 34 | i | 735 | C | O3'-P | -5.00 | 1.55 | 1.61 |
| 34 | i | 1466 | C | C2'-C1' | -5.00 | 1.47 | 1.53 |

All (3231) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 8 | H | 109 | ARG | NE-CZ-NH2 | -53.45 | 93.58 | 120.30 |
| 8 | H | 109 | ARG | NE-CZ-NH1 | 42.58 | 141.59 | 120.30 |
| 34 | i | 1774 | G | P-O3'-C3' | 38.31 | 165.68 | 119.70 |
| 34 | i | 1114 | C | O4'-C1'-N1 | 35.28 | 136.42 | 108.20 |
| 34 | i | 582 | C | O4'-C1'-N1 | 32.53 | 134.22 | 108.20 |
| 34 | i | 67 | C | O4'-C1'-N1 | 31.27 | 133.22 | 108.20 |
| 34 | i | 72 | C | O4'-C1'-N1 | 30.36 | 132.49 | 108.20 |
| 8 | H | 118 | ARG | NE-CZ-NH1 | 29.49 | 135.04 | 120.30 |
| 34 | i | 678 | U | O4'-C1'-N1 | 29.07 | 131.46 | 108.20 |
| 34 | i | 1548 | C | O4'-C1'-N1 | 28.61 | 131.09 | 108.20 |
| 34 | i | 883 | U | P-O3'-C3' | 28.23 | 153.58 | 119.70 |
| 34 | i | 793 | C | O4'-C1'-N1 | 28.18 | 130.74 | 108.20 |
| 34 | i | 1299 | C | O4'-C1'-N1 | 27.70 | 130.36 | 108.20 |
| 34 | i | 1113 | C | O4'-C1'-N1 | 27.45 | 130.16 | 108.20 |
| 34 | i | 418 | U | O4'-C1'-N1 | 27.33 | 130.06 | 108.20 |
| 34 | i | 1817 | A | P-O3'-C3' | 27.26 | 152.41 | 119.70 |
| 34 | i | 1080 | A | P-O3'-C3' | 27.15 | 152.28 | 119.70 |
| 34 | i | 521 | A | P-O3'-C3' | 26.77 | 151.82 | 119.70 |
| 34 | i | 1105 | C | O4'-C1'-N1 | 25.52 | 128.61 | 108.20 |
| 34 | i | 1311 | U | O4'-C1'-N1 | 25.33 | 128.47 | 108.20 |
| 34 | i | 1392 | A | O4'-C1'-N9 | 24.78 | 128.02 | 108.20 |
| 34 | i | 1627 | G | P-O3'-C3' | 24.30 | 148.86 | 119.70 |
| 34 | i | 867 | U | O4'-C1'-N1 | 24.18 | 127.54 | 108.20 |
| 34 | i | 730 | C | P-O3'-C3' | 23.82 | 148.28 | 119.70 |
| 34 | i | 317 | G | P-O3'-C3' | 23.79 | 148.24 | 119.70 |
| 34 | i | 1470 | A | P-O3'-C3' | 23.57 | 147.99 | 119.70 |
| 34 | i | 1564 | A | O4'-C1'-N9 | 23.47 | 126.98 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 165 | G | O4'-C1'-N9 | 23.38 | 126.90 | 108.20 |
| 34 | i | 1150 | U | O4'-C1'-N1 | 23.23 | 126.78 | 108.20 |
| 34 | i | 66 | G | P-O3'-C3' | 23.04 | 147.35 | 119.70 |
| 34 | i | 1472 | A | O4'-C1'-N9 | 22.98 | 126.58 | 108.20 |
| 34 | i | 211 | U | P-O3'-C3' | 22.94 | 147.23 | 119.70 |
| 34 | i | 1304 | U | O4'-C1'-N1 | 22.81 | 126.45 | 108.20 |
| 34 | i | 544 | A | O4'-C1'-N9 | 22.76 | 126.41 | 108.20 |
| 10 | J | 146 | SER | O-C-N | -22.68 | 86.41 | 122.70 |
| 34 | i | 793 | C | P-O3'-C3' | 22.64 | 146.87 | 119.70 |
| 34 | i | 140 | U | P-O3'-C3' | 22.44 | 146.63 | 119.70 |
| 34 | i | 314 | U | O4'-C1'-N1 | 22.32 | 126.06 | 108.20 |
| 34 | i | 836 | C | P-O3'-C3' | 22.23 | 146.38 | 119.70 |
| 34 | i | 876 | G | O4'-C1'-N9 | 22.07 | 125.86 | 108.20 |
| 34 | i | 1573 | U | O4'-C1'-N1 | 22.03 | 125.83 | 108.20 |
| 34 | i | 1776 | G | O4'-C1'-N9 | 21.95 | 125.76 | 108.20 |
| 8 | H | 118 | ARG | NE-CZ-NH2 | -21.86 | 109.37 | 120.30 |
| 34 | i | 1552 | C | O4'-C1'-N1 | 21.78 | 125.62 | 108.20 |
| 34 | i | 685 | G | P-O3'-C3' | 21.73 | 145.77 | 119.70 |
| 34 | i | 1296 | U | O4'-C1'-N1 | 21.54 | 125.43 | 108.20 |
| 34 | i | 1516 | C | P-O3'-C3' | 21.53 | 145.54 | 119.70 |
| 34 | i | 298 | G | O4'-C1'-N9 | 21.52 | 125.41 | 108.20 |
| 34 | i | 743 | U | P-O3'-C3' | 21.38 | 145.35 | 119.70 |
| 34 | i | 1664 | G | P-O5'-C5' | 21.34 | 155.05 | 120.90 |
| 34 | i | 1562 | G | O4'-C1'-N9 | 21.26 | 125.20 | 108.20 |
| 34 | i | 722 | C | P-O3'-C3' | 21.22 | 145.16 | 119.70 |
| 34 | i | 1473 | U | P-O3'-C3' | 20.95 | 144.84 | 119.70 |
| 34 | i | 264 | U | P-O3'-C3' | 20.74 | 144.59 | 119.70 |
| 34 | i | 1503 | G | O4'-C1'-C2' | 20.66 | 126.46 | 105.80 |
| 34 | i | 1391 | C | P-O3'-C3' | 20.65 | 144.47 | 119.70 |
| 34 | i | 1819 | A | O4'-C1'-N9 | 20.57 | 124.65 | 108.20 |
| 34 | i | 325 | G | O4'-C1'-N9 | 20.08 | 124.26 | 108.20 |
| 34 | i | 618 | A | O4'-C1'-N9 | 20.01 | 124.21 | 108.20 |
| 34 | i | 1392 | A | P-O3'-C3' | 20.00 | 143.70 | 119.70 |
| 34 | i | 1112 | C | O4'-C1'-N1 | 19.97 | 124.17 | 108.20 |
| 34 | i | 1414 | C | C3'-C2'-C1' | -19.96 | 85.53 | 101.50 |
| 34 | i | 1716 | U | O4'-C1'-N1 | 19.89 | 124.11 | 108.20 |
| 34 | i | 1426 | C | O4'-C1'-N1 | 19.77 | 124.02 | 108.20 |
| 34 | i | 319 | G | P-O3'-C3' | 19.66 | 143.29 | 119.70 |
| 34 | i | 1819 | A | P-O3'-C3' | 19.53 | 143.13 | 119.70 |
| 18 | R | 1 | MET | CA-C-N | -19.48 | 77.23 | 116.20 |
| 34 | i | 317 | G | O4'-C1'-N9 | 19.30 | 123.64 | 108.20 |
| 34 | i | 1358 | U | O4'-C1'-N1 | 19.25 | 123.60 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 34 | i | 225 | C | P-O3'-C3' | 19.18 | 142.72 | 119.70 |
| 34 | i | 1471 | G | P-O3'-C3' | 19.14 | 142.67 | 119.70 |
| 34 | i | 142 | C | O4'-C1'-N1 | 18.96 | 123.37 | 108.20 |
| 34 | i | 1151 | U | N1-C1'-C2' | 18.87 | 138.53 | 114.00 |
| 34 | i | 697 | G | P-O3'-C3' | 18.75 | 142.21 | 119.70 |
| 34 | i | 688 | U | P-O3'-C3' | 18.72 | 142.16 | 119.70 |
| 34 | i | 1673 | A | O4'-C1'-N9 | 18.69 | 123.15 | 108.20 |
| 34 | i | 78 | C | P-O3'-C3' | 18.68 | 142.12 | 119.70 |
| 34 | i | 126 | G | P-O3'-C3' | 18.67 | 142.11 | 119.70 |
| 34 | i | 954 | G | O4'-C1'-N9 | 18.61 | 123.09 | 108.20 |
| 34 | i | 180 | G | P-O3'-C3' | -18.56 | 97.43 | 119.70 |
| 34 | i | 911 | G | O4'-C1'-N9 | 18.41 | 122.93 | 108.20 |
| 34 | i | 883 | U | O4'-C1'-N1 | 18.32 | 122.85 | 108.20 |
| 34 | i | 899 | A | O4'-C1'-N9 | 18.20 | 122.76 | 108.20 |
| 34 | i | 1393 | U | N1-C1'-C2' | 18.17 | 137.62 | 114.00 |
| 34 | i | 72 | C | P-O3'-C3' | 18.13 | 141.45 | 119.70 |
| 34 | i | 1544 | U | P-O3'-C3' | 18.06 | 141.37 | 119.70 |
| 34 | i | 1226 | C | N1-C1'-C2' | 18.03 | 137.44 | 114.00 |
| 34 | i | 1133 | U | P-O3'-C3' | 17.98 | 141.28 | 119.70 |
| 34 | i | 1740 | A | O4'-C1'-N9 | 17.91 | 122.52 | 108.20 |
| 34 | i | 1377 | G | O4'-C1'-N9 | 17.85 | 122.48 | 108.20 |
| 34 | i | 727 | G | P-O3'-C3' | 17.72 | 140.97 | 119.70 |
| 34 | i | 428 | G | O4'-C1'-N9 | 17.71 | 122.37 | 108.20 |
| 34 | i | 1316 | G | O4'-C1'-N9 | 17.61 | 122.29 | 108.20 |
| 34 | i | 1012 | U | N1-C1'-C2' | 17.57 | 136.85 | 114.00 |
| 34 | i | 257 | G | P-O3'-C3' | 17.52 | 140.72 | 119.70 |
| 34 | i | 189 | G | P-O3'-C3' | 17.46 | 140.65 | 119.70 |
| 7 | G | 131 | ARG | CB-CA-C | 17.40 | 145.21 | 110.40 |
| 34 | i | 346 | C | O4'-C1'-N1 | 17.28 | 122.02 | 108.20 |
| 27 | a | 10 | ARG | NE-CZ-NH2 | 17.28 | 128.94 | 120.30 |
| 34 | i | 524 | G | P-O3'-C3' | 17.26 | 140.42 | 119.70 |
| 18 | R | 1 | MET | N-CA-CB | 17.23 | 141.61 | 110.60 |
| 34 | i | 1045 | A | O4'-C1'-N9 | 17.18 | 121.95 | 108.20 |
| 34 | i | 135 | U | P-O3'-C3' | 17.18 | 140.31 | 119.70 |
| 34 | i | 1149 | C | O4'-C1'-N1 | 17.12 | 121.89 | 108.20 |
| 34 | i | 1322 | U | N1-C1'-C2' | 17.10 | 136.23 | 114.00 |
| 34 | i | 1399 | C | O4'-C1'-N1 | 16.97 | 121.78 | 108.20 |
| 34 | i | 819 | U | O4'-C1'-N1 | 16.96 | 121.77 | 108.20 |
| 34 | i | 136 | C | P-O3'-C3' | 16.95 | 140.04 | 119.70 |
| 34 | i | 885 | U | O4'-C1'-N1 | 16.92 | 121.74 | 108.20 |
| 34 | i | 1618 | A | O4'-C1'-N9 | 16.90 | 121.72 | 108.20 |
| 34 | i | 222 | G | P-O3'-C3' | 16.88 | 139.95 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 74 | G | O4'-C1'-N9 | 16.85 | 121.68 | 108.20 |
| 34 | i | 826 | A | O4'-C1'-N9 | 16.84 | 121.67 | 108.20 |
| 34 | i | 868 | A | O4'-C1'-N9 | 16.80 | 121.64 | 108.20 |
| 34 | i | 239 | U | P-O3'-C3' | 16.79 | 139.84 | 119.70 |
| 22 | V | 61 | ARG | NE-CZ-NH2 | -16.76 | 111.92 | 120.30 |
| 34 | i | 1563 | C | N1-C1'-C2' | 16.75 | 135.77 | 114.00 |
| 34 | i | 1470 | A | O4'-C1'-N9 | 16.71 | 121.57 | 108.20 |
| 7 | G | 131 | ARG | CB-CG-CD | 16.61 | 154.79 | 111.60 |
| 36 | k | 22 | C | O4'-C1'-N1 | -16.58 | 94.94 | 108.20 |
| 34 | i | 1294 | G | O4'-C1'-N9 | 16.54 | 121.43 | 108.20 |
| 16 | P | 37 | TYR | N-CA-CB | -16.44 | 81.01 | 110.60 |
| 34 | i | 358 | U | P-O3'-C3' | 16.39 | 139.37 | 119.70 |
| 34 | i | 171 | A | O4'-C1'-N9 | 16.36 | 121.29 | 108.20 |
| 34 | i | 299 | G | N9-C1'-C2' | 16.20 | 135.05 | 114.00 |
| 34 | i | 1144 | A | O4'-C1'-N9 | 15.99 | 121.00 | 108.20 |
| 34 | i | 1233 | C | N1-C1'-C2' | 15.96 | 134.75 | 114.00 |
| 34 | i | 141 | A | P-O3'-C3' | 15.86 | 138.74 | 119.70 |
| 9 | I | 134 | GLU | N-CA-CB | 15.83 | 139.09 | 110.60 |
| 34 | i | 73 | C | O4'-C1'-N1 | 15.80 | 120.84 | 108.20 |
| 34 | i | 620 | U | O4'-C1'-N1 | 15.73 | 120.78 | 108.20 |
| 34 | i | 138 | C | P-O3'-C3' | 15.70 | 138.53 | 119.70 |
| 34 | i | 1006 | G | O4'-C1'-N9 | 15.67 | 120.73 | 108.20 |
| 4 | D | 5 | ILE | O-C-N | -15.62 | 97.70 | 122.70 |
| 34 | i | 1425 | G | P-O3'-C3' | 15.55 | 138.36 | 119.70 |
| 25 | Y | 86 | GLU | C-N-CD | -15.50 | 86.49 | 120.60 |
| 34 | i | 1056 | A | O4'-C1'-N9 | 15.50 | 120.60 | 108.20 |
| 34 | i | 1327 | C | N1-C1'-C2' | 15.46 | 134.09 | 114.00 |
| 34 | i | 295 | C | P-O3'-C3' | 15.41 | 138.19 | 119.70 |
| 34 | i | 79 | A | O4'-C1'-C2' | -15.29 | 90.51 | 105.80 |
| 10 | J | 146 | SER | CA-C-N | 15.27 | 150.78 | 117.20 |
| 27 | a | 102 | ARG | C-N-CD | -15.24 | 87.07 | 120.60 |
| 34 | i | 1279 | C | P-O3'-C3' | 15.21 | 137.95 | 119.70 |
| 34 | i | 396 | U | P-O3'-C3' | 15.19 | 137.93 | 119.70 |
| 34 | i | 1663 | U | O4'-C1'-N1 | 15.18 | 120.35 | 108.20 |
| 34 | i | 1607 | G | O4'-C1'-N9 | 15.13 | 120.31 | 108.20 |
| 34 | i | 64 | A | O4'-C1'-N9 | 15.12 | 120.30 | 108.20 |
| 34 | i | 60 | A | O4'-C1'-N9 | 15.08 | 120.26 | 108.20 |
| 9 | I | 43 | ILE | O-C-N | -15.07 | 98.59 | 122.70 |
| 34 | i | 1670 | A | O4'-C1'-N9 | 14.94 | 120.15 | 108.20 |
| 34 | i | 1543 | G | O4'-C1'-N9 | 14.93 | 120.14 | 108.20 |
| 34 | i | 734 | C | P-O3'-C3' | 14.92 | 137.61 | 119.70 |
| 8 | H | 109 | ARG | CD-NE-CZ | 14.90 | 144.46 | 123.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 1492 | U | P-O3'-C3' | 14.85 | 137.52 | 119.70 |
| 27 | a | 97 | PRO | N-CA-C | 14.83 | 150.66 | 112.10 |
| 34 | i | 111 | A | O4'-C1'-N9 | 14.80 | 120.04 | 108.20 |
| 34 | i | 478 | U | P-O3'-C3' | 14.74 | 137.39 | 119.70 |
| 34 | i | 215 | U | N1-C1'-C2' | 14.72 | 133.13 | 114.00 |
| 34 | i | 835 | C | N1-C1'-C2' | 14.71 | 133.13 | 114.00 |
| 34 | i | 857 | A | O4'-C1'-N9 | 14.66 | 119.93 | 108.20 |
| 34 | i | 1424 | G | O4'-C1'-N9 | 14.62 | 119.90 | 108.20 |
| 34 | i | 538 | C | P-O3'-C3' | 14.59 | 137.20 | 119.70 |
| 34 | i | 835 | C | C3'-C2'-C1' | -14.56 | 89.85 | 101.50 |
| 34 | i | 1773 | G | O4'-C1'-N9 | 14.55 | 119.84 | 108.20 |
| 34 | i | 720 | A | P-O3'-C3' | 14.54 | 137.15 | 119.70 |
| 34 | i | 1475 | G | O4'-C1'-N9 | 14.51 | 119.81 | 108.20 |
| 34 | i | 1594 | U | O4'-C1'-N1 | 14.49 | 119.79 | 108.20 |
| 34 | i | 1390 | G | P-O3'-C3' | 14.48 | 137.08 | 119.70 |
| 34 | i | 383 | U | O4'-C1'-N1 | 14.47 | 119.78 | 108.20 |
| 34 | i | 1227 | C | N1-C1'-C2' | 14.46 | 132.80 | 114.00 |
| 20 | T | 93 | SER | N-CA-CB | 14.45 | 132.17 | 110.50 |
| 34 | i | 1344 | G | O4'-C1'-N9 | 14.43 | 119.74 | 108.20 |
| 34 | i | 1010 | G | O4'-C1'-C2' | 14.41 | 120.57 | 107.60 |
| 34 | i | 543 | U | O4'-C1'-N1 | 14.40 | 119.72 | 108.20 |
| 34 | i | 1412 | C | O4'-C1'-N1 | 14.40 | 119.72 | 108.20 |
| 34 | i | 133 | C | P-O3'-C3' | 14.39 | 136.97 | 119.70 |
| 34 | i | 581 | U | O4'-C1'-N1 | 14.39 | 119.72 | 108.20 |
| 36 | k | 22 | C | C2-N1-C1' | -14.38 | 102.98 | 118.80 |
| 34 | i | 210 | G | O4'-C1'-N9 | 14.38 | 119.70 | 108.20 |
| 34 | i | 1412 | C | P-O3'-C3' | 14.31 | 136.87 | 119.70 |
| 25 | Y | 103 | SER | O-C-N | -14.27 | 99.87 | 122.70 |
| 14 | N | 81 | ALA | C-N-CD | -14.22 | 89.32 | 120.60 |
| 34 | i | 682 | G | P-O3'-C3' | 14.20 | 136.74 | 119.70 |
| 9 | I | 184 | ARG | NE-CZ-NH1 | -14.18 | 113.21 | 120.30 |
| 19 | S | 40 | TYR | CB-CG-CD1 | 14.18 | 129.51 | 121.00 |
| 34 | i | 1235 | U | P-O3'-C3' | -14.18 | 102.69 | 119.70 |
| 7 | G | 170 | ARG | CA-CB-CG | 14.15 | 144.53 | 113.40 |
| 34 | i | 1824 | U | P-O3'-C3' | 14.15 | 136.68 | 119.70 |
| 34 | i | 1414 | C | O4'-C1'-N1 | 14.13 | 119.50 | 108.20 |
| 25 | Y | 86 | GLU | N-CA-C | 14.09 | 149.03 | 111.00 |
| 34 | i | 912 | A | O4'-C1'-N9 | 14.07 | 119.45 | 108.20 |
| 34 | i | 649 | G | O4'-C1'-N9 | 14.05 | 119.44 | 108.20 |
| 34 | i | 1637 | U | O4'-C1'-N1 | 14.04 | 119.43 | 108.20 |
| 34 | i | 677 | C | O4'-C1'-N1 | 14.03 | 119.42 | 108.20 |
| 34 | i | 1861 | U | O4'-C1'-N1 | 13.97 | 119.38 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 1293 | U | O4'-C1'-N1 | 13.95 | 119.36 | 108.20 |
| 34 | i | 794 | G | P-O3'-C3' | 13.93 | 136.41 | 119.70 |
| 34 | i | 295 | C | C4'-C3'-O3' | -13.92 | 80.17 | 109.40 |
| 34 | i | 1818 | A | O4'-C1'-N9 | 13.91 | 119.33 | 108.20 |
| 34 | i | 240 | C | P-O3'-C3' | 13.88 | 136.36 | 119.70 |
| 34 | i | 1721 | G | O4'-C1'-N9 | 13.83 | 119.26 | 108.20 |
| 34 | i | 1413 | C | O4'-C1'-C2' | -13.82 | 91.98 | 105.80 |
| 34 | i | 1018 | U | N1-C1'-C2' | 13.80 | 131.94 | 114.00 |
| 34 | i | 454 | A | P-O3'-C3' | -13.76 | 103.19 | 119.70 |
| 19 | S | 141 | ARG | O-C-N | -13.70 | 100.78 | 122.70 |
| 28 | b | 36 | LYS | C-N-CA | 13.69 | 155.92 | 121.70 |
| 34 | i | 313 | C | P-O3'-C3' | 13.66 | 136.09 | 119.70 |
| 34 | i | 1773 | G | P-O3'-C3' | 13.65 | 136.08 | 119.70 |
| 34 | i | 276 | U | P-O3'-C3' | 13.62 | 136.04 | 119.70 |
| 34 | i | 1754 | G | O4'-C1'-N9 | 13.62 | 119.09 | 108.20 |
| 34 | i | 1449 | C | O4'-C1'-N1 | 13.58 | 119.06 | 108.20 |
| 34 | i | 1393 | U | O4'-C1'-N1 | -13.56 | 97.35 | 108.20 |
| 34 | i | 478 | U | O4'-C1'-N1 | 13.55 | 119.04 | 108.20 |
| 34 | i | 548 | G | O4'-C1'-N9 | 13.55 | 119.04 | 108.20 |
| 34 | i | 287 | U | N1-C1'-C2' | 13.51 | 131.56 | 114.00 |
| 20 | T | 4 | VAL | N-CA-C | 13.48 | 147.39 | 111.00 |
| 34 | i | 1510 | G | O4'-C1'-N9 | 13.47 | 118.98 | 108.20 |
| 34 | i | 1769 | U | O4'-C1'-N1 | 13.46 | 118.97 | 108.20 |
| 34 | i | 1862 | U | P-O3'-C3' | 13.46 | 135.85 | 119.70 |
| 34 | i | 1741 | U | P-O3'-C3' | 13.41 | 135.80 | 119.70 |
| 34 | i | 960 | A | O4'-C1'-N9 | 13.41 | 118.93 | 108.20 |
| 34 | i | 889 | U | O4'-C1'-N1 | 13.40 | 118.92 | 108.20 |
| 34 | i | 829 | C | P-O3'-C3' | 13.39 | 135.77 | 119.70 |
| 34 | i | 519 | A | P-O3'-C3' | -13.39 | 103.63 | 119.70 |
| 34 | i | 1011 | U | O4'-C1'-N1 | 13.37 | 118.89 | 108.20 |
| 34 | i | 830 | C | N1-C1'-C2' | 13.33 | 131.32 | 114.00 |
| 34 | i | 556 | U | O4'-C1'-N1 | 13.32 | 118.86 | 108.20 |
| 34 | i | 837 | G | O4'-C1'-N9 | 13.32 | 118.86 | 108.20 |
| 7 | G | 131 | ARG | CA-CB-CG | 13.32 | 142.69 | 113.40 |
| 36 | k | 22 | C | C6-N1-C1' | 13.27 | 136.73 | 120.80 |
| 34 | i | 1261 | A | N9-C1'-C2' | 13.27 | 131.25 | 114.00 |
| 34 | i | 530 | U | O4'-C1'-N1 | 13.26 | 118.81 | 108.20 |
| 34 | i | 438 | A | O4'-C1'-N9 | 13.22 | 118.78 | 108.20 |
| 34 | i | 1548 | C | C3'-C2'-C1' | -13.22 | 90.92 | 101.50 |
| 34 | i | 1482 | A | O4'-C1'-N9 | 13.22 | 118.77 | 108.20 |
| 34 | i | 24 | C | P-O3'-C3' | 13.19 | 135.53 | 119.70 |
| 27 | a | 97 | PRO | CB-CA-C | -13.18 | 79.04 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 277 | U | O4'-C1'-N1 | -13.18 | 97.66 | 108.20 |
| 34 | i | 1257 | C | N1-C1'-C2' | 13.18 | 131.13 | 114.00 |
| 34 | i | 627 | U | O4'-C1'-N1 | 13.16 | 118.73 | 108.20 |
| 34 | i | 415 | G | O4'-C1'-N9 | 13.15 | 118.72 | 108.20 |
| 34 | i | 1841 | G | O4'-C1'-N9 | 13.14 | 118.71 | 108.20 |
| 34 | i | 1616 | U | O4'-C1'-N1 | 13.13 | 118.70 | 108.20 |
| 34 | i | 1514 | U | O4'-C1'-N1 | 13.13 | 118.70 | 108.20 |
| 34 | i | 742 | C | P-O3'-C3' | 13.12 | 135.45 | 119.70 |
| 34 | i | 406 | U | O4'-C1'-N1 | 13.12 | 118.69 | 108.20 |
| 34 | i | 1715 | U | P-O3'-C3' | 13.10 | 135.42 | 119.70 |
| 34 | i | 147 | A | O4'-C1'-N9 | 13.09 | 118.67 | 108.20 |
| 11 | K | 55 | ARG | CG-CD-NE | 13.09 | 139.28 | 111.80 |
| 34 | i | 1523 | G | O4'-C1'-N9 | 13.05 | 118.64 | 108.20 |
| 34 | i | 1459 | U | C4'-C3'-O3' | -13.04 | 82.02 | 109.40 |
| 34 | i | 876 | G | P-O3'-C3' | 13.03 | 135.34 | 119.70 |
| 34 | i | 869 | G | P-O3'-C3' | 12.95 | 135.24 | 119.70 |
| 34 | i | 1503 | G | O4'-C1'-N9 | 12.95 | 118.56 | 108.20 |
| 34 | i | 1406 | C | N1-C1'-C2' | 12.95 | 130.83 | 114.00 |
| 34 | i | 456 | G | O4'-C1'-N9 | 12.91 | 118.53 | 108.20 |
| 34 | i | 594 | A | P-O3'-C3' | 12.86 | 135.13 | 119.70 |
| 34 | i | 1307 | C | N1-C1'-C2' | 12.85 | 130.70 | 114.00 |
| 34 | i | 1533 | C | P-O3'-C3' | 12.84 | 135.11 | 119.70 |
| 34 | i | 123 | G | O4'-C1'-N9 | 12.84 | 118.47 | 108.20 |
| 34 | i | 721 | C | P-O3'-C3' | 12.81 | 135.07 | 119.70 |
| 34 | i | 1429 | C | O3'-P-O5' | -12.80 | 79.68 | 104.00 |
| 34 | i | 126 | G | C4'-C3'-O3' | -12.79 | 82.54 | 109.40 |
| 34 | i | 1 | U | O4'-C1'-N1 | 12.77 | 118.42 | 108.20 |
| 34 | i | 622 | C | N1-C1'-C2' | 12.77 | 130.60 | 114.00 |
| 34 | i | 59 | U | O4'-C1'-N1 | 12.76 | 118.41 | 108.20 |
| 34 | i | 1402 | G | P-O3'-C3' | 12.75 | 135.00 | 119.70 |
| 34 | i | 139 | C | P-O3'-C3' | 12.75 | 135.00 | 119.70 |
| 34 | i | 1168 | U | O4'-C1'-N1 | 12.74 | 118.39 | 108.20 |
| 34 | i | 1565 | G | O4'-C1'-N9 | 12.70 | 118.36 | 108.20 |
| 34 | i | 1238 | U | N1-C1'-C2' | 12.70 | 130.51 | 114.00 |
| 34 | i | 75 | G | O4'-C1'-N9 | 12.63 | 118.30 | 108.20 |
| 34 | i | 38 | A | O4'-C1'-N9 | 12.62 | 118.29 | 108.20 |
| 17 | Q | 18 | THR | N-CA-CB | 12.61 | 134.26 | 110.30 |
| 34 | i | 1240 | U | O4'-C1'-N1 | 12.61 | 118.29 | 108.20 |
| 18 | R | 88 | VAL | O-C-N | -12.60 | 102.53 | 122.70 |
| 34 | i | 170 | A | O4'-C1'-C2' | 12.60 | 118.94 | 107.60 |
| 34 | i | 1249 | A | O4'-C1'-N9 | 12.59 | 118.27 | 108.20 |
| 18 | R | 89 | SER | N-CA-C | 12.56 | 144.91 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 816 | U | O4'-C1'-N1 | 12.56 | 118.25 | 108.20 |
| 34 | i | 1588 | C | P-O3'-C3' | 12.55 | 134.76 | 119.70 |
| 24 | X | 23 | HIS | O-C-N | -12.52 | 102.67 | 122.70 |
| 34 | i | 24 | C | C1'-C2'-O2' | -12.52 | 73.04 | 110.60 |
| 34 | i | 1104 | G | O4'-C1'-N9 | 12.45 | 118.16 | 108.20 |
| 34 | i | 1145 | A | O4'-C1'-N9 | 12.44 | 118.15 | 108.20 |
| 34 | i | 77 | A | P-O3'-C3' | 12.44 | 134.63 | 119.70 |
| 7 | G | 170 | ARG | N-CA-CB | 12.41 | 132.94 | 110.60 |
| 34 | i | 1753 | G | O4'-C1'-N9 | 12.41 | 118.12 | 108.20 |
| 34 | i | 696 | G | P-O3'-C3' | 12.39 | 134.57 | 119.70 |
| 34 | i | 66 | G | C1'-O4'-C4' | -12.38 | 99.99 | 109.90 |
| 34 | i | 831 | C | P-O5'-C5' | 12.37 | 140.69 | 120.90 |
| 34 | i | 881 | U | O4'-C1'-N1 | 12.35 | 118.08 | 108.20 |
| 34 | i | 616 | G | C3'-C2'-C1' | 12.32 | 111.35 | 101.50 |
| 34 | i | 1044 | G | N9-C1'-C2' | 12.31 | 130.01 | 114.00 |
| 16 | P | 17 | TYR | CB-CG-CD2 | -12.31 | 113.62 | 121.00 |
| 34 | i | 542 | G | P-O3'-C3' | 12.28 | 134.44 | 119.70 |
| 34 | i | 1414 | C | O4'-C1'-C2' | 12.27 | 118.64 | 107.60 |
| 34 | i | 1126 | G | O4'-C1'-N9 | 12.25 | 118.00 | 108.20 |
| 34 | i | 359 | C | O4'-C1'-N1 | 12.24 | 117.99 | 108.20 |
| 34 | i | 866 | A | O4'-C1'-N9 | 12.23 | 117.99 | 108.20 |
| 34 | i | 280 | G | O4'-C1'-N9 | 12.22 | 117.97 | 108.20 |
| 34 | i | 986 | A | N9-C1'-C2' | 12.22 | 129.88 | 114.00 |
| 34 | i | 1430 | C | P-O3'-C3' | 12.21 | 134.35 | 119.70 |
| 34 | i | 1081 | C | P-O5'-C5' | -12.19 | 101.39 | 120.90 |
| 34 | i | 1716 | U | N1-C1'-C2' | -12.19 | 98.15 | 114.00 |
| 34 | i | 1372 | A | O4'-C1'-N9 | 12.18 | 117.95 | 108.20 |
| 34 | i | 20 | G | O4'-C1'-N9 | 12.17 | 117.94 | 108.20 |
| 34 | i | 531 | U | O4'-C1'-N1 | 12.16 | 117.93 | 108.20 |
| 34 | i | 1097 | U | O4'-C1'-N1 | 12.16 | 117.93 | 108.20 |
| 4 | D | 4 | GLN | CG-CD-OE1 | -12.14 | 97.31 | 121.60 |
| 34 | i | 237 | G | P-O3'-C3' | 12.14 | 134.27 | 119.70 |
| 34 | i | 329 | A | C4'-C3'-O3' | -12.14 | 83.90 | 109.40 |
| 34 | i | 1188 | U | O4'-C1'-N1 | 12.11 | 117.89 | 108.20 |
| 34 | i | 1167 | G | O4'-C1'-N9 | 12.10 | 117.88 | 108.20 |
| 34 | i | 1838 | U | O4'-C1'-N1 | 12.10 | 117.88 | 108.20 |
| 33 | g | 24 | THR | C-N-CD | -12.09 | 94.00 | 120.60 |
| 34 | i | 4 | C | N1-C1'-C2' | 12.09 | 129.71 | 114.00 |
| 34 | i | 857 | A | N9-C1'-C2' | -12.07 | 98.30 | 114.00 |
| 25 | Y | 86 | GLU | CA-C-O | -12.06 | 94.78 | 120.10 |
| 34 | i | 1469 | G | O3'-P-O5' | 12.05 | 126.91 | 104.00 |
| 34 | i | 1550 | U | O4'-C1'-N1 | 12.05 | 117.84 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 1310 | U | O4'-C1'-N1 | 12.05 | 117.84 | 108.20 |
| 34 | i | 224 | U | O4'-C1'-N1 | 12.03 | 117.83 | 108.20 |
| 34 | i | 1255 | A | O4'-C1'-N9 | 12.02 | 117.82 | 108.20 |
| 34 | i | 1562 | G | C3'-C2'-C1' | -12.01 | 91.89 | 101.50 |
| 31 | e | 95 | LYS | O-C-N | -12.00 | 103.50 | 122.70 |
| 17 | Q | 146 | ARG | NE-CZ-NH2 | 11.99 | 126.30 | 120.30 |
| 34 | i | 915 | A | P-O3'-C3' | 11.99 | 134.09 | 119.70 |
| 34 | i | 520 | U | O4'-C1'-N1 | 11.99 | 117.79 | 108.20 |
| 34 | i | 1397 | A | P-O3'-C3' | 11.99 | 134.09 | 119.70 |
| 34 | i | 736 | C | N1-C1'-C2' | 11.98 | 129.58 | 114.00 |
| 34 | i | 146 | G | O4'-C1'-N9 | 11.97 | 117.78 | 108.20 |
| 34 | i | 835 | C | O4'-C1'-N1 | 11.97 | 117.78 | 108.20 |
| 34 | i | 1659 | A | P-O3'-C3' | 11.96 | 134.06 | 119.70 |
| 11 | K | 1 | MET | N-CA-CB | -11.96 | 89.08 | 110.60 |
| 34 | i | 412 | U | O4'-C1'-N1 | 11.95 | 117.76 | 108.20 |
| 34 | i | 807 | A | P-O3'-C3' | 11.94 | 134.03 | 119.70 |
| 34 | i | 426 | G | O4'-C1'-N9 | 11.91 | 117.73 | 108.20 |
| 34 | i | 868 | A | P-O3'-C3' | 11.91 | 133.99 | 119.70 |
| 34 | i | 179 | C | N1-C1'-C2' | 11.90 | 129.47 | 114.00 |
| 34 | i | 1355 | U | O4'-C1'-N1 | 11.90 | 117.72 | 108.20 |
| 34 | i | 596 | G | O4'-C1'-N9 | 11.88 | 117.70 | 108.20 |
| 34 | i | 1549 | C | O3'-P-O5' | -11.86 | 81.47 | 104.00 |
| 34 | i | 1538 | U | P-O3'-C3' | 11.85 | 133.92 | 119.70 |
| 34 | i | 1671 | U | O4'-C1'-N1 | 11.85 | 117.68 | 108.20 |
| 4 | D | 4 | GLN | N-CA-CB | -11.84 | 89.28 | 110.60 |
| 34 | i | 1418 | G | O4'-C1'-N9 | 11.84 | 117.67 | 108.20 |
| 34 | i | 278 | U | P-O3'-C3' | 11.84 | 133.91 | 119.70 |
| 34 | i | 1607 | G | N9-C1'-C2' | -11.84 | 98.61 | 114.00 |
| 18 | R | 1 | MET | C-N-CA | -11.82 | 97.48 | 122.30 |
| 34 | i | 1103 | G | O4'-C1'-N9 | 11.81 | 117.65 | 108.20 |
| 34 | i | 1315 | U | O4'-C1'-N1 | 11.80 | 117.64 | 108.20 |
| 34 | i | 1233 | C | C1'-O4'-C4' | -11.71 | 100.53 | 109.90 |
| 2 | B | 41 | ILE | CB-CA-C | 11.71 | 135.01 | 111.60 |
| 34 | i | 796 | U | O4'-C1'-N1 | 11.70 | 117.56 | 108.20 |
| 34 | i | 1494 | A | C1'-O4'-C4' | -11.70 | 100.54 | 109.90 |
| 34 | i | 225 | C | C3'-C2'-C1' | 11.70 | 110.86 | 101.50 |
| 34 | i | 1670 | A | N9-C1'-C2' | -11.70 | 98.80 | 114.00 |
| 34 | i | 1157 | U | O4'-C1'-N1 | 11.69 | 117.55 | 108.20 |
| 34 | i | 1828 | A | N9-C1'-C2' | 11.68 | 129.19 | 114.00 |
| 34 | i | 1515 | G | N9-C1'-C2' | 11.68 | 129.18 | 114.00 |
| 13 | M | 99 | LYS | C-N-CD | -11.68 | 94.92 | 120.60 |
| 34 | i | 570 | U | P-O3'-C3' | -11.65 | 105.72 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 1833 | U | O4'-C1'-N1 | 11.65 | 117.52 | 108.20 |
| 34 | i | 1231 | G | O4'-C1'-N9 | 11.65 | 117.52 | 108.20 |
| 9 | I | 134 | GLU | CB-CA-C | -11.63 | 87.13 | 110.40 |
| 34 | i | 526 | A | P-O3'-C3' | -11.63 | 105.74 | 119.70 |
| 34 | i | 734 | C | N1-C1'-C2' | 11.63 | 129.11 | 114.00 |
| 34 | i | 1319 | U | O4'-C1'-N1 | 11.62 | 117.50 | 108.20 |
| 34 | i | 461 | G | O4'-C1'-N9 | 11.59 | 117.48 | 108.20 |
| 34 | i | 817 | G | O4'-C1'-N9 | 11.59 | 117.47 | 108.20 |
| 34 | i | 1437 | U | O4'-C1'-N1 | 11.59 | 117.47 | 108.20 |
| 34 | i | 1446 | G | O4'-C1'-N9 | 11.58 | 117.47 | 108.20 |
| 34 | i | 365 | U | O4'-C1'-N1 | 11.58 | 117.47 | 108.20 |
| 34 | i | 1806 | U | O4'-C1'-N1 | 11.58 | 117.46 | 108.20 |
| 34 | i | 277 | U | C3'-C2'-C1' | 11.57 | 110.75 | 101.50 |
| 18 | R | 1 | MET | N-CA-C | -11.55 | 79.80 | 111.00 |
| 34 | i | 417 | U | O4'-C1'-N1 | 11.55 | 117.44 | 108.20 |
| 34 | i | 1007 | A | O4'-C1'-N9 | 11.54 | 117.44 | 108.20 |
| 34 | i | 31 | U | O4'-C1'-N1 | 11.52 | 117.42 | 108.20 |
| 34 | i | 800 | U | O4'-C1'-N1 | 11.51 | 117.41 | 108.20 |
| 34 | i | 413 | U | O4'-C1'-N1 | 11.49 | 117.40 | 108.20 |
| 34 | i | 929 | G | C1'-O4'-C4' | -11.49 | 100.70 | 109.90 |
| 10 | J | 146 | SER | C-N-CA | 11.49 | 150.43 | 121.70 |
| 12 | L | 153 | LYS | O-C-N | -11.48 | 104.33 | 122.70 |
| 34 | i | 728 | U | P-O3'-C3' | 11.48 | 133.47 | 119.70 |
| 34 | i | 672 | U | O4'-C1'-N1 | 11.44 | 117.35 | 108.20 |
| 34 | i | 1000 | U | O4'-C1'-N1 | 11.43 | 117.35 | 108.20 |
| 34 | i | 1206 | G | O4'-C1'-N9 | 11.43 | 117.34 | 108.20 |
| 34 | i | 1552 | C | P-O3'-C3' | 11.37 | 133.35 | 119.70 |
| 34 | i | 728 | U | P-O5'-C5' | 11.37 | 139.09 | 120.90 |
| 34 | i | 368 | U | O4'-C1'-N1 | 11.36 | 117.29 | 108.20 |
| 34 | i | 1718 | G | O4'-C1'-N9 | 11.34 | 117.27 | 108.20 |
| 34 | i | 474 | A | P-O3'-C3' | 11.33 | 133.30 | 119.70 |
| 9 | I | 6 | ASP | CB-CG-OD2 | -11.31 | 108.12 | 118.30 |
| 34 | i | 1643 | G | C4'-C3'-O3' | 11.30 | 135.61 | 113.00 |
| 34 | i | 145 | G | C1'-O4'-C4' | -11.30 | 100.86 | 109.90 |
| 34 | i | 536 | G | P-O3'-C3' | 11.28 | 133.24 | 119.70 |
| 34 | i | 1237 | A | C3'-C2'-C1' | 11.27 | 110.52 | 101.50 |
| 34 | i | 1500 | U | O4'-C1'-N1 | 11.27 | 117.22 | 108.20 |
| 34 | i | 358 | U | O4'-C1'-N1 | 11.26 | 117.20 | 108.20 |
| 34 | i | 861 | A | O4'-C1'-N9 | 11.23 | 117.18 | 108.20 |
| 34 | i | 1815 | U | O4'-C1'-N1 | 11.22 | 117.18 | 108.20 |
| 4 | D | 5 | ILE | CA-C-N | 11.22 | 141.89 | 117.20 |
| 12 | L | 20 | LYS | N-CA-CB | -11.20 | 90.44 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 1414 | C | P-O3'-C3' | 11.19 | 133.12 | 119.70 |
| 34 | i | 1742 | C | P-O3'-C3' | 11.16 | 133.09 | 119.70 |
| 34 | i | 1496 | G | N9-C1'-C2' | 11.15 | 128.49 | 114.00 |
| 27 | a | 98 | PRO | C-N-CD | -11.15 | 96.08 | 120.60 |
| 34 | i | 520 | U | C4'-C3'-O3' | -11.12 | 86.04 | 109.40 |
| 34 | i | 1348 | G | C1'-O4'-C4' | -11.12 | 101.00 | 109.90 |
| 34 | i | 1405 | A | P-O3'-C3' | 11.12 | 133.05 | 119.70 |
| 34 | i | 947 | C | C3'-C2'-C1' | 11.12 | 110.39 | 101.50 |
| 34 | i | 1738 | G | N9-C1'-C2' | 11.12 | 128.45 | 114.00 |
| 34 | i | 385 | G | O4'-C1'-N9 | 11.09 | 117.07 | 108.20 |
| 34 | i | 1414 | C | C1'-O4'-C4' | -11.09 | 101.03 | 109.90 |
| 34 | i | 918 | A | O4'-C1'-N9 | 11.07 | 117.05 | 108.20 |
| 34 | i | 1024 | A | P-O3'-C3' | -11.06 | 106.43 | 119.70 |
| 34 | i | 1715 | U | O4'-C1'-N1 | 11.05 | 117.04 | 108.20 |
| 34 | i | 1194 | G | O4'-C1'-C2' | 11.04 | 117.53 | 107.60 |
| 34 | i | 170 | A | C1'-O4'-C4' | -11.03 | 101.08 | 109.90 |
| 34 | i | 1154 | G | O4'-C1'-N9 | 11.02 | 117.02 | 108.20 |
| 34 | i | 913 | U | O4'-C1'-N1 | 11.02 | 117.01 | 108.20 |
| 34 | i | 1772 | C | O4'-C1'-N1 | 11.02 | 117.01 | 108.20 |
| 34 | i | 411 | G | O4'-C1'-N9 | 11.00 | 117.00 | 108.20 |
| 34 | i | 1648 | U | O4'-C1'-N1 | 11.00 | 117.00 | 108.20 |
| 34 | i | 948 | G | O4'-C1'-N9 | 11.00 | 117.00 | 108.20 |
| 34 | i | 1255 | A | O4'-C1'-C2' | 10.97 | 117.47 | 107.60 |
| 34 | i | 340 | C | O4'-C1'-C2' | -10.97 | 94.83 | 105.80 |
| 34 | i | 207 | U | P-O3'-C3' | 10.95 | 132.84 | 119.70 |
| 34 | i | 1432 | C | C3'-C2'-C1' | 10.95 | 110.26 | 101.50 |
| 34 | i | 1848 | U | O4'-C1'-N1 | 10.94 | 116.96 | 108.20 |
| 34 | i | 684 | A | O4'-C1'-C2' | 10.94 | 117.45 | 107.60 |
| 34 | i | 1408 | C | P-O3'-C3' | 10.94 | 132.83 | 119.70 |
| 34 | i | 1062 | U | O4'-C1'-N1 | 10.93 | 116.94 | 108.20 |
| 34 | i | 631 | A | O4'-C1'-N9 | 10.91 | 116.93 | 108.20 |
| 34 | i | 827 | G | O4'-C1'-N9 | 10.90 | 116.92 | 108.20 |
| 34 | i | 862 | U | O4'-C1'-N1 | 10.89 | 116.91 | 108.20 |
| 24 | X | 91 | LEU | CA-CB-CG | 10.89 | 140.34 | 115.30 |
| 34 | i | 684 | A | O4'-C1'-N9 | 10.87 | 116.90 | 108.20 |
| 34 | i | 61 | A | O4'-C1'-N9 | 10.87 | 116.89 | 108.20 |
| 34 | i | 103 | A | O4'-C1'-N9 | 10.86 | 116.89 | 108.20 |
| 34 | i | 1193 | G | O4'-C1'-N9 | 10.86 | 116.88 | 108.20 |
| 34 | i | 1672 | U | O4'-C1'-N1 | 10.84 | 116.87 | 108.20 |
| 26 | Z | 107 | VAL | N-CA-CB | -10.83 | 87.67 | 111.50 |
| 34 | i | 832 | G | O4'-C1'-N9 | 10.82 | 116.86 | 108.20 |
| 34 | i | 200 | U | O4'-C1'-N1 | 10.80 | 116.84 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 436 | G | N9-C1'-C2' | 10.80 | 128.04 | 114.00 |
| 18 | R | 86 | PRO | CA-N-CD | -10.80 | 96.39 | 111.50 |
| 34 | i | 1138 | G | O4'-C1'-N9 | 10.79 | 116.83 | 108.20 |
| 18 | R | 89 | SER | CA-C-N | 10.78 | 140.91 | 117.20 |
| 34 | i | 1290 | G | O4'-C1'-N9 | 10.77 | 116.82 | 108.20 |
| 19 | S | 40 | TYR | CB-CG-CD2 | -10.77 | 114.54 | 121.00 |
| 34 | i | 907 | C | P-O5'-C5' | 10.75 | 138.10 | 120.90 |
| 34 | i | 1632 | A | P-O3'-C3' | 10.75 | 132.60 | 119.70 |
| 34 | i | 991 | G | O4'-C1'-N9 | 10.74 | 116.79 | 108.20 |
| 34 | i | 671 | U | O4'-C1'-N1 | 10.74 | 116.79 | 108.20 |
| 34 | i | 1037 | G | C1'-O4'-C4' | -10.73 | 101.31 | 109.90 |
| 34 | i | 1111 | U | O4'-C1'-N1 | 10.70 | 116.76 | 108.20 |
| 34 | i | 835 | C | C1'-O4'-C4' | -10.69 | 101.35 | 109.90 |
| 34 | i | 57 | U | O4'-C1'-N1 | 10.68 | 116.75 | 108.20 |
| 34 | i | 521 | A | C1'-O4'-C4' | -10.68 | 101.36 | 109.90 |
| 34 | i | 676 | U | O4'-C1'-N1 | 10.68 | 116.74 | 108.20 |
| 34 | i | 1724 | U | O4'-C1'-N1 | 10.65 | 116.72 | 108.20 |
| 34 | i | 1354 | U | O4'-C1'-N1 | 10.65 | 116.72 | 108.20 |
| 34 | i | 858 | A | N9-C1'-C2' | 10.64 | 127.84 | 114.00 |
| 34 | i | 1536 | G | O4'-C1'-N9 | 10.63 | 116.71 | 108.20 |
| 34 | i | 143 | U | N1-C1'-C2' | 10.63 | 127.82 | 114.00 |
| 34 | i | 682 | G | O4'-C1'-N9 | 10.63 | 116.70 | 108.20 |
| 34 | i | 878 | U | O4'-C1'-N1 | 10.63 | 116.70 | 108.20 |
| 34 | i | 405 | A | O4'-C1'-N9 | 10.62 | 116.69 | 108.20 |
| 34 | i | 477 | U | P-O3'-C3' | 10.62 | 132.44 | 119.70 |
| 34 | i | 1329 | U | O4'-C1'-N1 | 10.61 | 116.69 | 108.20 |
| 34 | i | 522 | C | O4'-C1'-C2' | -10.61 | 95.19 | 105.80 |
| 34 | i | 1546 | U | O4'-C1'-C2' | 10.60 | 117.14 | 107.60 |
| 27 | a | 10 | ARG | CD-NE-CZ | 10.60 | 138.44 | 123.60 |
| 19 | S | 87 | GLN | O-C-N | -10.59 | 105.75 | 122.70 |
| 34 | i | 1615 | A | N9-C1'-C2' | 10.59 | 127.77 | 114.00 |
| 34 | i | 19 | A | O4'-C1'-N9 | 10.58 | 116.67 | 108.20 |
| 34 | i | 1308 | G | O4'-C1'-N9 | -10.58 | 99.73 | 108.20 |
| 34 | i | 1856 | G | O4'-C1'-C2' | -10.57 | 95.23 | 105.80 |
| 34 | i | 1012 | U | C3'-C2'-C1' | 10.57 | 109.96 | 101.50 |
| 34 | i | 1743 | G | O4'-C1'-N9 | 10.57 | 116.65 | 108.20 |
| 34 | i | 592 | G | O4'-C1'-N9 | 10.55 | 116.64 | 108.20 |
| 34 | i | 894 | U | P-O3'-C3' | 10.55 | 132.36 | 119.70 |
| 34 | i | 1079 | A | C1'-O4'-C4' | -10.55 | 101.46 | 109.90 |
| 34 | i | 1674 | A | P-O3'-C3' | 10.53 | 132.34 | 119.70 |
| 34 | i | 1346 | U | O4'-C1'-N1 | 10.53 | 116.62 | 108.20 |
| 19 | S | 88 | LYS | CB-CA-C | 10.53 | 131.45 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 1299 | C | C3'-C2'-C1' | -10.53 | 93.08 | 101.50 |
| 34 | i | 1555 | U | O4'-C1'-N1 | 10.50 | 116.60 | 108.20 |
| 34 | i | 1570 | G | O4'-C1'-N9 | 10.49 | 116.59 | 108.20 |
| 34 | i | 739 | U | O4'-C1'-N1 | 10.48 | 116.59 | 108.20 |
| 34 | i | 1021 | U | O4'-C1'-N1 | 10.48 | 116.58 | 108.20 |
| 34 | i | 1210 | A | P-O3'-C3' | 10.48 | 132.27 | 119.70 |
| 34 | i | 154 | U | O4'-C1'-N1 | 10.47 | 116.58 | 108.20 |
| 34 | i | 1584 | A | O4'-C1'-N9 | 10.46 | 116.57 | 108.20 |
| 9 | I | 6 | ASP | CB-CG-OD1 | 10.46 | 127.72 | 118.30 |
| 34 | i | 1074 | C | N1-C1'-C2' | 10.46 | 127.59 | 114.00 |
| 34 | i | 79 | A | O4'-C1'-N9 | 10.44 | 116.56 | 108.20 |
| 34 | i | 1295 | A | O4'-C1'-N9 | 10.44 | 116.56 | 108.20 |
| 34 | i | 1255 | A | C3'-C2'-C1' | -10.44 | 93.15 | 101.50 |
| 34 | i | 385 | G | C1'-O4'-C4' | -10.44 | 101.55 | 109.90 |
| 34 | i | 322 | G | O4'-C1'-N9 | 10.44 | 116.55 | 108.20 |
| 34 | i | 915 | A | N9-C1'-C2' | 10.41 | 127.53 | 114.00 |
| 34 | i | 93 | U | O4'-C1'-N1 | 10.41 | 116.53 | 108.20 |
| 34 | i | 815 | G | O4'-C1'-N9 | 10.40 | 116.52 | 108.20 |
| 34 | i | 1288 | C | C3'-C2'-C1' | 10.40 | 109.82 | 101.50 |
| 34 | i | 542 | G | O4'-C1'-N9 | 10.40 | 116.52 | 108.20 |
| 34 | i | 1407 | G | C1'-O4'-C4' | -10.40 | 101.58 | 109.90 |
| 34 | i | 490 | A | O3'-P-O5' | -10.39 | 84.25 | 104.00 |
| 15 | O | 129 | ILE | CB-CA-C | -10.39 | 90.83 | 111.60 |
| 34 | i | 789 | G | O4'-C1'-N9 | 10.39 | 116.51 | 108.20 |
| 7 | G | 170 | ARG | CB-CG-CD | 10.37 | 138.56 | 111.60 |
| 34 | i | 794 | G | O4'-C1'-C2' | -10.37 | 95.43 | 105.80 |
| 34 | i | 1404 | U | N1-C1'-C2' | 10.37 | 127.48 | 114.00 |
| 34 | i | 1479 | A | O4'-C1'-N9 | 10.36 | 116.49 | 108.20 |
| 34 | i | 204 | G | O4'-C1'-N9 | 10.35 | 116.48 | 108.20 |
| 34 | i | 167 | G | O4'-C1'-N9 | 10.34 | 116.47 | 108.20 |
| 34 | i | 170 | A | C3'-C2'-C1' | -10.32 | 93.25 | 101.50 |
| 34 | i | 1170 | U | O4'-C1'-N1 | 10.30 | 116.44 | 108.20 |
| 34 | i | 792 | G | O4'-C1'-N9 | 10.30 | 116.44 | 108.20 |
| 34 | i | 585 | U | O4'-C1'-N1 | 10.29 | 116.43 | 108.20 |
| 10 | J | 138 | ARG | N-CA-C | 10.28 | 138.77 | 111.00 |
| 34 | i | 1857 | A | O4'-C1'-C2' | -10.27 | 95.53 | 105.80 |
| 34 | i | 349 | U | O4'-C1'-N1 | 10.27 | 116.41 | 108.20 |
| 34 | i | 546 | U | P-O5'-C5' | 10.23 | 137.28 | 120.90 |
| 34 | i | 1010 | G | O4'-C1'-N9 | 10.22 | 116.38 | 108.20 |
| 34 | i | 1774 | G | C1'-O4'-C4' | -10.22 | 101.73 | 109.90 |
| 34 | i | 971 | G | O4'-C1'-N9 | 10.22 | 116.37 | 108.20 |
| 34 | i | 1551 | A | P-O3'-C3' | 10.21 | 131.96 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 34 | i | 300 | G | O4'-C1'-N9 | 10.21 | 116.37 | 108.20 |
| 18 | R | 2 | GLY | O-C-N | -10.21 | 106.37 | 122.70 |
| 34 | i | 65 | C | P-O3'-C3' | 10.19 | 131.93 | 119.70 |
| 34 | i | 168 | C | N1-C1'-C2' | 10.19 | 127.25 | 114.00 |
| 34 | i | 1232 | G | O4'-C1'-C2' | 10.17 | 116.76 | 107.60 |
| 5 | E | 171 | ASP | N-CA-C | 10.17 | 138.46 | 111.00 |
| 34 | i | 662 | A | O4'-C1'-N9 | 10.15 | 116.32 | 108.20 |
| 34 | i | 141 | A | O4'-C1'-C2' | -10.14 | 95.66 | 105.80 |
| 34 | i | 102 | A | P-O3'-C3' | 10.13 | 131.86 | 119.70 |
| 11 | K | 43 | LEU | CA-CB-CG | 10.12 | 138.57 | 115.30 |
| 34 | i | 1075 | C | C3'-C2'-C1' | 10.11 | 109.59 | 101.50 |
| 34 | i | 517 | C | O4'-C1'-N1 | 10.11 | 116.29 | 108.20 |
| 34 | i | 865 | A | P-O3'-C3' | 10.11 | 131.83 | 119.70 |
| 34 | i | 590 | G | O4'-C1'-N9 | 10.10 | 116.28 | 108.20 |
| 21 | U | 71 | GLY | N-CA-C | 10.10 | 138.35 | 113.10 |
| 34 | i | 31 | U | P-O3'-C3' | 10.10 | 131.82 | 119.70 |
| 34 | i | 1416 | G | C1'-O4'-C4' | -10.10 | 101.82 | 109.90 |
| 34 | i | 1662 | U | O4'-C1'-N1 | 10.10 | 116.28 | 108.20 |
| 34 | i | 287 | U | C1'-O4'-C4' | -10.08 | 101.84 | 109.90 |
| 34 | i | 935 | U | O4'-C1'-N1 | 10.08 | 116.26 | 108.20 |
| 34 | i | 1276 | G | O4'-C1'-N9 | 10.07 | 116.26 | 108.20 |
| 34 | i | 73 | C | O4'-C1'-C2' | -10.06 | 95.74 | 105.80 |
| 34 | i | 1811 | G | O4'-C1'-N9 | 10.06 | 116.25 | 108.20 |
| 34 | i | 1414 | C | P-O5'-C5' | 10.06 | 137.00 | 120.90 |
| 34 | i | 74 | G | C3'-C2'-C1' | 10.06 | 109.55 | 101.50 |
| 34 | i | 1408 | C | O3'-P-O5' | -10.06 | 84.88 | 104.00 |
| 34 | i | 1722 | G | O4'-C1'-N9 | 10.05 | 116.24 | 108.20 |
| 11 | K | 55 | ARG | NE-CZ-NH1 | 10.05 | 125.33 | 120.30 |
| 34 | i | 1615 | A | O4'-C1'-N9 | 10.04 | 116.23 | 108.20 |
| 34 | i | 1281 | G | C4'-C3'-O3' | 10.03 | 133.06 | 113.00 |
| 34 | i | 1211 | C | O4'-C1'-C2' | -10.02 | 95.78 | 105.80 |
| 34 | i | 1258 | C | N1-C1'-C2' | 9.99 | 126.99 | 114.00 |
| 34 | i | 1303 | U | P-O3'-C3' | 9.99 | 131.69 | 119.70 |
| 4 | D | 4 | GLN | CG-CD-NE2 | 9.99 | 140.67 | 116.70 |
| 34 | i | 547 | U | N1-C1'-C2' | 9.98 | 126.98 | 114.00 |
| 34 | i | 1532 | A | O4'-C1'-C2' | -9.98 | 95.82 | 105.80 |
| 34 | i | 344 | U | O4'-C1'-N1 | 9.98 | 116.18 | 108.20 |
| 34 | i | 1715 | U | C1'-O4'-C4' | 9.98 | 117.88 | 109.90 |
| 34 | i | 546 | U | C4'-C3'-C2' | -9.96 | 92.64 | 102.60 |
| 11 | K | 1 | MET | CB-CG-SD | 9.96 | 142.28 | 112.40 |
| 34 | i | 1472 | A | N9-C1'-C2' | -9.96 | 101.05 | 112.00 |
| 9 | I | 43 | ILE | CA-C-O | 9.95 | 141.00 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8 | H | 110 | THR | CA-C-O | -9.95 | 99.20 | 120.10 |
| 34 | i | 1036 | G | O4'-C1'-N9 | 9.94 | 116.15 | 108.20 |
| 34 | i | 1643 | G | P-O3'-C3' | 9.94 | 131.62 | 119.70 |
| 24 | X | 23 | HIS | CB-CA-C | 9.93 | 130.26 | 110.40 |
| 34 | i | 795 | U | O4'-C1'-N1 | 9.93 | 116.14 | 108.20 |
| 34 | i | 1435 | A | O4'-C1'-N9 | 9.93 | 116.14 | 108.20 |
| 7 | G | 180 | VAL | CB-CA-C | -9.93 | 92.54 | 111.40 |
| 34 | i | 204 | G | N9-C1'-C2' | -9.93 | 101.08 | 112.00 |
| 34 | i | 189 | G | C1'-O4'-C4' | -9.92 | 101.97 | 109.90 |
| 34 | i | 1771 | G | C3'-C2'-C1' | -9.92 | 93.57 | 101.50 |
| 34 | i | 92 | A | N9-C1'-C2' | 9.90 | 126.87 | 114.00 |
| 34 | i | 1397 | A | O4'-C1'-N9 | 9.90 | 116.12 | 108.20 |
| 34 | i | 1115 | A | O4'-C1'-N9 | 9.89 | 116.11 | 108.20 |
| 34 | i | 1010 | G | C1'-O4'-C4' | -9.88 | 102.00 | 109.90 |
| 34 | i | 663 | G | O4'-C1'-N9 | 9.87 | 116.09 | 108.20 |
| 34 | i | 1234 | U | O4'-C1'-N1 | 9.86 | 116.08 | 108.20 |
| 34 | i | 616 | G | O4'-C1'-C2' | -9.83 | 95.97 | 105.80 |
| 34 | i | 1151 | U | O4'-C1'-N1 | 9.83 | 116.07 | 108.20 |
| 18 | R | 42 | PRO | CA-N-CD | -9.83 | 97.74 | 111.50 |
| 34 | i | 1803 | A | O4'-C1'-N9 | 9.82 | 116.06 | 108.20 |
| 34 | i | 1004 | A | P-O3'-C3' | 9.82 | 131.48 | 119.70 |
| 34 | i | 5 | U | O4'-C1'-N1 | 9.82 | 116.05 | 108.20 |
| 34 | i | 914 | U | N1-C1'-C2' | 9.82 | 126.76 | 114.00 |
| 34 | i | 1194 | G | C1'-O4'-C4' | -9.81 | 102.05 | 109.90 |
| 34 | i | 80 | G | C3'-C2'-C1' | 9.80 | 109.34 | 101.50 |
| 34 | i | 105 | U | O4'-C1'-N1 | 9.79 | 116.03 | 108.20 |
| 34 | i | 1333 | C | O4'-C1'-N1 | 9.78 | 116.03 | 108.20 |
| 34 | i | 665 | U | O4'-C1'-N1 | 9.78 | 116.02 | 108.20 |
| 33 | g | 142 | VAL | CA-C-N | -9.78 | 95.69 | 117.20 |
| 34 | i | 1798 | U | O4'-C1'-N1 | 9.77 | 116.02 | 108.20 |
| 34 | i | 1659 | A | N9-C1'-C2' | 9.76 | 126.69 | 114.00 |
| 34 | i | 1771 | G | O4'-C1'-N9 | 9.76 | 116.00 | 108.20 |
| 34 | i | 1432 | C | P-O3'-C3' | 9.75 | 131.40 | 119.70 |
| 19 | S | 91 | LYS | CG-CD-CE | 9.74 | 141.11 | 111.90 |
| 34 | i | 928 | G | O4'-C1'-N9 | 9.74 | 115.99 | 108.20 |
| 28 | b | 36 | LYS | N-CA-C | 9.73 | 137.28 | 111.00 |
| 34 | i | 1126 | G | N9-C1'-C2' | -9.73 | 101.30 | 112.00 |
| 34 | i | 810 | U | O4'-C1'-N1 | 9.73 | 115.98 | 108.20 |
| 34 | i | 999 | U | O4'-C1'-N1 | 9.72 | 115.98 | 108.20 |
| 21 | U | 104 | ILE | N-CA-C | -9.71 | 84.77 | 111.00 |
| 1 | A | 200 | ASP | CB-CA-C | -9.71 | 90.99 | 110.40 |
| 34 | i | 1072 | G | O4'-C1'-N9 | 9.70 | 115.96 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1413 | C | C3'-C2'-C1' | 9.70 | 109.26 | 101.50 |
| 34 | i | 520 | U | O4'-C4'-C3' | -9.70 | 94.30 | 104.00 |
| 34 | i | 121 | U | O4'-C1'-N1 | 9.70 | 115.96 | 108.20 |
| 34 | i | 1328 | A | O4'-C1'-C2' | -9.70 | 96.10 | 105.80 |
| 34 | i | 321 | C | O4'-C1'-N1 | 9.70 | 115.96 | 108.20 |
| 34 | i | 743 | U | O4'-C1'-N1 | 9.70 | 115.96 | 108.20 |
| 34 | i | 1716 | U | P-O3'-C3' | 9.69 | 131.33 | 119.70 |
| 10 | J | 89 | GLU | N-CA-C | 9.69 | 137.16 | 111.00 |
| 34 | i | 381 | C | O4'-C1'-N1 | 9.68 | 115.94 | 108.20 |
| 34 | i | 879 | U | O4'-C1'-N1 | 9.68 | 115.94 | 108.20 |
| 34 | i | 1232 | G | O4'-C1'-N9 | 9.67 | 115.94 | 108.20 |
| 34 | i | 397 | G | O4'-C1'-N9 | 9.67 | 115.94 | 108.20 |
| 34 | i | 1551 | A | O4'-C1'-N9 | 9.66 | 115.93 | 108.20 |
| 34 | i | 1490 | U | O4'-C1'-N1 | 9.65 | 115.92 | 108.20 |
| 19 | S | 54 | LYS | N-CA-C | 9.65 | 137.06 | 111.00 |
| 33 | g | 159 | ASN | N-CA-C | 9.65 | 137.05 | 111.00 |
| 34 | i | 66 | G | N9-C1'-C2' | 9.65 | 126.54 | 114.00 |
| 3 | C | 93 | LYS | C-N-CA | 9.64 | 145.81 | 121.70 |
| 18 | R | 1 | MET | CA-C-O | 9.64 | 140.35 | 120.10 |
| 34 | i | 1599 | G | O4'-C1'-N9 | 9.64 | 115.91 | 108.20 |
| 34 | i | 1546 | U | O4'-C1'-N1 | 9.62 | 115.90 | 108.20 |
| 34 | i | 1288 | C | O4'-C1'-N1 | -9.61 | 100.52 | 108.20 |
| 34 | i | 434 | G | O4'-C1'-N9 | 9.60 | 115.88 | 108.20 |
| 34 | i | 1503 | G | C1'-O4'-C4' | -9.60 | 102.22 | 109.90 |
| 34 | i | 824 | G | O4'-C1'-C2' | 9.60 | 116.24 | 107.60 |
| 34 | i | 1249 | A | P-O3'-C3' | 9.59 | 131.21 | 119.70 |
| 34 | i | 468 | G | O4'-C1'-N9 | 9.59 | 115.87 | 108.20 |
| 34 | i | 1077 | U | O4'-C1'-N1 | 9.59 | 115.87 | 108.20 |
| 18 | R | 3 | ARG | N-CA-CB | 9.58 | 127.85 | 110.60 |
| 34 | i | 1530 | U | P-O3'-C3' | 9.58 | 131.20 | 119.70 |
| 34 | i | 830 | C | C1'-O4'-C4' | -9.57 | 102.24 | 109.90 |
| 34 | i | 1132 | U | O4'-C1'-N1 | 9.57 | 115.85 | 108.20 |
| 34 | i | 1490 | U | P-O3'-C3' | 9.54 | 131.14 | 119.70 |
| 34 | i | 394 | G | O4'-C1'-N9 | 9.53 | 115.83 | 108.20 |
| 34 | i | 545 | A | P-O3'-C3' | 9.52 | 131.13 | 119.70 |
| 34 | i | 909 | A | C3'-C2'-C1' | 9.52 | 109.12 | 101.50 |
| 34 | i | 626 | C | C3'-C2'-C1' | 9.51 | 109.11 | 101.50 |
| 4 | D | 193 | ASP | N-CA-C | -9.51 | 85.33 | 111.00 |
| 34 | i | 961 | U | O4'-C1'-N1 | 9.51 | 115.80 | 108.20 |
| 34 | i | 1585 | C | N1-C1'-C2' | 9.50 | 126.35 | 114.00 |
| 34 | i | 1251 | G | C1'-O4'-C4' | -9.50 | 102.30 | 109.90 |
| 34 | i | 1582 | G | O4'-C1'-N9 | 9.49 | 115.79 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 647 | U | O4'-C1'-N1 | 9.49 | 115.79 | 108.20 |
| 34 | i | 1163 | G | O4'-C1'-N9 | 9.48 | 115.78 | 108.20 |
| 34 | i | 838 | C | C3'-C2'-C1' | 9.48 | 109.08 | 101.50 |
| 34 | i | 67 | C | C3'-C2'-C1' | -9.47 | 93.92 | 101.50 |
| 34 | i | 504 | U | O4'-C1'-N1 | 9.46 | 115.77 | 108.20 |
| 34 | i | 987 | G | O4'-C1'-N9 | 9.46 | 115.77 | 108.20 |
| 9 | I | 105 | ASP | CB-CG-OD2 | 9.46 | 126.82 | 118.30 |
| 34 | i | 1845 | A | O4'-C1'-C2' | -9.46 | 96.34 | 105.80 |
| 34 | i | 1215 | C | O4'-C1'-N1 | 9.45 | 115.76 | 108.20 |
| 34 | i | 1802 | U | O4'-C1'-N1 | 9.45 | 115.76 | 108.20 |
| 34 | i | 883 | U | P-O5'-C5' | 9.45 | 136.02 | 120.90 |
| 25 | Y | 103 | SER | CA-C-N | 9.45 | 137.98 | 117.20 |
| 34 | i | 826 | A | C3'-C2'-C1' | -9.45 | 93.94 | 101.50 |
| 27 | a | 63 | VAL | C-N-CA | 9.44 | 145.31 | 121.70 |
| 34 | i | 160 | U | P-O3'-C3' | 9.44 | 131.02 | 119.70 |
| 34 | i | 1291 | A | O4'-C1'-N9 | 9.43 | 115.74 | 108.20 |
| 34 | i | 1564 | A | O5'-P-OP2 | -9.43 | 97.22 | 105.70 |
| 34 | i | 1140 | A | N9-C1'-C2' | 9.41 | 126.23 | 114.00 |
| 34 | i | 79 | A | C5'-C4'-O4' | 9.40 | 120.39 | 109.10 |
| 34 | i | 1125 | G | O4'-C1'-N9 | 9.40 | 115.72 | 108.20 |
| 34 | i | 1013 | U | O4'-C1'-N1 | 9.40 | 115.72 | 108.20 |
| 8 | H | 111 | LYS | N-CA-CB | 9.39 | 127.50 | 110.60 |
| 27 | a | 10 | ARG | CB-CG-CD | 9.39 | 136.01 | 111.60 |
| 34 | i | 207 | U | C4'-C3'-O3' | 9.38 | 131.77 | 113.00 |
| 34 | i | 793 | C | C3'-C2'-C1' | 9.38 | 109.00 | 101.50 |
| 34 | i | 642 | U | O4'-C1'-N1 | 9.38 | 115.70 | 108.20 |
| 34 | i | 855 | G | O4'-C1'-N9 | 9.37 | 115.70 | 108.20 |
| 34 | i | 1197 | U | O4'-C1'-N1 | 9.37 | 115.70 | 108.20 |
| 34 | i | 840 | U | O4'-C1'-N1 | 9.37 | 115.69 | 108.20 |
| 34 | i | 1037 | G | O4'-C1'-C2' | 9.36 | 116.03 | 107.60 |
| 34 | i | 1204 | A | O4'-C1'-N9 | 9.36 | 115.69 | 108.20 |
| 34 | i | 1444 | A | P-O3'-C3' | 9.35 | 130.92 | 119.70 |
| 34 | i | 951 | A | O4'-C1'-N9 | 9.35 | 115.68 | 108.20 |
| 34 | i | 728 | U | N1-C1'-C2' | 9.35 | 126.15 | 114.00 |
| 34 | i | 1266 | G | O4'-C1'-N9 | 9.35 | 115.68 | 108.20 |
| 34 | i | 1317 | G | O4'-C1'-N9 | 9.34 | 115.67 | 108.20 |
| 34 | i | 431 | C | N1-C1'-C2' | 9.33 | 126.12 | 114.00 |
| 34 | i | 214 | A | C3'-C2'-C1' | 9.32 | 108.96 | 101.50 |
| 34 | i | 424 | G | C4'-C3'-O3' | -9.32 | 89.84 | 109.40 |
| 34 | i | 905 | G | O3'-P-O5' | 9.32 | 121.70 | 104.00 |
| 34 | i | 408 | A | N9-C1'-C2' | 9.30 | 126.09 | 114.00 |
| 34 | i | 524 | G | O3'-P-O5' | -9.30 | 86.33 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1786 | G | O4'-C1'-C2' | 9.30 | 115.97 | 107.60 |
| 34 | i | 1617 | U | O4'-C1'-N1 | -9.30 | 100.76 | 108.20 |
| 4 | D | 82 | GLY | C-N-CA | -9.29 | 98.46 | 121.70 |
| 22 | V | 61 | ARG | NE-CZ-NH1 | 9.29 | 124.94 | 120.30 |
| 34 | i | 651 | U | O4'-C1'-N1 | 9.29 | 115.63 | 108.20 |
| 7 | G | 122 | PRO | CA-N-CD | -9.29 | 98.50 | 111.50 |
| 34 | i | 1068 | U | O4'-C1'-N1 | 9.28 | 115.63 | 108.20 |
| 34 | i | 619 | A | O4'-C1'-N9 | 9.27 | 115.62 | 108.20 |
| 34 | i | 1228 | U | O4'-C1'-N1 | 9.27 | 115.62 | 108.20 |
| 34 | i | 892 | U | O4'-C1'-N1 | 9.26 | 115.61 | 108.20 |
| 34 | i | 51 | U | O4'-C1'-N1 | 9.25 | 115.60 | 108.20 |
| 19 | S | 40 | TYR | N-CA-C | 9.25 | 135.98 | 111.00 |
| 34 | i | 147 | A | N9-C1'-C2' | -9.24 | 101.83 | 112.00 |
| 34 | i | 1360 | U | O3'-P-O5' | 9.24 | 121.56 | 104.00 |
| 34 | i | 1810 | G | O4'-C1'-N9 | 9.24 | 115.59 | 108.20 |
| 21 | U | 94 | PRO | CA-N-CD | -9.24 | 98.56 | 111.50 |
| 34 | i | 1065 | U | P-O3'-C3' | 9.24 | 130.79 | 119.70 |
| 26 | Z | 104 | ARG | CD-NE-CZ | -9.24 | 110.67 | 123.60 |
| 34 | i | 1288 | C | N1-C1'-C2' | 9.22 | 125.99 | 114.00 |
| 34 | i | 641 | U | O4'-C1'-N1 | 9.22 | 115.58 | 108.20 |
| 34 | i | 1102 | C | O4'-C1'-N1 | 9.22 | 115.58 | 108.20 |
| 16 | P | 37 | TYR | CB-CG-CD2 | -9.22 | 115.47 | 121.00 |
| 33 | g | 274 | VAL | O-C-N | -9.22 | 107.95 | 122.70 |
| 34 | i | 660 | A | O4'-C1'-N9 | 9.22 | 115.57 | 108.20 |
| 34 | i | 1642 | A | O4'-C1'-N9 | 9.20 | 115.56 | 108.20 |
| 34 | i | 551 | A | C4'-C3'-O3' | -9.20 | 90.08 | 109.40 |
| 34 | i | 89 | C | O4'-C1'-N1 | 9.20 | 115.56 | 108.20 |
| 7 | G | 157 | VAL | N-CA-C | 9.19 | 135.82 | 111.00 |
| 34 | i | 446 | C | N1-C1'-C2' | 9.19 | 125.95 | 114.00 |
| 34 | i | 1403 | U | N1-C1'-C2' | 9.19 | 125.95 | 114.00 |
| 34 | i | 1199 | G | N9-C1'-C2' | 9.19 | 125.95 | 114.00 |
| 2 | B | 40 | ASN | C-N-CA | -9.18 | 98.74 | 121.70 |
| 34 | i | 60 | A | C3'-C2'-C1' | -9.18 | 94.16 | 101.50 |
| 34 | i | 1736 | U | N1-C1'-C2' | 9.17 | 125.92 | 114.00 |
| 34 | i | 53 | C | O4'-C1'-C2' | -9.17 | 96.63 | 105.80 |
| 34 | i | 1153 | G | O4'-C1'-N9 | 9.17 | 115.53 | 108.20 |
| 34 | i | 1455 | G | C1'-O4'-C4' | -9.17 | 102.57 | 109.90 |
| 21 | U | 53 | PRO | CA-N-CD | -9.14 | 98.70 | 111.50 |
| 34 | i | 114 | G | O4'-C1'-N9 | 9.13 | 115.50 | 108.20 |
| 12 | L | 17 | PHE | O-C-N | 9.13 | 137.30 | 122.70 |
| 34 | i | 1743 | G | P-O5'-C5' | 9.13 | 135.50 | 120.90 |
| 34 | i | 561 | U | O4'-C1'-N1 | 9.12 | 115.50 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 484 | C | C3'-C2'-C1' | 9.12 | 108.80 | 101.50 |
| 34 | i | 995 | G | O4'-C1'-N9 | 9.12 | 115.49 | 108.20 |
| 34 | i | 298 | G | C3'-C2'-C1' | -9.11 | 94.21 | 101.50 |
| 34 | i | 735 | C | N1-C1'-C2' | 9.10 | 125.83 | 114.00 |
| 34 | i | 107 | A | O4'-C1'-N9 | 9.09 | 115.47 | 108.20 |
| 34 | i | 1022 | C | C3'-C2'-C1' | 9.09 | 108.77 | 101.50 |
| 34 | i | 1261 | A | C3'-C2'-C1' | 9.09 | 108.77 | 101.50 |
| 34 | i | 910 | U | O4'-C1'-N1 | 9.08 | 115.47 | 108.20 |
| 34 | i | 152 | U | O4'-C1'-N1 | 9.08 | 115.46 | 108.20 |
| 34 | i | 99 | A | O4'-C1'-N9 | 9.07 | 115.46 | 108.20 |
| 4 | D | 5 | ILE | C-N-CA | 9.06 | 144.36 | 121.70 |
| 12 | L | 17 | PHE | CA-C-N | -9.06 | 97.27 | 117.20 |
| 34 | i | 824 | G | C3'-C2'-C1' | -9.06 | 94.25 | 101.50 |
| 34 | i | 1076 | A | O4'-C1'-N9 | 9.06 | 115.45 | 108.20 |
| 19 | S | 53 | THR | O-C-N | -9.06 | 108.21 | 122.70 |
| 34 | i | 501 | U | O4'-C1'-N1 | 9.04 | 115.44 | 108.20 |
| 34 | i | 414 | C | N1-C1'-C2' | 9.03 | 125.73 | 114.00 |
| 9 | I | 105 | ASP | CB-CG-OD1 | -9.02 | 110.18 | 118.30 |
| 34 | i | 405 | A | N9-C1'-C2' | -9.02 | 102.08 | 112.00 |
| 34 | i | 640 | A | C3'-C2'-C1' | 9.02 | 108.72 | 101.50 |
| 34 | i | 56 | G | O4'-C1'-N9 | 9.01 | 115.41 | 108.20 |
| 34 | i | 1469 | G | P-O3'-C3' | 9.01 | 130.51 | 119.70 |
| 34 | i | 1427 | G | O4'-C1'-N9 | 9.00 | 115.40 | 108.20 |
| 34 | i | 1189 | U | O4'-C1'-N1 | 8.99 | 115.40 | 108.20 |
| 34 | i | 24 | C | O3'-P-O5' | -8.99 | 86.92 | 104.00 |
| 34 | i | 1129 | A | O4'-C1'-N9 | 8.98 | 115.39 | 108.20 |
| 27 | a | 10 | ARG | NH1-CZ-NH2 | -8.98 | 109.53 | 119.40 |
| 34 | i | 1631 | G | O4'-C1'-N9 | 8.98 | 115.38 | 108.20 |
| 21 | U | 93 | SER | C-N-CD | 8.97 | 147.24 | 128.40 |
| 34 | i | 653 | C | N1-C1'-C2' | 8.97 | 125.66 | 114.00 |
| 34 | i | 733 | G | C1'-O4'-C4' | 8.96 | 117.07 | 109.90 |
| 34 | i | 437 | A | O4'-C1'-C2' | -8.95 | 96.85 | 105.80 |
| 34 | i | 1523 | G | C3'-C2'-C1' | -8.95 | 94.34 | 101.50 |
| 27 | a | 97 | PRO | N-CA-CB | -8.95 | 92.57 | 103.30 |
| 34 | i | 542 | G | P-O5'-C5' | 8.94 | 135.21 | 120.90 |
| 34 | i | 730 | C | O4'-C1'-C2' | -8.94 | 96.86 | 105.80 |
| 34 | i | 652 | G | N9-C1'-C2' | 8.94 | 125.62 | 114.00 |
| 34 | i | 482 | C | O4'-C1'-C2' | -8.94 | 96.86 | 105.80 |
| 24 | X | 62 | PRO | CA-N-CD | -8.93 | 98.99 | 111.50 |
| 34 | i | 1405 | A | P-O5'-C5' | 8.93 | 135.18 | 120.90 |
| 34 | i | 1515 | G | C1'-O4'-C4' | -8.93 | 102.76 | 109.90 |
| 34 | i | 947 | C | P-O5'-C5' | 8.93 | 135.18 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1335 | U | O4'-C1'-N1 | 8.93 | 115.34 | 108.20 |
| 34 | i | 1775 | A | P-O3'-C3' | 8.93 | 130.41 | 119.70 |
| 34 | i | 1184 | A | O4'-C1'-C2' | -8.92 | 96.88 | 105.80 |
| 34 | i | 1687 | U | O4'-C1'-N1 | 8.92 | 115.34 | 108.20 |
| 34 | i | 1716 | U | O4'-C1'-C2' | -8.92 | 96.88 | 105.80 |
| 34 | i | 1473 | U | P-O5'-C5' | 8.91 | 135.16 | 120.90 |
| 34 | i | 1472 | A | C1'-O4'-C4' | 8.91 | 117.03 | 109.90 |
| 34 | i | 189 | G | N9-C1'-C2' | 8.91 | 125.58 | 114.00 |
| 34 | i | 609 | A | O4'-C1'-N9 | 8.90 | 115.32 | 108.20 |
| 34 | i | 1847 | C | N1-C1'-C2' | 8.90 | 125.57 | 114.00 |
| 34 | i | 1272 | A | N9-C1'-C2' | -8.89 | 102.22 | 112.00 |
| 34 | i | 847 | C | O3'-P-O5' | -8.88 | 87.12 | 104.00 |
| 34 | i | 1501 | U | O4'-C1'-N1 | 8.88 | 115.31 | 108.20 |
| 28 | b | 12 | PRO | CA-N-CD | -8.88 | 99.07 | 111.50 |
| 34 | i | 1824 | U | C3'-C2'-C1' | 8.88 | 108.60 | 101.50 |
| 34 | i | 951 | A | P-O3'-C3' | 8.87 | 130.35 | 119.70 |
| 34 | i | 611 | C | N1-C1'-C2' | 8.87 | 125.53 | 114.00 |
| 34 | i | 1191 | A | O4'-C1'-N9 | 8.87 | 115.30 | 108.20 |
| 34 | i | 543 | U | O4'-C1'-C2' | -8.86 | 96.94 | 105.80 |
| 34 | i | 1855 | G | O4'-C1'-C2' | 8.86 | 115.57 | 107.60 |
| 34 | i | 201 | G | O4'-C1'-N9 | 8.86 | 115.28 | 108.20 |
| 34 | i | 956 | U | N1-C1'-C2' | 8.86 | 125.51 | 114.00 |
| 34 | i | 1159 | C | N1-C1'-C2' | 8.86 | 125.51 | 114.00 |
| 34 | i | 325 | G | N9-C1'-C2' | -8.85 | 102.27 | 112.00 |
| 10 | J | 165 | TYR | CB-CA-C | 8.85 | 128.09 | 110.40 |
| 19 | S | 88 | LYS | C-N-CA | -8.84 | 99.59 | 121.70 |
| 19 | S | 142 | ARG | CB-CA-C | -8.84 | 92.72 | 110.40 |
| 34 | i | 444 | U | O4'-C1'-N1 | 8.84 | 115.27 | 108.20 |
| 34 | i | 1596 | A | P-O3'-C3' | 8.84 | 130.30 | 119.70 |
| 34 | i | 212 | G | O4'-C1'-N9 | 8.83 | 115.27 | 108.20 |
| 34 | i | 1214 | C | N1-C1'-C2' | 8.83 | 125.48 | 114.00 |
| 19 | S | 94 | LYS | CA-C-N | -8.83 | 97.78 | 117.20 |
| 33 | g | 145 | GLU | N-CA-C | -8.83 | 87.16 | 111.00 |
| 34 | i | 299 | G | C1'-O4'-C4' | -8.83 | 102.84 | 109.90 |
| 34 | i | 1676 | U | O4'-C1'-N1 | 8.83 | 115.26 | 108.20 |
| 34 | i | 25 | A | N9-C1'-C2' | -8.82 | 102.29 | 112.00 |
| 34 | i | 548 | G | C3'-C2'-C1' | -8.82 | 94.44 | 101.50 |
| 34 | i | 224 | U | N1-C1'-C2' | -8.82 | 102.30 | 112.00 |
| 6 | F | 130 | ARG | NE-CZ-NH1 | 8.81 | 124.71 | 120.30 |
| 34 | i | 140 | U | O4'-C1'-N1 | 8.81 | 115.25 | 108.20 |
| 34 | i | 1068 | U | C1'-O4'-C4' | 8.81 | 116.95 | 109.90 |
| 34 | i | 1861 | U | C3'-C2'-C1' | -8.81 | 94.45 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 963 | C | O4'-C1'-N1 | 8.80 | 115.24 | 108.20 |
| 34 | i | 1436 | C | C3'-C2'-C1' | 8.80 | 108.54 | 101.50 |
| 34 | i | 689 | G | P-O3'-C3' | 8.80 | 130.26 | 119.70 |
| 22 | V | 67 | ASP | CB-CA-C | 8.79 | 127.98 | 110.40 |
| 34 | i | 1466 | C | O4'-C1'-N1 | 8.79 | 115.23 | 108.20 |
| 34 | i | 108 | G | O4'-C1'-N9 | 8.78 | 115.23 | 108.20 |
| 34 | i | 583 | C | C3'-C2'-C1' | 8.78 | 108.52 | 101.50 |
| 34 | i | 564 | A | C3'-C2'-C1' | 8.76 | 108.51 | 101.50 |
| 25 | Y | 52 | PRO | CA-N-CD | -8.76 | 99.24 | 111.50 |
| 3 | C | 104 | GLY | N-CA-C | 8.75 | 134.97 | 113.10 |
| 34 | i | 903 | G | N9-C1'-C2' | 8.75 | 125.37 | 114.00 |
| 34 | i | 234 | C | C1'-O4'-C4' | 8.74 | 116.89 | 109.90 |
| 34 | i | 837 | G | C1'-C2'-O2' | -8.74 | 84.39 | 110.60 |
| 34 | i | 1776 | G | C3'-C2'-C1' | -8.74 | 94.51 | 101.50 |
| 34 | i | 1546 | U | C1'-O4'-C4' | -8.73 | 102.91 | 109.90 |
| 34 | i | 1601 | G | O4'-C1'-N9 | 8.73 | 115.18 | 108.20 |
| 34 | i | 43 | U | O4'-C1'-N1 | 8.72 | 115.18 | 108.20 |
| 34 | i | 161 | U | O4'-C1'-C2' | -8.72 | 97.08 | 105.80 |
| 34 | i | 1548 | C | P-O3'-C3' | 8.71 | 130.16 | 119.70 |
| 34 | i | 872 | C | O4'-C1'-N1 | 8.71 | 115.17 | 108.20 |
| 34 | i | 234 | C | O4'-C1'-C2' | -8.70 | 97.10 | 105.80 |
| 10 | J | 118 | GLY | O-C-N | -8.70 | 108.79 | 122.70 |
| 34 | i | 1425 | G | O4'-C1'-N9 | 8.70 | 115.16 | 108.20 |
| 34 | i | 79 | A | C4'-C3'-C2' | -8.69 | 93.91 | 102.60 |
| 34 | i | 792 | G | P-O3'-C3' | 8.69 | 130.13 | 119.70 |
| 25 | Y | 86 | GLU | CB-CA-C | -8.69 | 93.02 | 110.40 |
| 34 | i | 455 | A | P-O3'-C3' | 8.69 | 130.12 | 119.70 |
| 17 | Q | 134 | GLY | C-N-CD | -8.68 | 101.50 | 120.60 |
| 34 | i | 1232 | G | C3'-C2'-C1' | -8.68 | 94.55 | 101.50 |
| 34 | i | 604 | G | C3'-C2'-C1' | 8.68 | 108.44 | 101.50 |
| 34 | i | 1104 | G | P-O3'-C3' | 8.68 | 130.12 | 119.70 |
| 34 | i | 1131 | C | O4'-C1'-N1 | 8.68 | 115.14 | 108.20 |
| 34 | i | 222 | G | C1'-O4'-C4' | -8.68 | 102.96 | 109.90 |
| 34 | i | 1428 | U | C3'-C2'-C1' | 8.67 | 108.44 | 101.50 |
| 34 | i | 1706 | U | O4'-C1'-N1 | 8.67 | 115.14 | 108.20 |
| 34 | i | 959 | A | O4'-C1'-N9 | 8.66 | 115.13 | 108.20 |
| 34 | i | 58 | C | O4'-C1'-N1 | 8.66 | 115.13 | 108.20 |
| 34 | i | 929 | G | O4'-C1'-N9 | 8.66 | 115.12 | 108.20 |
| 21 | U | 67 | LYS | C-N-CA | -8.65 | 100.08 | 121.70 |
| 34 | i | 1222 | G | N9-C1'-C2' | 8.65 | 125.24 | 114.00 |
| 34 | i | 1576 | C | O4'-C1'-C2' | -8.65 | 97.15 | 105.80 |
| 8 | H | 111 | LYS | N-CA-C | -8.64 | 87.67 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 153 | G | O4'-C1'-N9 | 8.64 | 115.11 | 108.20 |
| 34 | i | 234 | C | O4'-C1'-N1 | 8.63 | 115.10 | 108.20 |
| 34 | i | 472 | G | O4'-C1'-N9 | 8.63 | 115.10 | 108.20 |
| 34 | i | 848 | G | P-O3'-C3' | 8.62 | 130.05 | 119.70 |
| 34 | i | 1199 | G | C1'-O4'-C4' | -8.62 | 103.00 | 109.90 |
| 16 | P | 17 | TYR | CB-CA-C | 8.62 | 127.64 | 110.40 |
| 34 | i | 1208 | G | N9-C1'-C2' | 8.62 | 125.21 | 114.00 |
| 34 | i | 1272 | A | O4'-C1'-C2' | -8.62 | 97.18 | 105.80 |
| 34 | i | 25 | A | O4'-C1'-C2' | -8.61 | 97.19 | 105.80 |
| 34 | i | 795 | U | N1-C1'-C2' | 8.61 | 125.20 | 114.00 |
| 34 | i | 835 | C | P-O3'-C3' | 8.61 | 130.03 | 119.70 |
| 34 | i | 518 | A | C1'-O4'-C4' | -8.60 | 103.02 | 109.90 |
| 34 | i | 1067 | G | O4'-C1'-N9 | 8.60 | 115.08 | 108.20 |
| 34 | i | 180 | G | C4'-C3'-O3' | 8.59 | 130.18 | 113.00 |
| 34 | i | 849 | C | O3'-P-O5' | 8.59 | 120.32 | 104.00 |
| 34 | i | 296 | U | P-O3'-C3' | -8.59 | 109.39 | 119.70 |
| 34 | i | 21 | U | O4'-C1'-N1 | 8.58 | 115.06 | 108.20 |
| 34 | i | 1388 | U | O4'-C1'-N1 | 8.58 | 115.06 | 108.20 |
| 32 | f | 122 | PRO | CA-N-CD | -8.58 | 99.49 | 111.50 |
| 34 | i | 1003 | C | C3'-C2'-C1' | 8.58 | 108.36 | 101.50 |
| 6 | F | 45 | TYR | CA-CB-CG | -8.57 | 97.11 | 113.40 |
| 8 | H | 36 | LEU | CA-CB-CG | -8.57 | 95.58 | 115.30 |
| 34 | i | 1726 | A | O4'-C1'-N9 | 8.56 | 115.05 | 108.20 |
| 34 | i | 1108 | U | O4'-C1'-N1 | 8.56 | 115.05 | 108.20 |
| 28 | b | 10 | PRO | CA-N-CD | -8.56 | 99.52 | 111.50 |
| 34 | i | 972 | G | P-O5'-C5' | 8.55 | 134.58 | 120.90 |
| 34 | i | 159 | A | O4'-C1'-N9 | 8.54 | 115.03 | 108.20 |
| 34 | i | 144 | U | N1-C1'-C2' | 8.54 | 125.10 | 114.00 |
| 34 | i | 1646 | A | N9-C1'-C2' | -8.53 | 102.61 | 112.00 |
| 34 | i | 1325 | U | C1'-O4'-C4' | -8.53 | 103.08 | 109.90 |
| 10 | J | 161 | LEU | O-C-N | -8.53 | 109.05 | 122.70 |
| 9 | I | 184 | ARG | N-CA-CB | 8.53 | 125.94 | 110.60 |
| 34 | i | 1229 | G | C1'-O4'-C4' | -8.52 | 103.08 | 109.90 |
| 16 | P | 69 | PRO | CA-N-CD | -8.51 | 99.58 | 111.50 |
| 34 | i | 1002 | C | N1-C1'-C2' | 8.51 | 125.07 | 114.00 |
| 34 | i | 1728 | U | O4'-C1'-N1 | 8.51 | 115.01 | 108.20 |
| 34 | i | 1517 | A | O4'-C1'-N9 | 8.51 | 115.01 | 108.20 |
| 27 | a | 80 | HIS | N-CA-CB | -8.51 | 95.29 | 110.60 |
| 34 | i | 929 | G | O4'-C1'-C2' | 8.51 | 115.25 | 107.60 |
| 34 | i | 1109 | A | O4'-C1'-N9 | 8.51 | 115.00 | 108.20 |
| 34 | i | 1770 | G | O4'-C1'-N9 | 8.51 | 115.00 | 108.20 |
| 11 | K | 87 | PRO | C-N-CA | 8.50 | 142.96 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1425 | G | N9-C1'-C2' | -8.50 | 102.65 | 112.00 |
| 34 | i | 1581 | U | O4'-C1'-N1 | 8.50 | 115.00 | 108.20 |
| 34 | i | 859 | U | C1'-O4'-C4' | -8.49 | 103.11 | 109.90 |
| 34 | i | 669 | A | O4'-C1'-N9 | 8.49 | 114.99 | 108.20 |
| 34 | i | 602 | U | O4'-C1'-N1 | 8.48 | 114.98 | 108.20 |
| 34 | i | 727 | G | O3'-P-O5' | 8.48 | 120.11 | 104.00 |
| 34 | i | 1198 | U | N1-C1'-C2' | -8.47 | 102.68 | 112.00 |
| 34 | i | 1513 | C | O4'-C1'-N1 | 8.47 | 114.98 | 108.20 |
| 34 | i | 343 | C | C5'-C4'-C3' | 8.47 | 129.55 | 116.00 |
| 34 | i | 1526 | A | O4'-C1'-N9 | 8.47 | 114.97 | 108.20 |
| 34 | i | 131 | C | P-O3'-C3' | 8.46 | 129.85 | 119.70 |
| 8 | H | 108 | SER | N-CA-CB | 8.46 | 123.18 | 110.50 |
| 34 | i | 824 | G | O4'-C1'-N9 | 8.46 | 114.97 | 108.20 |
| 34 | i | 849 | C | P-O3'-C3' | -8.45 | 109.56 | 119.70 |
| 34 | i | 1442 | A | P-O3'-C3' | 8.45 | 129.84 | 119.70 |
| 34 | i | 28 | U | O4'-C1'-N1 | 8.44 | 114.95 | 108.20 |
| 17 | Q | 18 | THR | CA-CB-OG1 | 8.44 | 126.72 | 109.00 |
| 19 | S | 95 | TYR | N-CA-CB | -8.44 | 95.41 | 110.60 |
| 34 | i | 1411 | C | N1-C1'-C2' | 8.44 | 124.97 | 114.00 |
| 34 | i | 739 | U | O4'-C1'-C2' | -8.43 | 97.37 | 105.80 |
| 34 | i | 1137 | G | O4'-C1'-N9 | 8.43 | 114.94 | 108.20 |
| 21 | U | 70 | CYS | C-N-CA | 8.43 | 140.00 | 122.30 |
| 31 | e | 95 | LYS | CA-C-N | 8.42 | 135.73 | 117.20 |
| 34 | i | 1205 | A | O4'-C1'-N9 | 8.42 | 114.94 | 108.20 |
| 4 | D | 193 | ASP | C-N-CD | 8.42 | 146.08 | 128.40 |
| 34 | i | 1014 | U | N1-C1'-C2' | 8.42 | 124.94 | 114.00 |
| 34 | i | 1504 | A | N9-C1'-C2' | -8.41 | 102.75 | 112.00 |
| 34 | i | 733 | G | N9-C1'-C2' | -8.40 | 102.75 | 112.00 |
| 34 | i | 1272 | A | C3'-C2'-C1' | 8.40 | 108.22 | 101.50 |
| 10 | J | 180 | LYS | C-N-CA | 8.40 | 139.93 | 122.30 |
| 34 | i | 276 | U | O4'-C1'-N1 | -8.39 | 101.49 | 108.20 |
| 34 | i | 1110 | U | O4'-C1'-N1 | 8.39 | 114.92 | 108.20 |
| 34 | i | 1198 | U | O4'-C1'-N1 | 8.39 | 114.91 | 108.20 |
| 34 | i | 1458 | U | C4'-C3'-O3' | 8.39 | 129.78 | 113.00 |
| 34 | i | 1685 | U | O4'-C1'-N1 | 8.39 | 114.91 | 108.20 |
| 34 | i | 442 | G | C3'-C2'-C1' | 8.39 | 108.21 | 101.50 |
| 34 | i | 691 | G | P-O3'-C3' | 8.39 | 129.77 | 119.70 |
| 34 | i | 964 | U | O4'-C1'-C2' | -8.39 | 97.41 | 105.80 |
| 34 | i | 1322 | U | C3'-C2'-C1' | 8.39 | 108.21 | 101.50 |
| 34 | i | 1006 | G | C3'-C2'-C1' | -8.38 | 94.79 | 101.50 |
| 34 | i | 1474 | U | O4'-C1'-N1 | 8.38 | 114.91 | 108.20 |
| 34 | i | 276 | U | C3'-C2'-C1' | 8.38 | 108.21 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1082 | G | O3'-P-O5' | -8.38 | 88.08 | 104.00 |
| 34 | i | 385 | G | C3'-C2'-C1' | -8.38 | 94.80 | 101.50 |
| 34 | i | 512 | A | O4'-C1'-N9 | 8.38 | 114.90 | 108.20 |
| 34 | i | 103 | A | C3'-C2'-C1' | -8.37 | 94.80 | 101.50 |
| 34 | i | 1044 | G | C1'-O4'-C4' | -8.37 | 103.20 | 109.90 |
| 5 | E | 43 | PRO | CA-N-CD | -8.36 | 99.79 | 111.50 |
| 34 | i | 1691 | C | N1-C1'-C2' | 8.36 | 124.87 | 114.00 |
| 34 | i | 1434 | A | O4'-C1'-C2' | -8.36 | 97.44 | 105.80 |
| 7 | G | 170 | ARG | CB-CA-C | -8.36 | 93.69 | 110.40 |
| 34 | i | 1468 | C | C4'-C3'-O3' | 8.35 | 129.70 | 113.00 |
| 34 | i | 97 | U | N1-C1'-C2' | 8.35 | 124.85 | 114.00 |
| 34 | i | 1118 | A | O4'-C1'-C2' | -8.35 | 97.45 | 105.80 |
| 34 | i | 1014 | U | C1'-O4'-C4' | -8.34 | 103.23 | 109.90 |
| 34 | i | 389 | C | C3'-C2'-C1' | 8.34 | 108.17 | 101.50 |
| 34 | i | 543 | U | C4'-C3'-C2' | -8.33 | 94.27 | 102.60 |
| 34 | i | 291 | U | O4'-C1'-N1 | 8.32 | 114.86 | 108.20 |
| 34 | i | 546 | U | O4'-C1'-N1 | 8.31 | 114.85 | 108.20 |
| 34 | i | 1655 | C | O4'-C1'-N1 | 8.31 | 114.84 | 108.20 |
| 34 | i | 1316 | G | C3'-C2'-C1' | -8.30 | 94.86 | 101.50 |
| 34 | i | 966 | G | P-O3'-C3' | 8.30 | 129.66 | 119.70 |
| 34 | i | 1336 | U | O4'-C1'-N1 | 8.30 | 114.84 | 108.20 |
| 34 | i | 82 | G | O4'-C1'-C2' | -8.29 | 97.51 | 105.80 |
| 34 | i | 544 | A | C3'-C2'-C1' | -8.29 | 94.87 | 101.50 |
| 34 | i | 639 | U | C1'-O4'-C4' | -8.29 | 103.27 | 109.90 |
| 34 | i | 1376 | C | C3'-C2'-C1' | 8.29 | 108.13 | 101.50 |
| 34 | i | 520 | U | P-O3'-C3' | 8.29 | 129.64 | 119.70 |
| 34 | i | 1226 | C | C1'-O4'-C4' | -8.29 | 103.27 | 109.90 |
| 27 | a | 58 | VAL | CB-CA-C | -8.28 | 95.66 | 111.40 |
| 26 | Z | 104 | ARG | NE-CZ-NH1 | -8.28 | 116.16 | 120.30 |
| 34 | i | 1688 | G | C1'-O4'-C4' | -8.27 | 103.29 | 109.90 |
| 34 | i | 357 | U | O4'-C1'-N1 | 8.27 | 114.81 | 108.20 |
| 34 | i | 1292 | U | O4'-C1'-N1 | 8.27 | 114.81 | 108.20 |
| 12 | L | 147 | LYS | N-CA-C | 8.26 | 133.31 | 111.00 |
| 34 | i | 376 | C | N1-C1'-C2' | 8.26 | 124.74 | 114.00 |
| 34 | i | 905 | G | P-O3'-C3' | -8.26 | 109.79 | 119.70 |
| 34 | i | 1529 | C | O4'-C1'-C2' | -8.26 | 97.54 | 105.80 |
| 34 | i | 313 | C | C3'-C2'-C1' | 8.26 | 108.11 | 101.50 |
| 19 | S | 6 | PRO | N-CA-C | 8.25 | 133.56 | 112.10 |
| 34 | i | 1151 | U | C5'-C4'-O4' | 8.25 | 119.00 | 109.10 |
| 34 | i | 1464 | C | O4'-C1'-N1 | 8.25 | 114.80 | 108.20 |
| 11 | K | 55 | ARG | NE-CZ-NH2 | -8.24 | 116.18 | 120.30 |
| 34 | i | 1305 | C | O4'-C1'-C2' | -8.24 | 97.56 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9 | I | 5 | ARG | O-C-N | -8.23 | 109.52 | 122.70 |
| 34 | i | 351 | U | O4'-C1'-N1 | 8.23 | 114.78 | 108.20 |
| 34 | i | 546 | U | N1-C1'-C2' | 8.23 | 124.70 | 114.00 |
| 32 | f | 87 | THR | N-CA-C | -8.22 | 88.80 | 111.00 |
| 34 | i | 744 | C | C3'-C2'-C1' | 8.22 | 108.08 | 101.50 |
| 34 | i | 36 | U | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 34 | i | 334 | U | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 34 | i | 1208 | G | C1'-O4'-C4' | -8.22 | 103.33 | 109.90 |
| 25 | Y | 87 | PRO | CA-N-CD | -8.21 | 100.00 | 111.50 |
| 14 | N | 7 | PRO | CA-N-CD | -8.21 | 100.00 | 111.50 |
| 34 | i | 38 | A | N9-C1'-C2' | -8.21 | 102.97 | 112.00 |
| 34 | i | 578 | G | O3'-P-O5' | -8.21 | 88.40 | 104.00 |
| 34 | i | 1836 | C | O4'-C1'-N1 | 8.21 | 114.77 | 108.20 |
| 34 | i | 303 | G | O4'-C1'-N9 | 8.21 | 114.77 | 108.20 |
| 34 | i | 1344 | G | N9-C1'-C2' | -8.21 | 102.97 | 112.00 |
| 34 | i | 1615 | A | C1'-O4'-C4' | -8.21 | 103.33 | 109.90 |
| 34 | i | 1804 | U | O4'-C1'-N1 | 8.20 | 114.76 | 108.20 |
| 34 | i | 1178 | A | O4'-C1'-N9 | 8.20 | 114.76 | 108.20 |
| 1 | A | 133 | PRO | CA-N-CD | -8.20 | 100.02 | 111.50 |
| 34 | i | 80 | G | P-O5'-C5' | 8.20 | 134.01 | 120.90 |
| 34 | i | 630 | A | C1'-O4'-C4' | -8.20 | 103.34 | 109.90 |
| 34 | i | 887 | G | C1'-O4'-C4' | -8.20 | 103.34 | 109.90 |
| 34 | i | 1026 | A | O4'-C1'-N9 | 8.19 | 114.75 | 108.20 |
| 34 | i | 1618 | A | C3'-C2'-C1' | -8.19 | 94.95 | 101.50 |
| 34 | i | 1632 | A | O4'-C1'-N9 | 8.18 | 114.75 | 108.20 |
| 34 | i | 156 | G | P-O3'-C3' | -8.18 | 109.89 | 119.70 |
| 34 | i | 1010 | G | C3'-C2'-C1' | -8.18 | 94.96 | 101.50 |
| 21 | U | 93 | SER | CA-C-N | -8.17 | 94.21 | 117.10 |
| 34 | i | 281 | U | O4'-C1'-N1 | 8.17 | 114.74 | 108.20 |
| 34 | i | 1660 | G | O4'-C1'-C2' | 8.17 | 114.95 | 107.60 |
| 34 | i | 1715 | U | O4'-C1'-C2' | -8.17 | 97.63 | 105.80 |
| 21 | U | 57 | PRO | CA-N-CD | -8.16 | 100.08 | 111.50 |
| 34 | i | 186 | G | C1'-O4'-C4' | -8.15 | 103.38 | 109.90 |
| 34 | i | 605 | C | N1-C1'-C2' | 8.15 | 124.60 | 114.00 |
| 34 | i | 1307 | C | C1'-O4'-C4' | -8.14 | 103.39 | 109.90 |
| 34 | i | 435 | A | C1'-O4'-C4' | -8.14 | 103.39 | 109.90 |
| 34 | i | 1034 | U | O4'-C1'-N1 | 8.14 | 114.71 | 108.20 |
| 34 | i | 908 | C | C3'-C2'-C1' | 8.13 | 108.01 | 101.50 |
| 34 | i | 1332 | C | O4'-C1'-N1 | 8.13 | 114.71 | 108.20 |
| 16 | P | 37 | TYR | CB-CG-CD1 | 8.13 | 125.88 | 121.00 |
| 21 | U | 103 | SER | C-N-CA | -8.13 | 101.37 | 121.70 |
| 34 | i | 1651 | G | O4'-C1'-N9 | 8.13 | 114.71 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 909 | A | O4'-C1'-C2' | -8.13 | 97.67 | 105.80 |
| 34 | i | 145 | G | N9-C1'-C2' | 8.13 | 124.56 | 114.00 |
| 34 | i | 1322 | U | C1'-O4'-C4' | -8.12 | 103.40 | 109.90 |
| 34 | i | 837 | G | O4'-C4'-C3' | -8.12 | 95.88 | 104.00 |
| 3 | C | 93 | LYS | O-C-N | -8.12 | 109.71 | 122.70 |
| 34 | i | 315 | C | P-O3'-C3' | 8.12 | 129.44 | 119.70 |
| 34 | i | 1777 | C | O4'-C1'-C2' | -8.12 | 97.68 | 105.80 |
| 34 | i | 851 | G | O4'-C1'-N9 | 8.11 | 114.69 | 108.20 |
| 34 | i | 927 | C | C5'-C4'-C3' | -8.12 | 103.02 | 116.00 |
| 34 | i | 311 | C | C3'-C2'-C1' | 8.11 | 107.99 | 101.50 |
| 34 | i | 495 | G | O4'-C1'-N9 | 8.11 | 114.69 | 108.20 |
| 34 | i | 451 | U | O4'-C1'-N1 | 8.11 | 114.69 | 108.20 |
| 12 | L | 153 | LYS | C-N-CA | 8.10 | 141.95 | 121.70 |
| 34 | i | 562 | U | O4'-C1'-N1 | 8.10 | 114.68 | 108.20 |
| 34 | i | 1233 | C | C3'-C2'-C1' | 8.10 | 107.98 | 101.50 |
| 34 | i | 162 | C | P-O3'-C3' | 8.09 | 129.41 | 119.70 |
| 34 | i | 1714 | A | C1'-O4'-C4' | 8.09 | 116.37 | 109.90 |
| 34 | i | 854 | A | O4'-C1'-C2' | -8.09 | 97.71 | 105.80 |
| 21 | U | 93 | SER | O-C-N | 8.08 | 136.46 | 121.10 |
| 34 | i | 333 | A | O4'-C1'-N9 | 8.08 | 114.67 | 108.20 |
| 34 | i | 520 | U | N1-C1'-C2' | -8.07 | 103.12 | 112.00 |
| 34 | i | 619 | A | O4'-C1'-C2' | -8.06 | 97.74 | 105.80 |
| 34 | i | 1133 | U | C2'-C3'-O3' | 8.06 | 127.24 | 109.50 |
| 34 | i | 217 | U | O4'-C1'-N1 | 8.06 | 114.65 | 108.20 |
| 34 | i | 1467 | C | N1-C1'-C2' | 8.06 | 124.48 | 114.00 |
| 34 | i | 1191 | A | O4'-C4'-C3' | -8.06 | 95.94 | 104.00 |
| 34 | i | 598 | C | C3'-C2'-C1' | 8.06 | 107.94 | 101.50 |
| 34 | i | 1030 | A | O4'-C1'-N9 | 8.05 | 114.64 | 108.20 |
| 17 | Q | 31 | LEU | N-CA-C | 8.04 | 132.71 | 111.00 |
| 34 | i | 917 | G | O4'-C1'-N9 | 8.04 | 114.63 | 108.20 |
| 34 | i | 1060 | C | O4'-C1'-C2' | -8.04 | 97.76 | 105.80 |
| 34 | i | 491 | C | P-O3'-C3' | 8.04 | 129.34 | 119.70 |
| 34 | i | 1046 | A | O4'-C1'-N9 | 8.04 | 114.63 | 108.20 |
| 34 | i | 464 | G | N9-C1'-C2' | 8.03 | 124.44 | 114.00 |
| 34 | i | 1161 | G | N9-C1'-C2' | -8.03 | 103.17 | 112.00 |
| 34 | i | 1655 | C | P-O3'-C3' | -8.02 | 110.08 | 119.70 |
| 34 | i | 844 | U | N1-C1'-C2' | 8.01 | 124.42 | 114.00 |
| 34 | i | 1359 | C | C3'-C2'-C1' | 8.01 | 107.91 | 101.50 |
| 34 | i | 570 | U | C4'-C3'-O3' | 8.01 | 129.02 | 113.00 |
| 34 | i | 1117 | G | O4'-C1'-N9 | 8.01 | 114.61 | 108.20 |
| 34 | i | 1707 | A | O4'-C1'-N9 | 8.00 | 114.60 | 108.20 |
| 11 | K | 84 | HIS | CB-CA-C | -8.00 | 94.40 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 41 | G | O4'-C1'-N9 | -8.00 | 101.80 | 108.20 |
| 34 | i | 435 | A | N9-C1'-C2' | 7.99 | 124.39 | 114.00 |
| 34 | i | 490 | A | P-O3'-C3' | 7.99 | 129.29 | 119.70 |
| 34 | i | 1289 | A | N9-C1'-C2' | 7.99 | 124.39 | 114.00 |
| 34 | i | 1850 | C | O4'-C1'-N1 | 7.99 | 114.59 | 108.20 |
| 34 | i | 205 | G | N9-C1'-C2' | 7.99 | 124.39 | 114.00 |
| 34 | i | 342 | U | C3'-C2'-C1' | 7.98 | 107.89 | 101.50 |
| 34 | i | 1786 | G | C3'-C2'-C1' | -7.98 | 95.11 | 101.50 |
| 34 | i | 1068 | U | O4'-C1'-C2' | -7.98 | 97.82 | 105.80 |
| 34 | i | 939 | U | O4'-C1'-N1 | 7.97 | 114.58 | 108.20 |
| 34 | i | 1303 | U | O4'-C1'-N1 | 7.97 | 114.58 | 108.20 |
| 34 | i | 366 | A | O4'-C1'-N9 | 7.97 | 114.57 | 108.20 |
| 34 | i | 1534 | U | O4'-C1'-C2' | -7.97 | 97.83 | 105.80 |
| 34 | i | 1093 | G | O4'-C1'-N9 | 7.96 | 114.57 | 108.20 |
| 7 | G | 131 | ARG | C-N-CA | -7.96 | 101.81 | 121.70 |
| 34 | i | 986 | A | C3'-C2'-C1' | 7.96 | 107.87 | 101.50 |
| 34 | i | 1650 | C | N1-C1'-C2' | 7.96 | 124.34 | 114.00 |
| 34 | i | 735 | C | O4'-C1'-C2' | -7.95 | 97.85 | 105.80 |
| 34 | i | 429 | A | N9-C1'-C2' | -7.95 | 103.25 | 112.00 |
| 34 | i | 1348 | G | O4'-C1'-C2' | 7.95 | 114.75 | 107.60 |
| 34 | i | 890 | G | O4'-C1'-N9 | 7.95 | 114.56 | 108.20 |
| 34 | i | 238 | G | O4'-C1'-N9 | 7.95 | 114.56 | 108.20 |
| 34 | i | 1677 | C | O4'-C1'-C2' | -7.95 | 97.85 | 105.80 |
| 34 | i | 1725 | U | O4'-C1'-N1 | 7.95 | 114.56 | 108.20 |
| 34 | i | 525 | G | P-O3'-C3' | 7.94 | 129.23 | 119.70 |
| 26 | Z | 70 | PRO | CA-N-CD | -7.94 | 100.39 | 111.50 |
| 34 | i | 960 | A | C1'-O4'-C4' | 7.94 | 116.25 | 109.90 |
| 34 | i | 1136 | G | O4'-C1'-N9 | 7.94 | 114.55 | 108.20 |
| 34 | i | 520 | U | P-O5'-C5' | -7.94 | 108.20 | 120.90 |
| 34 | i | 650 | C | N1-C1'-C2' | 7.93 | 124.31 | 114.00 |
| 34 | i | 1095 | G | O4'-C1'-N9 | 7.93 | 114.54 | 108.20 |
| 34 | i | 1111 | U | P-O3'-C3' | 7.92 | 129.21 | 119.70 |
| 34 | i | 80 | G | O4'-C1'-C2' | -7.92 | 97.88 | 105.80 |
| 34 | i | 1741 | U | C4'-C3'-O3' | 7.92 | 128.85 | 113.00 |
| 34 | i | 872 | C | O4'-C1'-C2' | -7.92 | 97.88 | 105.80 |
| 9 | I | 184 | ARG | CB-CA-C | -7.92 | 94.56 | 110.40 |
| 34 | i | 207 | U | O3'-P-O5' | -7.91 | 88.97 | 104.00 |
| 34 | i | 1312 | C | N1-C1'-C2' | 7.91 | 124.28 | 114.00 |
| 34 | i | 905 | G | C4'-C3'-O3' | 7.90 | 128.81 | 113.00 |
| 34 | i | 1786 | G | C1'-O4'-C4' | -7.90 | 103.58 | 109.90 |
| 34 | i | 1297 | A | C4'-C3'-O3' | 7.90 | 128.81 | 113.00 |
| 34 | i | 1660 | G | C1'-O4'-C4' | -7.90 | 103.58 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1369 | C | C3'-C2'-C1' | 7.90 | 107.82 | 101.50 |
| 34 | i | 626 | C | P-O5'-C5' | 7.90 | 133.53 | 120.90 |
| 34 | i | 1537 | C | C1'-O4'-C4' | -7.89 | 103.59 | 109.90 |
| 34 | i | 817 | G | P-O3'-C3' | 7.88 | 129.16 | 119.70 |
| 34 | i | 1515 | G | O3'-P-O5' | 7.88 | 118.97 | 104.00 |
| 34 | i | 1779 | C | O4'-C1'-C2' | -7.88 | 97.92 | 105.80 |
| 34 | i | 33 | G | O4'-C1'-N9 | 7.87 | 114.50 | 108.20 |
| 34 | i | 1229 | G | O4'-C1'-C2' | 7.87 | 114.69 | 107.60 |
| 34 | i | 467 | G | O4'-C1'-N9 | 7.87 | 114.50 | 108.20 |
| 34 | i | 1471 | G | P-O5'-C5' | 7.87 | 133.49 | 120.90 |
| 34 | i | 82 | G | O4'-C1'-N9 | 7.86 | 114.49 | 108.20 |
| 34 | i | 342 | U | O4'-C1'-C2' | -7.86 | 97.94 | 105.80 |
| 34 | i | 1678 | C | N1-C1'-C2' | 7.86 | 124.22 | 114.00 |
| 34 | i | 1524 | C | N1-C1'-C2' | 7.86 | 124.21 | 114.00 |
| 8 | H | 15 | LYS | C-N-CD | -7.85 | 103.33 | 120.60 |
| 34 | i | 329 | A | C2'-C3'-O3' | 7.84 | 126.75 | 109.50 |
| 34 | i | 1539 | C | C3'-C2'-C1' | 7.84 | 107.77 | 101.50 |
| 34 | i | 1653 | G | O4'-C1'-C2' | 7.84 | 114.65 | 107.60 |
| 34 | i | 549 | G | O4'-C1'-N9 | 7.84 | 114.47 | 108.20 |
| 34 | i | 907 | C | N1-C1'-C2' | 7.83 | 124.19 | 114.00 |
| 7 | G | 161 | PRO | CA-N-CD | -7.83 | 100.53 | 111.50 |
| 34 | i | 169 | U | P-O3'-C3' | 7.83 | 129.10 | 119.70 |
| 34 | i | 791 | A | O4'-C1'-N9 | 7.83 | 114.47 | 108.20 |
| 26 | Z | 104 | ARG | N-CA-CB | -7.83 | 96.51 | 110.60 |
| 34 | i | 316 | C | O4'-C1'-C2' | -7.83 | 97.97 | 105.80 |
| 34 | i | 1709 | U | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 34 | i | 77 | A | N9-C1'-C2' | -7.83 | 103.39 | 112.00 |
| 34 | i | 117 | C | O4'-C1'-N1 | 7.83 | 114.46 | 108.20 |
| 34 | i | 1632 | A | N9-C1'-C2' | -7.83 | 103.39 | 112.00 |
| 34 | i | 1666 | G | N9-C1'-C2' | 7.82 | 124.16 | 114.00 |
| 34 | i | 1860 | A | P-O3'-C3' | 7.82 | 129.08 | 119.70 |
| 34 | i | 96 | C | N1-C1'-C2' | 7.81 | 124.16 | 114.00 |
| 34 | i | 147 | A | C1'-O4'-C4' | 7.81 | 116.15 | 109.90 |
| 34 | i | 541 | U | N1-C1'-C2' | 7.80 | 124.15 | 114.00 |
| 34 | i | 594 | A | O4'-C1'-C2' | -7.80 | 98.00 | 105.80 |
| 34 | i | 987 | G | O4'-C1'-C2' | 7.80 | 114.62 | 107.60 |
| 11 | K | 35 | LEU | CA-CB-CG | -7.80 | 97.37 | 115.30 |
| 34 | i | 1686 | U | O4'-C1'-N1 | 7.79 | 114.44 | 108.20 |
| 34 | i | 446 | C | C3'-C2'-C1' | 7.79 | 107.73 | 101.50 |
| 34 | i | 524 | G | C4'-C3'-O3' | 7.79 | 128.58 | 113.00 |
| 34 | i | 612 | C | N1-C1'-C2' | 7.79 | 124.12 | 114.00 |
| 34 | i | 1091 | U | N1-C1'-C2' | 7.79 | 124.12 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 222 | G | O4'-C1'-C2' | 7.78 | 114.60 | 107.60 |
| 34 | i | 429 | A | O4'-C1'-N9 | 7.77 | 114.42 | 108.20 |
| 34 | i | 733 | G | O4'-C1'-N9 | 7.77 | 114.42 | 108.20 |
| 34 | i | 821 | A | P-O3'-C3' | -7.77 | 110.38 | 119.70 |
| 34 | i | 368 | U | C1'-O4'-C4' | -7.77 | 103.69 | 109.90 |
| 34 | i | 1655 | C | C5'-C4'-C3' | -7.77 | 103.57 | 116.00 |
| 34 | i | 3 | C | O4'-C1'-C2' | -7.77 | 98.03 | 105.80 |
| 34 | i | 1420 | G | O4'-C1'-N9 | 7.77 | 114.41 | 108.20 |
| 34 | i | 904 | A | O3'-P-O5' | -7.76 | 89.25 | 104.00 |
| 34 | i | 1386 | U | O4'-C1'-N1 | 7.76 | 114.41 | 108.20 |
| 9 | I | 5 | ARG | C-N-CA | 7.76 | 141.10 | 121.70 |
| 25 | Y | 51 | THR | C-N-CD | -7.76 | 103.54 | 120.60 |
| 34 | i | 191 | C | C4'-C3'-O3' | 7.75 | 128.50 | 113.00 |
| 34 | i | 977 | A | C3'-C2'-C1' | 7.75 | 107.70 | 101.50 |
| 34 | i | 1692 | A | O4'-C1'-N9 | 7.75 | 114.40 | 108.20 |
| 7 | G | 155 | GLN | O-C-N | -7.74 | 110.31 | 122.70 |
| 16 | P | 36 | LEU | CA-C-N | -7.74 | 100.17 | 117.20 |
| 34 | i | 1841 | G | N9-C1'-C2' | -7.74 | 103.48 | 112.00 |
| 34 | i | 1485 | A | O4'-C1'-N9 | 7.74 | 114.39 | 108.20 |
| 34 | i | 40 | A | O4'-C1'-N9 | 7.74 | 114.39 | 108.20 |
| 20 | T | 42 | HIS | CB-CA-C | -7.74 | 94.93 | 110.40 |
| 9 | I | 178 | ARG | CG-CD-NE | -7.73 | 95.56 | 111.80 |
| 17 | Q | 146 | ARG | NE-CZ-NH1 | -7.72 | 116.44 | 120.30 |
| 34 | i | 1449 | C | N1-C1'-C2' | 7.72 | 124.04 | 114.00 |
| 24 | X | 23 | HIS | CA-C-N | 7.72 | 134.19 | 117.20 |
| 34 | i | 645 | A | O4'-C1'-N9 | 7.72 | 114.37 | 108.20 |
| 34 | i | 1405 | A | C5'-C4'-C3' | 7.71 | 128.34 | 116.00 |
| 3 | C | 148 | VAL | C-N-CD | -7.71 | 103.64 | 120.60 |
| 10 | J | 166 | GLY | C-N-CA | -7.71 | 106.10 | 122.30 |
| 34 | i | 1003 | C | N1-C1'-C2' | 7.71 | 124.03 | 114.00 |
| 34 | i | 1696 | C | O4'-C1'-C2' | -7.71 | 98.09 | 105.80 |
| 34 | i | 2 | A | P-O3'-C3' | 7.70 | 128.94 | 119.70 |
| 34 | i | 171 | A | N9-C1'-C2' | -7.70 | 103.53 | 112.00 |
| 34 | i | 1606 | G | O4'-C1'-N9 | 7.70 | 114.36 | 108.20 |
| 34 | i | 164 | A | C1'-O4'-C4' | -7.69 | 103.75 | 109.90 |
| 34 | i | 1215 | C | C3'-C2'-C1' | 7.69 | 107.66 | 101.50 |
| 34 | i | 484 | C | O4'-C1'-C2' | -7.69 | 98.11 | 105.80 |
| 34 | i | 227 | A | C1'-O4'-C4' | 7.68 | 116.05 | 109.90 |
| 34 | i | 521 | A | O4'-C4'-C3' | -7.68 | 96.32 | 104.00 |
| 34 | i | 690 | C | O4'-C1'-N1 | 7.68 | 114.34 | 108.20 |
| 34 | i | 1134 | C | O3'-P-O5' | 7.68 | 118.58 | 104.00 |
| 2 | B | 37 | ALA | C-N-CA | -7.67 | 102.51 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 76 | U | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 34 | i | 959 | A | O4'-C1'-C2' | 7.67 | 114.50 | 107.60 |
| 31 | e | 77 | HIS | C-N-CA | 7.67 | 138.41 | 122.30 |
| 19 | S | 6 | PRO | CA-C-N | 7.67 | 134.07 | 117.20 |
| 34 | i | 1448 | A | C3'-C2'-C1' | 7.66 | 107.63 | 101.50 |
| 34 | i | 522 | C | O4'-C1'-N1 | 7.66 | 114.33 | 108.20 |
| 34 | i | 689 | G | O4'-C1'-C2' | -7.65 | 98.15 | 105.80 |
| 18 | R | 89 | SER | O-C-N | -7.64 | 110.47 | 122.70 |
| 34 | i | 301 | C | O4'-C1'-N1 | 7.64 | 114.31 | 108.20 |
| 34 | i | 1396 | U | O4'-C1'-N1 | 7.63 | 114.31 | 108.20 |
| 34 | i | 385 | G | O4'-C1'-C2' | 7.63 | 114.47 | 107.60 |
| 34 | i | 1597 | U | O3'-P-O5' | -7.63 | 89.50 | 104.00 |
| 34 | i | 1859 | C | C4'-C3'-O3' | 7.63 | 128.26 | 113.00 |
| 34 | i | 630 | A | N9-C1'-C2' | 7.63 | 123.92 | 114.00 |
| 34 | i | 1056 | A | N9-C1'-C2' | 7.63 | 123.91 | 114.00 |
| 5 | E | 259 | LYS | N-CA-C | 7.62 | 131.59 | 111.00 |
| 34 | i | 1092 | G | O4'-C1'-N9 | 7.62 | 114.30 | 108.20 |
| 34 | i | 296 | U | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 34 | i | 526 | A | C4'-C3'-O3' | 7.62 | 128.24 | 113.00 |
| 34 | i | 1690 | A | O4'-C1'-C2' | -7.62 | 98.19 | 105.80 |
| 12 | L | 153 | LYS | CA-C-N | 7.61 | 133.95 | 117.20 |
| 10 | J | 93 | LYS | C-N-CA | 7.61 | 140.73 | 121.70 |
| 34 | i | 595 | A | O4'-C1'-N9 | 7.61 | 114.29 | 108.20 |
| 34 | i | 35 | C | C3'-C2'-C1' | 7.61 | 107.59 | 101.50 |
| 34 | i | 450 | A | O4'-C1'-N9 | 7.61 | 114.29 | 108.20 |
| 8 | H | 106 | ARG | NE-CZ-NH1 | -7.61 | 116.50 | 120.30 |
| 16 | P | 52 | LYS | C-N-CA | -7.60 | 102.69 | 121.70 |
| 34 | i | 865 | A | O4'-C1'-N9 | 7.60 | 114.28 | 108.20 |
| 34 | i | 1043 | C | C3'-C2'-C1' | 7.59 | 107.57 | 101.50 |
| 34 | i | 1517 | A | C5'-C4'-O4' | 7.59 | 118.21 | 109.10 |
| 34 | i | 628 | C | O4'-C1'-N1 | 7.59 | 114.27 | 108.20 |
| 34 | i | 1182 | U | O4'-C1'-N1 | 7.58 | 114.27 | 108.20 |
| 9 | I | 55 | TYR | CA-CB-CG | -7.58 | 99.00 | 113.40 |
| 34 | i | 606 | A | N9-C1'-C2' | 7.58 | 123.86 | 114.00 |
| 33 | g | 274 | VAL | C-N-CA | -7.58 | 102.76 | 121.70 |
| 34 | i | 1258 | C | C1'-O4'-C4' | -7.57 | 103.84 | 109.90 |
| 34 | i | 1828 | A | O4'-C1'-N9 | 7.57 | 114.25 | 108.20 |
| 6 | F | 36 | GLN | N-CA-C | -7.55 | 90.60 | 111.00 |
| 34 | i | 1771 | G | C1'-O4'-C4' | -7.55 | 103.86 | 109.90 |
| 34 | i | 436 | G | C3'-C2'-C1' | 7.55 | 107.54 | 101.50 |
| 6 | F | 131 | ALA | C-N-CA | -7.55 | 106.44 | 122.30 |
| 34 | i | 848 | G | C4'-C3'-O3' | -7.55 | 93.55 | 109.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1263 | C | N1-C1'-C2' | 7.55 | 123.81 | 114.00 |
| 34 | i | 1113 | C | C3'-C2'-C1' | -7.55 | 95.46 | 101.50 |
| 34 | i | 296 | U | P-O5'-C5' | 7.55 | 132.98 | 120.90 |
| 34 | i | 1447 | G | C3'-C2'-C1' | 7.54 | 107.53 | 101.50 |
| 34 | i | 1600 | G | C1'-O4'-C4' | -7.54 | 103.87 | 109.90 |
| 34 | i | 1771 | G | O4'-C1'-C2' | 7.54 | 114.39 | 107.60 |
| 34 | i | 1630 | C | O4'-C1'-N1 | 7.54 | 114.23 | 108.20 |
| 34 | i | 554 | A | O4'-C1'-N9 | 7.53 | 114.23 | 108.20 |
| 34 | i | 604 | G | N9-C1'-C2' | 7.53 | 123.80 | 114.00 |
| 34 | i | 659 | A | O4'-C1'-N9 | 7.53 | 114.23 | 108.20 |
| 4 | D | 94 | ARG | CB-CA-C | -7.53 | 95.34 | 110.40 |
| 34 | i | 902 | U | O4'-C1'-N1 | 7.53 | 114.22 | 108.20 |
| 34 | i | 1269 | C | P-O3'-C3' | -7.53 | 110.66 | 119.70 |
| 34 | i | 170 | A | O4'-C1'-N9 | 7.53 | 114.22 | 108.20 |
| 34 | i | 794 | G | P-O5'-C5' | 7.53 | 132.94 | 120.90 |
| 34 | i | 1289 | A | C3'-C2'-C1' | 7.52 | 107.51 | 101.50 |
| 21 | U | 104 | ILE | N-CA-CB | 7.51 | 128.07 | 110.80 |
| 34 | i | 78 | C | N1-C1'-C2' | -7.51 | 103.74 | 112.00 |
| 34 | i | 594 | A | C3'-C2'-C1' | 7.50 | 107.50 | 101.50 |
| 34 | i | 825 | C | O4'-C1'-C2' | -7.50 | 98.30 | 105.80 |
| 34 | i | 795 | U | P-O3'-C3' | 7.50 | 128.71 | 119.70 |
| 34 | i | 1499 | C | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 34 | i | 1591 | U | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 34 | i | 218 | A | O4'-C1'-N9 | 7.50 | 114.20 | 108.20 |
| 34 | i | 1055 | G | P-O3'-C3' | 7.50 | 128.70 | 119.70 |
| 34 | i | 1488 | U | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 34 | i | 1504 | A | C1'-O4'-C4' | 7.50 | 115.90 | 109.90 |
| 34 | i | 1720 | U | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 34 | i | 188 | U | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 13 | M | 10 | GLY | N-CA-C | 7.50 | 131.85 | 113.10 |
| 34 | i | 230 | C | O4'-C1'-N1 | 7.49 | 114.19 | 108.20 |
| 34 | i | 400 | G | O4'-C1'-N9 | 7.49 | 114.19 | 108.20 |
| 34 | i | 837 | G | P-O5'-C5' | 7.49 | 132.88 | 120.90 |
| 34 | i | 1505 | U | C4'-C3'-O3' | -7.49 | 93.67 | 109.40 |
| 10 | J | 17 | ARG | CB-CA-C | -7.49 | 95.42 | 110.40 |
| 34 | i | 1664 | G | O4'-C1'-N9 | 7.49 | 114.19 | 108.20 |
| 10 | J | 161 | LEU | C-N-CA | -7.48 | 103.00 | 121.70 |
| 34 | i | 1043 | C | O4'-C1'-C2' | -7.48 | 98.32 | 105.80 |
| 34 | i | 931 | G | O4'-C1'-N9 | 7.47 | 114.18 | 108.20 |
| 34 | i | 1413 | C | C1'-O4'-C4' | 7.47 | 115.88 | 109.90 |
| 34 | i | 1410 | A | O4'-C1'-N9 | 7.47 | 114.18 | 108.20 |
| 34 | i | 639 | U | N1-C1'-C2' | 7.47 | 123.71 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1667 | U | O4'-C1'-N1 | 7.47 | 114.18 | 108.20 |
| 34 | i | 1424 | G | N9-C1'-C2' | -7.46 | 103.79 | 112.00 |
| 34 | i | 1559 | C | N1-C1'-C2' | 7.46 | 123.70 | 114.00 |
| 34 | i | 1244 | U | O4'-C1'-N1 | 7.46 | 114.17 | 108.20 |
| 34 | i | 1530 | U | O3'-P-O5' | -7.46 | 89.83 | 104.00 |
| 34 | i | 35 | C | O4'-C1'-C2' | -7.46 | 98.34 | 105.80 |
| 34 | i | 853 | U | C1'-O4'-C4' | -7.45 | 103.94 | 109.90 |
| 34 | i | 1028 | C | N1-C1'-C2' | 7.45 | 123.68 | 114.00 |
| 34 | i | 1459 | U | P-O5'-C5' | 7.45 | 132.82 | 120.90 |
| 34 | i | 797 | U | O4'-C1'-N1 | 7.45 | 114.16 | 108.20 |
| 34 | i | 1270 | G | C3'-C2'-C1' | 7.44 | 107.46 | 101.50 |
| 18 | R | 1 | MET | CB-CA-C | 7.44 | 125.29 | 110.40 |
| 34 | i | 808 | A | O4'-C1'-N9 | 7.44 | 114.15 | 108.20 |
| 34 | i | 684 | A | C3'-C2'-C1' | -7.44 | 95.55 | 101.50 |
| 34 | i | 976 | A | C1'-O4'-C4' | -7.44 | 103.95 | 109.90 |
| 34 | i | 1590 | U | N1-C1'-C2' | -7.44 | 103.82 | 112.00 |
| 8 | H | 109 | ARG | CA-CB-CG | -7.44 | 97.04 | 113.40 |
| 34 | i | 689 | G | C3'-C2'-C1' | 7.42 | 107.44 | 101.50 |
| 34 | i | 514 | U | O4'-C1'-N1 | 7.42 | 114.14 | 108.20 |
| 34 | i | 1237 | A | P-O3'-C3' | 7.42 | 128.61 | 119.70 |
| 34 | i | 1406 | C | C3'-C2'-C1' | 7.42 | 107.44 | 101.50 |
| 34 | i | 927 | C | O4'-C1'-C2' | -7.42 | 98.38 | 105.80 |
| 34 | i | 1632 | A | C1'-O4'-C4' | 7.42 | 115.84 | 109.90 |
| 34 | i | 1068 | U | P-O3'-C3' | 7.42 | 128.60 | 119.70 |
| 34 | i | 980 | C | N1-C1'-C2' | 7.41 | 123.64 | 114.00 |
| 34 | i | 1776 | G | C5'-C4'-C3' | 7.41 | 127.86 | 116.00 |
| 34 | i | 34 | U | C1'-O4'-C4' | -7.41 | 103.97 | 109.90 |
| 5 | E | 75 | LYS | N-CA-C | 7.41 | 131.00 | 111.00 |
| 34 | i | 1127 | G | O4'-C1'-N9 | 7.41 | 114.12 | 108.20 |
| 19 | S | 9 | PHE | N-CA-C | 7.40 | 130.99 | 111.00 |
| 34 | i | 503 | G | O4'-C1'-N9 | 7.39 | 114.11 | 108.20 |
| 9 | I | 133 | GLU | O-C-N | -7.39 | 110.88 | 122.70 |
| 33 | g | 50 | THR | C-N-CA | -7.39 | 103.23 | 121.70 |
| 34 | i | 1186 | A | O4'-C1'-C2' | -7.39 | 98.41 | 105.80 |
| 34 | i | 1675 | G | O4'-C1'-N9 | 7.39 | 114.11 | 108.20 |
| 34 | i | 420 | C | O4'-C1'-N1 | 7.38 | 114.11 | 108.20 |
| 34 | i | 432 | C | C3'-C2'-C1' | 7.38 | 107.41 | 101.50 |
| 32 | f | 148 | TYR | CA-CB-CG | -7.38 | 99.37 | 113.40 |
| 34 | i | 1766 | C | C3'-C2'-C1' | 7.38 | 107.41 | 101.50 |
| 34 | i | 985 | C | O4'-C1'-C2' | -7.38 | 98.42 | 105.80 |
| 34 | i | 1433 | C | C1'-O4'-C4' | -7.38 | 104.00 | 109.90 |
| 34 | i | 1404 | U | C1'-O4'-C4' | -7.37 | 104.00 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1533 | C | C4'-C3'-C2' | -7.37 | 95.23 | 102.60 |
| 34 | i | 1019 | A | C1'-O4'-C4' | 7.37 | 115.79 | 109.90 |
| 10 | J | 144 | ILE | CA-CB-CG1 | -7.36 | 97.01 | 111.00 |
| 18 | R | 1 | MET | O-C-N | 7.36 | 135.71 | 123.20 |
| 24 | X | 115 | ILE | N-CA-C | -7.36 | 91.14 | 111.00 |
| 34 | i | 27 | A | O4'-C1'-N9 | 7.36 | 114.08 | 108.20 |
| 23 | W | 100 | GLY | N-CA-C | -7.35 | 94.71 | 113.10 |
| 28 | b | 9 | HIS | C-N-CD | -7.35 | 104.43 | 120.60 |
| 34 | i | 534 | G | O4'-C1'-N9 | 7.35 | 114.08 | 108.20 |
| 25 | Y | 64 | PHE | C-N-CA | -7.35 | 106.86 | 122.30 |
| 34 | i | 529 | C | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 34 | i | 76 | U | P-O5'-C5' | 7.35 | 132.66 | 120.90 |
| 34 | i | 410 | G | C1'-O4'-C4' | -7.35 | 104.02 | 109.90 |
| 34 | i | 547 | U | O4'-C1'-C2' | -7.35 | 98.45 | 105.80 |
| 34 | i | 841 | G | P-O3'-C3' | -7.34 | 110.89 | 119.70 |
| 18 | R | 3 | ARG | NE-CZ-NH2 | 7.34 | 123.97 | 120.30 |
| 34 | i | 731 | C | O4'-C1'-N1 | 7.34 | 114.07 | 108.20 |
| 34 | i | 1717 | G | P-O5'-C5' | 7.34 | 132.65 | 120.90 |
| 34 | i | 1818 | A | P-O3'-C3' | 7.34 | 128.51 | 119.70 |
| 34 | i | 1355 | U | C1'-O4'-C4' | 7.34 | 115.77 | 109.90 |
| 34 | i | 14 | C | O4'-C1'-N1 | 7.34 | 114.07 | 108.20 |
| 34 | i | 1175 | G | O4'-C1'-N9 | 7.34 | 114.07 | 108.20 |
| 34 | i | 608 | C | O4'-C1'-N1 | 7.33 | 114.07 | 108.20 |
| 34 | i | 893 | U | O3'-P-O5' | -7.33 | 90.06 | 104.00 |
| 34 | i | 1773 | G | N9-C1'-C2' | -7.33 | 103.93 | 112.00 |
| 34 | i | 81 | U | N1-C1'-C2' | 7.33 | 123.53 | 114.00 |
| 34 | i | 1194 | G | C3'-C2'-C1' | -7.33 | 95.64 | 101.50 |
| 34 | i | 1451 | A | O4'-C1'-C2' | -7.33 | 98.47 | 105.80 |
| 34 | i | 1773 | G | C3'-C2'-C1' | -7.33 | 95.64 | 101.50 |
| 34 | i | 798 | A | C1'-O4'-C4' | -7.33 | 104.04 | 109.90 |
| 10 | J | 180 | LYS | CB-CA-C | -7.32 | 95.75 | 110.40 |
| 34 | i | 210 | G | N9-C1'-C2' | -7.32 | 103.94 | 112.00 |
| 34 | i | 1845 | A | P-O3'-C3' | 7.32 | 128.49 | 119.70 |
| 34 | i | 57 | U | C1'-O4'-C4' | 7.32 | 115.76 | 109.90 |
| 34 | i | 1689 | U | O4'-C1'-N1 | 7.32 | 114.06 | 108.20 |
| 4 | D | 82 | GLY | O-C-N | -7.31 | 111.00 | 122.70 |
| 9 | I | 3 | ILE | N-CA-C | 7.31 | 130.74 | 111.00 |
| 34 | i | 574 | A | P-O5'-C5' | 7.30 | 132.59 | 120.90 |
| 34 | i | 168 | C | C3'-C2'-C1' | 7.30 | 107.34 | 101.50 |
| 34 | i | 1672 | U | N1-C1'-C2' | -7.30 | 103.97 | 112.00 |
| 34 | i | 545 | A | O4'-C1'-C2' | -7.30 | 98.50 | 105.80 |
| 34 | i | 332 | C | C3'-C2'-C1' | 7.29 | 107.34 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 225 | C | N1-C1'-C2' | 7.29 | 123.48 | 114.00 |
| 34 | i | 656 | U | O4'-C1'-C2' | -7.29 | 98.51 | 105.80 |
| 21 | U | 93 | SER | C-N-CA | -7.29 | 91.38 | 122.00 |
| 34 | i | 1648 | U | P-O3'-C3' | 7.29 | 128.45 | 119.70 |
| 34 | i | 1237 | A | O4'-C1'-C2' | -7.28 | 98.52 | 105.80 |
| 34 | i | 454 | A | O3'-P-O5' | 7.28 | 117.83 | 104.00 |
| 34 | i | 1325 | U | N1-C1'-C2' | 7.28 | 123.46 | 114.00 |
| 18 | R | 1 | MET | CA-CB-CG | 7.28 | 125.67 | 113.30 |
| 34 | i | 1504 | A | O4'-C1'-N9 | 7.28 | 114.02 | 108.20 |
| 34 | i | 187 | C | O4'-C1'-C2' | -7.27 | 98.53 | 105.80 |
| 24 | X | 23 | HIS | C-N-CA | 7.27 | 139.87 | 121.70 |
| 34 | i | 827 | G | C3'-C2'-C1' | -7.27 | 95.69 | 101.50 |
| 34 | i | 1204 | A | N9-C1'-C2' | -7.27 | 104.00 | 112.00 |
| 34 | i | 942 | U | O4'-C1'-N1 | 7.26 | 114.01 | 108.20 |
| 32 | f | 88 | PRO | O-C-N | -7.26 | 111.08 | 122.70 |
| 34 | i | 743 | U | O4'-C1'-C2' | -7.26 | 98.54 | 105.80 |
| 34 | i | 1527 | C | C3'-C2'-C1' | 7.26 | 107.31 | 101.50 |
| 34 | i | 64 | A | N9-C1'-C2' | -7.26 | 104.02 | 112.00 |
| 34 | i | 541 | U | P-O5'-C5' | 7.26 | 132.51 | 120.90 |
| 34 | i | 1557 | C | N1-C1'-C2' | 7.26 | 123.44 | 114.00 |
| 34 | i | 1693 | C | C3'-C2'-C1' | 7.26 | 107.31 | 101.50 |
| 34 | i | 873 | C | O4'-C1'-C2' | -7.25 | 98.55 | 105.80 |
| 34 | i | 1059 | C | C3'-C2'-C1' | 7.25 | 107.30 | 101.50 |
| 34 | i | 1161 | G | O4'-C1'-N9 | 7.25 | 114.00 | 108.20 |
| 34 | i | 1060 | C | C3'-C2'-C1' | 7.25 | 107.30 | 101.50 |
| 34 | i | 1275 | C | O4'-C1'-C2' | -7.25 | 98.55 | 105.80 |
| 34 | i | 498 | A | O4'-C1'-N9 | 7.25 | 114.00 | 108.20 |
| 18 | R | 89 | SER | C-N-CA | -7.25 | 103.58 | 121.70 |
| 34 | i | 798 | A | O4'-C1'-N9 | 7.24 | 114.00 | 108.20 |
| 34 | i | 1781 | G | O4'-C1'-N9 | 7.24 | 113.99 | 108.20 |
| 34 | i | 359 | C | N1-C1'-C2' | 7.24 | 123.41 | 114.00 |
| 34 | i | 60 | A | O4'-C1'-C2' | 7.24 | 114.11 | 107.60 |
| 34 | i | 277 | U | O4'-C1'-C2' | -7.24 | 98.56 | 105.80 |
| 34 | i | 299 | G | P-O3'-C3' | 7.24 | 128.38 | 119.70 |
| 34 | i | 1305 | C | C3'-C2'-C1' | 7.24 | 107.29 | 101.50 |
| 33 | g | 275 | ILE | N-CA-C | 7.23 | 130.53 | 111.00 |
| 34 | i | 997 | A | O4'-C1'-C2' | -7.23 | 98.57 | 105.80 |
| 34 | i | 1184 | A | C3'-C2'-C1' | 7.23 | 107.28 | 101.50 |
| 34 | i | 290 | A | O4'-C1'-N9 | 7.23 | 113.98 | 108.20 |
| 34 | i | 1637 | U | C1'-O4'-C4' | 7.22 | 115.68 | 109.90 |
| 34 | i | 106 | C | O4'-C1'-N1 | 7.22 | 113.98 | 108.20 |
| 34 | i | 1210 | A | O4'-C1'-N9 | 7.22 | 113.98 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 162 | C | C4'-C3'-O3' | 7.22 | 127.44 | 113.00 |
| 34 | i | 17 | C | O4'-C1'-N1 | 7.22 | 113.97 | 108.20 |
| 34 | i | 170 | A | C5'-C4'-C3' | -7.22 | 104.45 | 116.00 |
| 34 | i | 431 | C | C1'-O4'-C4' | -7.21 | 104.13 | 109.90 |
| 34 | i | 673 | G | O4'-C1'-N9 | 7.21 | 113.97 | 108.20 |
| 34 | i | 740 | G | C3'-C2'-C1' | 7.21 | 107.27 | 101.50 |
| 11 | K | 37 | ASP | CB-CG-OD2 | 7.21 | 124.79 | 118.30 |
| 10 | J | 91 | LYS | O-C-N | -7.21 | 111.17 | 122.70 |
| 34 | i | 542 | G | C3'-C2'-C1' | -7.21 | 95.73 | 101.50 |
| 34 | i | 1041 | U | O4'-C1'-N1 | 7.20 | 113.96 | 108.20 |
| 14 | N | 19 | ARG | N-CA-C | -7.20 | 91.56 | 111.00 |
| 34 | i | 1560 | C | O4'-C1'-C2' | -7.20 | 98.60 | 105.80 |
| 10 | J | 35 | TYR | CA-C-N | -7.20 | 101.81 | 116.20 |
| 34 | i | 635 | C | C3'-C2'-C1' | 7.19 | 107.25 | 101.50 |
| 34 | i | 791 | A | O4'-C1'-C2' | -7.19 | 98.61 | 105.80 |
| 34 | i | 1767 | C | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 4 | D | 52 | ALA | C-N-CA | -7.19 | 103.73 | 121.70 |
| 34 | i | 306 | C | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 34 | i | 1546 | U | C3'-C2'-C1' | -7.19 | 95.75 | 101.50 |
| 8 | H | 191 | GLU | O-C-N | -7.18 | 111.21 | 122.70 |
| 34 | i | 149 | A | C3'-C2'-C1' | 7.18 | 107.24 | 101.50 |
| 14 | N | 14 | SER | CB-CA-C | -7.18 | 96.46 | 110.10 |
| 34 | i | 364 | G | O4'-C1'-N9 | 7.18 | 113.94 | 108.20 |
| 34 | i | 1116 | U | N1-C1'-C2' | 7.18 | 123.33 | 114.00 |
| 34 | i | 1301 | C | O4'-C1'-N1 | 7.18 | 113.94 | 108.20 |
| 27 | a | 97 | PRO | CA-CB-CG | 7.17 | 118.43 | 104.80 |
| 34 | i | 279 | G | N9-C1'-C2' | -7.17 | 104.11 | 112.00 |
| 34 | i | 1517 | A | P-O3'-C3' | -7.16 | 111.10 | 119.70 |
| 34 | i | 145 | G | O4'-C1'-C2' | 7.16 | 114.05 | 107.60 |
| 18 | R | 111 | PHE | N-CA-C | 7.16 | 130.33 | 111.00 |
| 34 | i | 1452 | G | C1'-O4'-C4' | -7.16 | 104.17 | 109.90 |
| 34 | i | 1287 | A | P-O3'-C3' | 7.16 | 128.29 | 119.70 |
| 11 | K | 35 | LEU | N-CA-C | -7.15 | 91.69 | 111.00 |
| 34 | i | 1578 | C | C3'-C2'-C1' | 7.15 | 107.22 | 101.50 |
| 8 | H | 109 | ARG | O-C-N | 7.15 | 134.14 | 122.70 |
| 34 | i | 1788 | C | O4'-C1'-C2' | -7.15 | 98.65 | 105.80 |
| 34 | i | 1288 | C | P-O5'-C5' | -7.15 | 109.46 | 120.90 |
| 16 | P | 49 | LEU | CA-C-N | 7.14 | 132.91 | 117.20 |
| 24 | X | 22 | TRP | C-N-CA | -7.14 | 103.86 | 121.70 |
| 34 | i | 368 | U | C4'-C3'-C2' | -7.14 | 95.46 | 102.60 |
| 34 | i | 1852 | G | O4'-C1'-N9 | 7.14 | 113.91 | 108.20 |
| 2 | B | 147 | ASN | C-N-CA | -7.13 | 103.87 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 899 | A | C3'-C2'-C1' | -7.13 | 95.80 | 101.50 |
| 34 | i | 1118 | A | N9-C1'-C2' | -7.13 | 104.16 | 112.00 |
| 34 | i | 1045 | A | C4'-C3'-C2' | -7.13 | 95.47 | 102.60 |
| 8 | H | 110 | THR | CA-C-N | 7.12 | 132.87 | 117.20 |
| 34 | i | 834 | G | O4'-C1'-N9 | 7.12 | 113.90 | 108.20 |
| 34 | i | 1015 | C | N1-C1'-C2' | 7.12 | 123.26 | 114.00 |
| 34 | i | 1666 | G | C1'-O4'-C4' | -7.12 | 104.20 | 109.90 |
| 34 | i | 167 | G | N9-C1'-C2' | -7.12 | 104.17 | 112.00 |
| 34 | i | 1019 | A | N9-C1'-C2' | -7.11 | 104.17 | 112.00 |
| 34 | i | 1858 | U | P-O5'-C5' | 7.11 | 132.28 | 120.90 |
| 34 | i | 684 | A | C1'-O4'-C4' | -7.11 | 104.21 | 109.90 |
| 34 | i | 1738 | G | C1'-O4'-C4' | -7.11 | 104.21 | 109.90 |
| 34 | i | 1656 | A | C1'-O4'-C4' | -7.11 | 104.21 | 109.90 |
| 19 | S | 93 | GLY | CA-C-N | -7.11 | 101.56 | 117.20 |
| 20 | T | 4 | VAL | N-CA-CB | -7.11 | 95.86 | 111.50 |
| 34 | i | 227 | A | C3'-C2'-C1' | 7.11 | 107.18 | 101.50 |
| 34 | i | 1651 | G | C1'-O4'-C4' | -7.11 | 104.22 | 109.90 |
| 34 | i | 830 | C | P-O3'-C3' | 7.10 | 128.22 | 119.70 |
| 34 | i | 1459 | U | O4'-C1'-N1 | 7.10 | 113.88 | 108.20 |
| 34 | i | 894 | U | P-O5'-C5' | 7.10 | 132.25 | 120.90 |
| 34 | i | 1001 | G | O4'-C1'-N9 | 7.10 | 113.88 | 108.20 |
| 34 | i | 275 | C | O4'-C1'-C2' | -7.09 | 98.71 | 105.80 |
| 34 | i | 47 | G | O4'-C1'-N9 | 7.09 | 113.87 | 108.20 |
| 34 | i | 241 | A | O4'-C1'-C2' | -7.09 | 98.71 | 105.80 |
| 34 | i | 1634 | G | C3'-C2'-C1' | 7.09 | 107.17 | 101.50 |
| 34 | i | 567 | U | O4'-C1'-N1 | 7.08 | 113.87 | 108.20 |
| 34 | i | 906 | G | O4'-C1'-N9 | 7.08 | 113.87 | 108.20 |
| 34 | i | 1663 | U | O5'-P-OP2 | -7.08 | 99.32 | 105.70 |
| 18 | R | 2 | GLY | CA-C-N | 7.08 | 132.78 | 117.20 |
| 34 | i | 275 | C | C3'-C2'-C1' | 7.08 | 107.17 | 101.50 |
| 34 | i | 1363 | U | O4'-C1'-N1 | 7.08 | 113.86 | 108.20 |
| 15 | O | 145 | GLY | N-CA-C | 7.08 | 130.80 | 113.10 |
| 34 | i | 49 | C | N1-C1'-C2' | 7.08 | 123.20 | 114.00 |
| 34 | i | 1503 | G | C1'-C2'-O2' | 7.07 | 131.82 | 110.60 |
| 20 | T | 82 | ARG | NE-CZ-NH1 | 7.07 | 123.84 | 120.30 |
| 34 | i | 1311 | U | C3'-C2'-C1' | -7.07 | 95.84 | 101.50 |
| 34 | i | 792 | G | C3'-C2'-C1' | -7.07 | 95.84 | 101.50 |
| 34 | i | 279 | G | O4'-C1'-N9 | 7.07 | 113.86 | 108.20 |
| 34 | i | 1661 | C | O4'-C1'-N1 | 7.07 | 113.86 | 108.20 |
| 34 | i | 53 | C | C3'-C2'-C1' | 7.07 | 107.15 | 101.50 |
| 34 | i | 32 | U | O4'-C1'-N1 | 7.07 | 113.85 | 108.20 |
| 34 | i | 100 | U | O4'-C1'-N1 | 7.06 | 113.85 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 970 | C | N1-C1'-C2' | 7.06 | 123.18 | 114.00 |
| 34 | i | 1783 | G | O4'-C1'-C2' | -7.06 | 98.74 | 105.80 |
| 34 | i | 58 | C | N1-C1'-C2' | -7.06 | 104.23 | 112.00 |
| 34 | i | 1755 | U | P-O5'-C5' | 7.06 | 132.19 | 120.90 |
| 19 | S | 142 | ARG | N-CA-CB | -7.05 | 97.90 | 110.60 |
| 11 | K | 1 | MET | N-CA-C | 7.05 | 130.04 | 111.00 |
| 10 | J | 164 | PRO | N-CA-CB | -7.05 | 94.84 | 103.30 |
| 34 | i | 1668 | U | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 34 | i | 997 | A | C1'-O4'-C4' | 7.04 | 115.54 | 109.90 |
| 34 | i | 1105 | C | C3'-C2'-C1' | -7.04 | 95.86 | 101.50 |
| 10 | J | 123 | ILE | CB-CA-C | 7.04 | 125.69 | 111.60 |
| 34 | i | 166 | A | O4'-C1'-N9 | 7.04 | 113.83 | 108.20 |
| 34 | i | 274 | G | O4'-C1'-C2' | 7.04 | 113.94 | 107.60 |
| 34 | i | 342 | U | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 34 | i | 1093 | G | C5'-C4'-O4' | 7.04 | 117.55 | 109.10 |
| 34 | i | 1205 | A | N9-C1'-C2' | -7.04 | 104.26 | 112.00 |
| 34 | i | 1671 | U | P-O3'-C3' | -7.04 | 111.25 | 119.70 |
| 34 | i | 1837 | G | C1'-O4'-C4' | -7.03 | 104.28 | 109.90 |
| 34 | i | 518 | A | N9-C1'-C2' | 7.03 | 123.14 | 114.00 |
| 34 | i | 1478 | C | O4'-C1'-N1 | 7.03 | 113.82 | 108.20 |
| 34 | i | 1326 | G | C1'-O4'-C4' | -7.02 | 104.28 | 109.90 |
| 34 | i | 1827 | C | C3'-C2'-C1' | 7.02 | 107.11 | 101.50 |
| 34 | i | 41 | G | C1'-O4'-C4' | -7.02 | 104.29 | 109.90 |
| 34 | i | 908 | C | O4'-C1'-N1 | 7.02 | 113.81 | 108.20 |
| 34 | i | 267 | G | P-O3'-C3' | 7.01 | 128.12 | 119.70 |
| 34 | i | 1373 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 3 | C | 258 | LEU | CB-CG-CD2 | 7.01 | 122.92 | 111.00 |
| 34 | i | 1099 | C | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 34 | i | 1425 | G | P-O5'-C5' | 7.01 | 132.12 | 120.90 |
| 4 | D | 83 | SER | N-CA-CB | 7.01 | 121.01 | 110.50 |
| 34 | i | 1339 | U | O4'-C1'-N1 | 7.01 | 113.81 | 108.20 |
| 34 | i | 93 | U | O4'-C1'-C2' | -7.00 | 98.80 | 105.80 |
| 34 | i | 1405 | A | O4'-C1'-C2' | -7.00 | 98.80 | 105.80 |
| 34 | i | 956 | U | C1'-O4'-C4' | -7.00 | 104.30 | 109.90 |
| 34 | i | 1640 | C | P-O3'-C3' | 7.00 | 128.10 | 119.70 |
| 20 | T | 82 | ARG | NE-CZ-NH2 | 7.00 | 123.80 | 120.30 |
| 34 | i | 286 | C | N1-C1'-C2' | 7.00 | 123.10 | 114.00 |
| 34 | i | 945 | G | O4'-C1'-N9 | 7.00 | 113.80 | 108.20 |
| 34 | i | 1847 | C | C1'-O4'-C4' | -7.00 | 104.30 | 109.90 |
| 34 | i | 1438 | U | O4'-C1'-N1 | 6.99 | 113.80 | 108.20 |
| 20 | T | 82 | ARG | NH1-CZ-NH2 | -6.99 | 111.71 | 119.40 |
| 34 | i | 409 | G | O4'-C1'-C2' | -6.99 | 98.81 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20 | T | 4 | VAL | CA-C-N | 6.99 | 132.57 | 117.20 |
| 34 | i | 1542 | C | C3'-C2'-C1' | 6.98 | 107.09 | 101.50 |
| 34 | i | 53 | C | C1'-O4'-C4' | 6.98 | 115.49 | 109.90 |
| 34 | i | 315 | C | O4'-C1'-C2' | -6.98 | 98.82 | 105.80 |
| 34 | i | 1479 | A | N9-C1'-C2' | -6.98 | 104.32 | 112.00 |
| 11 | K | 55 | ARG | CB-CG-CD | 6.98 | 129.74 | 111.60 |
| 34 | i | 906 | G | C1'-O4'-C4' | -6.97 | 104.32 | 109.90 |
| 34 | i | 91 | A | O4'-C1'-N9 | 6.97 | 113.78 | 108.20 |
| 34 | i | 860 | A | O4'-C1'-N9 | 6.97 | 113.78 | 108.20 |
| 34 | i | 465 | C | C3'-C2'-C1' | 6.96 | 107.07 | 101.50 |
| 34 | i | 587 | G | O4'-C1'-N9 | 6.96 | 113.77 | 108.20 |
| 34 | i | 1053 | C | O4'-C1'-N1 | 6.96 | 113.76 | 108.20 |
| 34 | i | 726 | C | P-O3'-C3' | 6.95 | 128.04 | 119.70 |
| 34 | i | 1584 | A | N9-C1'-C2' | -6.95 | 104.35 | 112.00 |
| 34 | i | 499 | G | O4'-C1'-N9 | 6.95 | 113.76 | 108.20 |
| 34 | i | 510 | A | C1'-O4'-C4' | -6.95 | 104.34 | 109.90 |
| 25 | Y | 31 | GLY | N-CA-C | 6.94 | 130.45 | 113.10 |
| 34 | i | 74 | G | P-O3'-C3' | 6.94 | 128.03 | 119.70 |
| 34 | i | 1503 | G | C3'-C2'-C1' | -6.94 | 95.95 | 101.50 |
| 22 | V | 67 | ASP | CB-CG-OD2 | 6.93 | 124.54 | 118.30 |
| 32 | f | 148 | TYR | N-CA-C | 6.93 | 129.72 | 111.00 |
| 34 | i | 1693 | C | P-O3'-C3' | 6.93 | 128.02 | 119.70 |
| 34 | i | 262 | G | P-O3'-C3' | 6.93 | 128.02 | 119.70 |
| 34 | i | 1047 | G | O4'-C1'-N9 | 6.93 | 113.75 | 108.20 |
| 34 | i | 1648 | U | N1-C1'-C2' | -6.93 | 104.38 | 112.00 |
| 34 | i | 438 | A | C3'-C2'-C1' | -6.93 | 95.96 | 101.50 |
| 34 | i | 1052 | U | P-O3'-C3' | -6.93 | 111.39 | 119.70 |
| 21 | U | 118 | ASP | CB-CG-OD1 | 6.92 | 124.53 | 118.30 |
| 34 | i | 1328 | A | C3'-C2'-C1' | 6.92 | 107.04 | 101.50 |
| 19 | S | 93 | GLY | O-C-N | 6.92 | 133.77 | 122.70 |
| 34 | i | 1114 | C | C1'-O4'-C4' | 6.92 | 115.44 | 109.90 |
| 34 | i | 1042 | U | O4'-C1'-N1 | 6.92 | 113.74 | 108.20 |
| 34 | i | 597 | U | N1-C1'-C2' | 6.92 | 122.99 | 114.00 |
| 34 | i | 509 | A | O4'-C1'-C2' | -6.91 | 98.89 | 105.80 |
| 8 | H | 110 | THR | CA-CB-CG2 | 6.91 | 122.08 | 112.40 |
| 34 | i | 369 | C | C3'-C2'-C1' | 6.91 | 107.03 | 101.50 |
| 34 | i | 1426 | C | O4'-C1'-C2' | -6.91 | 98.89 | 105.80 |
| 34 | i | 127 | C | P-O3'-C3' | 6.91 | 127.99 | 119.70 |
| 34 | i | 637 | U | O4'-C1'-N1 | 6.91 | 113.73 | 108.20 |
| 34 | i | 1118 | A | C1'-O4'-C4' | 6.90 | 115.42 | 109.90 |
| 34 | i | 374 | U | N1-C1'-C2' | 6.90 | 122.97 | 114.00 |
| 28 | b | 79 | PHE | N-CA-C | 6.90 | 129.62 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 729 | C | O4'-C1'-C2' | -6.89 | 98.91 | 105.80 |
| 34 | i | 1329 | U | N1-C1'-C2' | -6.89 | 104.42 | 112.00 |
| 34 | i | 1497 | C | O3'-P-O5' | -6.89 | 90.91 | 104.00 |
| 1 | A | 53 | ARG | NE-CZ-NH1 | -6.89 | 116.86 | 120.30 |
| 18 | R | 123 | THR | CB-CA-C | -6.89 | 93.01 | 111.60 |
| 34 | i | 1173 | U | O4'-C1'-N1 | 6.89 | 113.71 | 108.20 |
| 2 | B | 77 | ASP | CB-CG-OD1 | 6.88 | 124.50 | 118.30 |
| 11 | K | 2 | LEU | N-CA-C | 6.88 | 129.59 | 111.00 |
| 34 | i | 63 | U | O4'-C1'-N1 | 6.88 | 113.71 | 108.20 |
| 34 | i | 507 | C | N1-C1'-C2' | 6.88 | 122.95 | 114.00 |
| 24 | X | 128 | VAL | N-CA-C | 6.88 | 129.58 | 111.00 |
| 34 | i | 299 | G | O4'-C1'-C2' | 6.88 | 113.79 | 107.60 |
| 34 | i | 1402 | G | N9-C1'-C2' | 6.88 | 122.94 | 114.00 |
| 34 | i | 636 | G | O4'-C1'-N9 | 6.88 | 113.70 | 108.20 |
| 11 | K | 2 | LEU | CA-CB-CG | -6.87 | 99.49 | 115.30 |
| 34 | i | 1775 | A | C3'-C2'-C1' | 6.87 | 107.00 | 101.50 |
| 34 | i | 389 | C | O4'-C1'-C2' | -6.87 | 98.93 | 105.80 |
| 34 | i | 1573 | U | C1'-O4'-C4' | 6.87 | 115.39 | 109.90 |
| 34 | i | 1642 | A | C3'-C2'-C1' | -6.87 | 96.00 | 101.50 |
| 34 | i | 1693 | C | O4'-C1'-C2' | -6.87 | 98.93 | 105.80 |
| 34 | i | 343 | C | N1-C1'-C2' | 6.86 | 122.92 | 114.00 |
| 34 | i | 1128 | C | O4'-C1'-N1 | 6.86 | 113.69 | 108.20 |
| 34 | i | 978 | G | O4'-C1'-N9 | 6.86 | 113.69 | 108.20 |
| 34 | i | 65 | C | C1'-O4'-C4' | 6.85 | 115.38 | 109.90 |
| 34 | i | 407 | C | C3'-C2'-C1' | 6.85 | 106.98 | 101.50 |
| 34 | i | 609 | A | N9-C1'-C2' | -6.85 | 104.46 | 112.00 |
| 34 | i | 845 | A | O4'-C1'-N9 | 6.85 | 113.68 | 108.20 |
| 34 | i | 571 | U | P-O3'-C3' | -6.85 | 111.48 | 119.70 |
| 34 | i | 839 | C | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 18 | R | 87 | GLU | CB-CA-C | -6.85 | 96.71 | 110.40 |
| 34 | i | 312 | C | C3'-C2'-C1' | 6.84 | 106.97 | 101.50 |
| 34 | i | 1171 | G | C1'-O4'-C4' | -6.84 | 104.42 | 109.90 |
| 3 | C | 105 | GLN | N-CA-C | 6.84 | 129.47 | 111.00 |
| 34 | i | 31 | U | N1-C1'-C2' | -6.84 | 104.48 | 112.00 |
| 34 | i | 447 | C | O4'-C1'-N1 | 6.84 | 113.67 | 108.20 |
| 34 | i | 1545 | G | P-O3'-C3' | 6.84 | 127.91 | 119.70 |
| 34 | i | 227 | A | O4'-C1'-C2' | -6.84 | 98.96 | 105.80 |
| 34 | i | 877 | G | C1'-O4'-C4' | -6.84 | 104.43 | 109.90 |
| 34 | i | 790 | A | C3'-C2'-C1' | 6.83 | 106.97 | 101.50 |
| 34 | i | 15 | U | O4'-C1'-N1 | 6.83 | 113.67 | 108.20 |
| 34 | i | 1782 | A | O4'-C1'-N9 | 6.83 | 113.67 | 108.20 |
| 13 | M | 13 | ASP | CB-CG-OD1 | -6.83 | 112.15 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 31 | U | C1'-O4'-C4' | 6.83 | 115.36 | 109.90 |
| 3 | C | 242 | LYS | N-CA-C | 6.83 | 129.44 | 111.00 |
| 34 | i | 365 | U | P-O5'-C5' | 6.83 | 131.83 | 120.90 |
| 34 | i | 981 | G | O4'-C1'-N9 | 6.83 | 113.66 | 108.20 |
| 34 | i | 1533 | C | O4'-C1'-C2' | -6.83 | 98.97 | 105.80 |
| 34 | i | 900 | A | C1'-O4'-C4' | -6.83 | 104.44 | 109.90 |
| 34 | i | 1638 | U | C3'-C2'-C1' | 6.83 | 106.96 | 101.50 |
| 34 | i | 1350 | G | C2'-C3'-O3' | 6.82 | 124.62 | 113.70 |
| 34 | i | 1199 | G | O4'-C1'-C2' | 6.82 | 113.74 | 107.60 |
| 34 | i | 1418 | G | N9-C1'-C2' | -6.82 | 104.50 | 112.00 |
| 34 | i | 312 | C | P-O3'-C3' | 6.82 | 127.88 | 119.70 |
| 34 | i | 1603 | U | O4'-C1'-N1 | 6.82 | 113.65 | 108.20 |
| 34 | i | 1779 | C | P-O3'-C3' | 6.81 | 127.87 | 119.70 |
| 34 | i | 683 | G | O4'-C4'-C3' | -6.81 | 97.19 | 104.00 |
| 34 | i | 920 | G | O4'-C1'-N9 | 6.80 | 113.64 | 108.20 |
| 34 | i | 1777 | C | C3'-C2'-C1' | 6.80 | 106.94 | 101.50 |
| 34 | i | 373 | G | C3'-C2'-C1' | 6.79 | 106.94 | 101.50 |
| 34 | i | 862 | U | C3'-C2'-C1' | -6.79 | 96.06 | 101.50 |
| 34 | i | 612 | C | C1'-O4'-C4' | -6.79 | 104.47 | 109.90 |
| 34 | i | 1647 | G | O4'-C1'-N9 | 6.79 | 113.63 | 108.20 |
| 34 | i | 1727 | G | O4'-C1'-N9 | 6.79 | 113.63 | 108.20 |
| 34 | i | 725 | C | O4'-C1'-C2' | -6.79 | 99.01 | 105.80 |
| 6 | F | 37 | ASP | N-CA-C | 6.79 | 129.33 | 111.00 |
| 34 | i | 1681 | G | O4'-C1'-N9 | 6.79 | 113.63 | 108.20 |
| 34 | i | 1222 | G | C1'-O4'-C4' | -6.78 | 104.47 | 109.90 |
| 27 | a | 58 | VAL | CG1-CB-CG2 | -6.78 | 100.05 | 110.90 |
| 34 | i | 850 | A | P-O5'-C5' | 6.78 | 131.74 | 120.90 |
| 34 | i | 1633 | G | C3'-C2'-C1' | 6.78 | 106.92 | 101.50 |
| 34 | i | 202 | U | O4'-C1'-N1 | 6.77 | 113.62 | 108.20 |
| 34 | i | 741 | C | C3'-C2'-C1' | 6.77 | 106.92 | 101.50 |
| 34 | i | 1239 | U | O4'-C1'-N1 | 6.77 | 113.62 | 108.20 |
| 34 | i | 1754 | G | N9-C1'-C2' | -6.77 | 104.55 | 112.00 |
| 34 | i | 125 | C | O3'-P-O5' | 6.77 | 116.86 | 104.00 |
| 34 | i | 876 | G | C3'-C2'-C1' | -6.77 | 96.09 | 101.50 |
| 34 | i | 1423 | C | O4'-C1'-C2' | -6.77 | 99.03 | 105.80 |
| 34 | i | 540 | C | O3'-P-O5' | -6.76 | 91.15 | 104.00 |
| 34 | i | 1024 | A | C5'-C4'-C3' | -6.76 | 105.18 | 116.00 |
| 34 | i | 1857 | A | C1'-O4'-C4' | 6.76 | 115.31 | 109.90 |
| 33 | g | 159 | ASN | C-N-CA | -6.76 | 104.80 | 121.70 |
| 34 | i | 193 | C | N1-C1'-C2' | 6.76 | 122.79 | 114.00 |
| 34 | i | 989 | G | O4'-C1'-N9 | 6.76 | 113.61 | 108.20 |
| 34 | i | 1859 | C | C2'-C3'-O3' | -6.76 | 94.64 | 109.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 377 | C | N1-C1'-C2' | 6.75 | 122.78 | 114.00 |
| 31 | e | 122 | THR | O-C-N | -6.75 | 111.90 | 122.70 |
| 34 | i | 243 | C | P-O3'-C3' | 6.75 | 127.80 | 119.70 |
| 34 | i | 318 | U | O4'-C1'-N1 | 6.75 | 113.60 | 108.20 |
| 34 | i | 1530 | U | C4'-C3'-O3' | 6.75 | 126.49 | 113.00 |
| 34 | i | 369 | C | P-O3'-C3' | 6.74 | 127.79 | 119.70 |
| 34 | i | 1038 | A | O4'-C1'-N9 | 6.74 | 113.59 | 108.20 |
| 33 | g | 142 | VAL | O-C-N | 6.74 | 133.48 | 122.70 |
| 34 | i | 421 | G | O4'-C1'-N9 | 6.73 | 113.59 | 108.20 |
| 2 | B | 133 | TYR | N-CA-CB | -6.73 | 98.48 | 110.60 |
| 10 | J | 179 | LYS | C-N-CA | 6.72 | 138.51 | 121.70 |
| 34 | i | 449 | C | C5'-C4'-O4' | 6.72 | 117.17 | 109.10 |
| 2 | B | 41 | ILE | CG1-CB-CG2 | -6.72 | 96.62 | 111.40 |
| 19 | S | 16 | LEU | CB-CG-CD2 | -6.72 | 99.58 | 111.00 |
| 34 | i | 1778 | G | N9-C1'-C2' | 6.72 | 122.73 | 114.00 |
| 34 | i | 278 | U | O4'-C1'-N1 | -6.71 | 102.83 | 108.20 |
| 34 | i | 823 | A | N9-C1'-C2' | 6.71 | 122.72 | 114.00 |
| 34 | i | 959 | A | C3'-C2'-C1' | -6.71 | 96.13 | 101.50 |
| 34 | i | 1216 | A | C1'-O4'-C4' | -6.71 | 104.53 | 109.90 |
| 34 | i | 1652 | G | C1'-O4'-C4' | -6.71 | 104.53 | 109.90 |
| 34 | i | 1739 | G | C1'-O4'-C4' | 6.71 | 115.27 | 109.90 |
| 34 | i | 1455 | G | N9-C1'-C2' | 6.70 | 122.71 | 114.00 |
| 34 | i | 1774 | G | O3'-P-O5' | 6.70 | 116.73 | 104.00 |
| 34 | i | 1511 | G | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 34 | i | 321 | C | O4'-C1'-C2' | -6.69 | 99.11 | 105.80 |
| 23 | W | 2 | VAL | C-N-CA | -6.69 | 104.98 | 121.70 |
| 34 | i | 1167 | G | O4'-C1'-C2' | -6.69 | 99.11 | 105.80 |
| 21 | U | 48 | LEU | CA-CB-CG | -6.68 | 99.93 | 115.30 |
| 34 | i | 550 | A | O4'-C1'-N9 | 6.68 | 113.55 | 108.20 |
| 7 | G | 157 | VAL | CA-C-N | -6.68 | 102.50 | 117.20 |
| 34 | i | 1251 | G | P-O3'-C3' | -6.68 | 111.68 | 119.70 |
| 34 | i | 548 | G | C1'-O4'-C4' | -6.68 | 104.56 | 109.90 |
| 34 | i | 541 | U | O4'-C1'-C2' | 6.68 | 113.61 | 107.60 |
| 34 | i | 94 | G | C1'-O4'-C4' | -6.67 | 104.56 | 109.90 |
| 34 | i | 657 | U | C1'-O4'-C4' | -6.67 | 104.56 | 109.90 |
| 34 | i | 512 | A | P-O5'-C5' | 6.67 | 131.57 | 120.90 |
| 10 | J | 144 | ILE | CB-CA-C | 6.67 | 124.94 | 111.60 |
| 34 | i | 1775 | A | P-O5'-C5' | 6.67 | 131.57 | 120.90 |
| 6 | F | 130 | ARG | N-CA-C | 6.66 | 128.99 | 111.00 |
| 34 | i | 82 | G | C1'-O4'-C4' | 6.66 | 115.23 | 109.90 |
| 11 | K | 89 | ILE | CA-CB-CG1 | -6.66 | 98.34 | 111.00 |
| 34 | i | 471 | C | N1-C1'-C2' | 6.66 | 122.66 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1779 | C | C1'-O4'-C4' | 6.66 | 115.23 | 109.90 |
| 34 | i | 391 | A | O4'-C1'-C2' | -6.66 | 99.14 | 105.80 |
| 34 | i | 1786 | G | O4'-C1'-N9 | 6.66 | 113.53 | 108.20 |
| 34 | i | 307 | G | P-O5'-C5' | 6.66 | 131.55 | 120.90 |
| 34 | i | 1347 | G | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 34 | i | 1243 | C | O4'-C1'-C2' | -6.65 | 99.15 | 105.80 |
| 34 | i | 728 | U | C1'-O4'-C4' | -6.65 | 104.58 | 109.90 |
| 34 | i | 1366 | A | O4'-C1'-C2' | -6.65 | 99.15 | 105.80 |
| 34 | i | 158 | A | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 18 | R | 121 | GLN | C-N-CD | -6.65 | 105.97 | 120.60 |
| 34 | i | 736 | C | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 34 | i | 1604 | C | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 22 | V | 64 | GLU | N-CA-C | 6.64 | 128.94 | 111.00 |
| 34 | i | 1105 | C | O4'-C1'-C2' | 6.64 | 113.58 | 107.60 |
| 34 | i | 1342 | U | O4'-C1'-N1 | 6.64 | 113.52 | 108.20 |
| 34 | i | 190 | A | O4'-C1'-C2' | -6.64 | 99.16 | 105.80 |
| 10 | J | 91 | LYS | N-CA-C | -6.63 | 93.09 | 111.00 |
| 27 | a | 63 | VAL | CB-CA-C | 6.63 | 124.00 | 111.40 |
| 34 | i | 144 | U | C1'-O4'-C4' | -6.63 | 104.59 | 109.90 |
| 34 | i | 622 | C | C3'-C2'-C1' | 6.63 | 106.80 | 101.50 |
| 34 | i | 807 | A | O4'-C1'-N9 | 6.63 | 113.50 | 108.20 |
| 2 | B | 155 | TYR | CB-CA-C | -6.63 | 97.15 | 110.40 |
| 34 | i | 1202 | G | O4'-C1'-N9 | 6.63 | 113.50 | 108.20 |
| 34 | i | 1541 | G | O4'-C1'-N9 | 6.63 | 113.50 | 108.20 |
| 34 | i | 1656 | A | C3'-C2'-C1' | -6.62 | 96.20 | 101.50 |
| 34 | i | 1250 | C | O4'-C1'-N1 | 6.62 | 113.50 | 108.20 |
| 34 | i | 616 | G | O4'-C1'-N9 | -6.62 | 102.90 | 108.20 |
| 34 | i | 550 | A | C3'-C2'-C1' | -6.62 | 96.20 | 101.50 |
| 34 | i | 1385 | C | P-O5'-C5' | 6.62 | 131.49 | 120.90 |
| 11 | K | 42 | ASN | CA-C-N | 6.62 | 131.76 | 117.20 |
| 34 | i | 1251 | G | N9-C1'-C2' | 6.61 | 122.60 | 114.00 |
| 34 | i | 274 | G | C1'-O4'-C4' | -6.61 | 104.61 | 109.90 |
| 34 | i | 1646 | A | C1'-O4'-C4' | 6.61 | 115.19 | 109.90 |
| 34 | i | 40 | A | C1'-O4'-C4' | 6.61 | 115.19 | 109.90 |
| 34 | i | 53 | C | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 34 | i | 541 | U | C1'-O4'-C4' | -6.61 | 104.61 | 109.90 |
| 34 | i | 340 | C | C3'-C2'-C1' | 6.60 | 106.78 | 101.50 |
| 34 | i | 554 | A | P-O3'-C3' | 6.60 | 127.62 | 119.70 |
| 34 | i | 1144 | A | O4'-C1'-C2' | 6.60 | 113.54 | 107.60 |
| 34 | i | 553 | G | O4'-C1'-C2' | -6.60 | 99.20 | 105.80 |
| 19 | S | 87 | GLN | CA-C-N | 6.60 | 131.71 | 117.20 |
| 34 | i | 1277 | G | O4'-C1'-N9 | 6.60 | 113.48 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27 | a | 85 | ARG | NE-CZ-NH2 | 6.59 | 123.60 | 120.30 |
| 34 | i | 983 | A | P-O5'-C5' | -6.59 | 110.35 | 120.90 |
| 34 | i | 984 | C | C3'-C2'-C1' | 6.59 | 106.78 | 101.50 |
| 34 | i | 1285 | U | P-O3'-C3' | 6.59 | 127.61 | 119.70 |
| 15 | O | 43 | HIS | N-CA-C | 6.59 | 128.79 | 111.00 |
| 34 | i | 1266 | G | N9-C1'-C2' | -6.59 | 104.75 | 112.00 |
| 34 | i | 285 | U | C3'-C2'-C1' | 6.59 | 106.77 | 101.50 |
| 16 | P | 36 | LEU | N-CA-C | -6.59 | 93.22 | 111.00 |
| 34 | i | 286 | C | O4'-C1'-C2' | -6.59 | 99.21 | 105.80 |
| 34 | i | 1071 | C | C1'-O4'-C4' | -6.59 | 104.63 | 109.90 |
| 34 | i | 208 | G | P-O5'-C5' | 6.58 | 131.43 | 120.90 |
| 34 | i | 1490 | U | C2'-C3'-O3' | 6.58 | 124.23 | 113.70 |
| 34 | i | 1816 | A | C4'-C3'-O3' | -6.58 | 95.58 | 109.40 |
| 34 | i | 432 | C | N1-C1'-C2' | 6.58 | 122.55 | 114.00 |
| 33 | g | 160 | SER | N-CA-C | 6.58 | 128.76 | 111.00 |
| 34 | i | 62 | G | C1'-O4'-C4' | -6.58 | 104.64 | 109.90 |
| 34 | i | 1461 | A | C1'-O4'-C4' | 6.58 | 115.16 | 109.90 |
| 34 | i | 1682 | C | C3'-C2'-C1' | 6.58 | 106.76 | 101.50 |
| 34 | i | 70 | G | O3'-P-O5' | -6.58 | 91.51 | 104.00 |
| 34 | i | 289 | G | N9-C1'-C2' | -6.58 | 104.77 | 112.00 |
| 34 | i | 1280 | A | O4'-C1'-C2' | -6.58 | 99.22 | 105.80 |
| 34 | i | 1525 | U | O4'-C1'-N1 | 6.57 | 113.46 | 108.20 |
| 9 | I | 8 | TRP | CG-CD2-CE3 | -6.57 | 127.99 | 133.90 |
| 34 | i | 272 | C | O3'-P-O5' | 6.57 | 116.48 | 104.00 |
| 34 | i | 1695 | C | O4'-C1'-C2' | -6.57 | 99.23 | 105.80 |
| 34 | i | 1455 | G | O4'-C1'-C2' | 6.57 | 113.51 | 107.60 |
| 3 | C | 217 | THR | C-N-CA | 6.57 | 138.12 | 121.70 |
| 34 | i | 1071 | C | N1-C1'-C2' | 6.56 | 122.53 | 114.00 |
| 33 | g | 274 | VAL | CA-C-N | 6.56 | 131.63 | 117.20 |
| 34 | i | 164 | A | N9-C1'-C2' | 6.56 | 122.53 | 114.00 |
| 9 | I | 207 | GLY | CA-C-O | -6.55 | 108.80 | 120.60 |
| 34 | i | 1819 | A | C3'-C2'-C1' | -6.55 | 96.26 | 101.50 |
| 34 | i | 342 | U | C5'-C4'-C3' | -6.55 | 105.52 | 116.00 |
| 34 | i | 1088 | G | O4'-C1'-N9 | 6.55 | 113.44 | 108.20 |
| 34 | i | 1861 | U | O4'-C1'-C2' | -6.55 | 99.25 | 105.80 |
| 17 | Q | 18 | THR | N-CA-C | -6.55 | 93.32 | 111.00 |
| 34 | i | 729 | C | C3'-C2'-C1' | 6.55 | 106.74 | 101.50 |
| 34 | i | 486 | C | O4'-C1'-C2' | -6.54 | 99.26 | 105.80 |
| 34 | i | 1639 | C | P-O3'-C3' | 6.54 | 127.55 | 119.70 |
| 34 | i | 1816 | A | O3'-P-O5' | -6.54 | 91.57 | 104.00 |
| 11 | K | 42 | ASN | CA-C-O | -6.54 | 106.36 | 120.10 |
| 34 | i | 428 | G | N9-C1'-C2' | -6.54 | 104.80 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1831 | G | O4'-C1'-N9 | 6.54 | 113.43 | 108.20 |
| 34 | i | 853 | U | N1-C1'-C2' | 6.54 | 122.50 | 114.00 |
| 34 | i | 957 | G | O4'-C1'-N9 | 6.54 | 113.43 | 108.20 |
| 34 | i | 1082 | G | P-O3'-C3' | 6.53 | 127.54 | 119.70 |
| 34 | i | 1550 | U | O4'-C4'-C3' | -6.53 | 97.47 | 104.00 |
| 34 | i | 1521 | G | O4'-C1'-N9 | 6.53 | 113.42 | 108.20 |
| 34 | i | 29 | G | O4'-C1'-N9 | 6.53 | 113.42 | 108.20 |
| 34 | i | 1377 | G | C3'-C2'-C1' | -6.53 | 96.28 | 101.50 |
| 34 | i | 1861 | U | P-O3'-C3' | 6.53 | 127.53 | 119.70 |
| 34 | i | 581 | U | P-O3'-C3' | 6.53 | 127.53 | 119.70 |
| 34 | i | 611 | C | C3'-C2'-C1' | 6.53 | 106.72 | 101.50 |
| 34 | i | 1656 | A | O4'-C1'-N9 | 6.53 | 113.42 | 108.20 |
| 34 | i | 1664 | G | O5'-P-OP2 | 6.53 | 118.53 | 110.70 |
| 34 | i | 192 | U | P-O5'-C5' | 6.52 | 131.34 | 120.90 |
| 34 | i | 459 | A | O4'-C1'-C2' | -6.52 | 99.28 | 105.80 |
| 19 | S | 92 | ASP | CB-CG-OD2 | -6.52 | 112.43 | 118.30 |
| 34 | i | 685 | G | O4'-C1'-C2' | -6.52 | 99.28 | 105.80 |
| 34 | i | 190 | A | O3'-P-O5' | 6.52 | 116.38 | 104.00 |
| 34 | i | 534 | G | C1'-O4'-C4' | 6.52 | 115.11 | 109.90 |
| 34 | i | 685 | G | O3'-P-O5' | 6.52 | 116.38 | 104.00 |
| 34 | i | 1859 | C | P-O3'-C3' | -6.52 | 111.88 | 119.70 |
| 34 | i | 1204 | A | O4'-C1'-C2' | -6.52 | 99.28 | 105.80 |
| 34 | i | 1387 | C | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 34 | i | 1154 | G | N9-C1'-C2' | -6.51 | 104.84 | 112.00 |
| 10 | J | 101 | LYS | N-CA-C | 6.51 | 128.58 | 111.00 |
| 34 | i | 1794 | A | C3'-C2'-C1' | 6.51 | 106.71 | 101.50 |
| 25 | Y | 128 | GLY | CA-C-O | -6.51 | 108.88 | 120.60 |
| 34 | i | 538 | C | N1-C1'-C2' | 6.51 | 122.46 | 114.00 |
| 34 | i | 974 | G | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |
| 22 | V | 81 | GLN | O-C-N | -6.51 | 112.29 | 122.70 |
| 34 | i | 1039 | G | C3'-C2'-C1' | 6.51 | 106.71 | 101.50 |
| 34 | i | 1519 | G | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |
| 34 | i | 1151 | U | C3'-C2'-C1' | 6.50 | 106.70 | 101.50 |
| 34 | i | 401 | G | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 34 | i | 1665 | C | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 34 | i | 1656 | A | N9-C1'-C2' | 6.50 | 122.45 | 114.00 |
| 26 | Z | 115 | GLY | CA-C-O | -6.50 | 108.90 | 120.60 |
| 34 | i | 443 | C | C3'-C2'-C1' | 6.50 | 106.70 | 101.50 |
| 34 | i | 1206 | G | C3'-C2'-C1' | -6.50 | 96.30 | 101.50 |
| 34 | i | 1496 | G | C1'-O4'-C4' | -6.50 | 104.70 | 109.90 |
| 34 | i | 1369 | C | O4'-C1'-C2' | -6.49 | 99.31 | 105.80 |
| 34 | i | 390 | C | O4'-C1'-C2' | -6.49 | 99.31 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 882 | A | C3'-C2'-C1' | 6.49 | 106.69 | 101.50 |
| 34 | i | 1169 | A | O4'-C1'-N9 | 6.49 | 113.39 | 108.20 |
| 34 | i | 1673 | A | C3'-C2'-C1' | -6.49 | 96.31 | 101.50 |
| 34 | i | 282 | G | N9-C1'-C2' | 6.49 | 122.44 | 114.00 |
| 34 | i | 962 | U | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 9 | I | 8 | TRP | CB-CG-CD1 | 6.49 | 135.43 | 127.00 |
| 34 | i | 1486 | G | O4'-C1'-N9 | 6.49 | 113.39 | 108.20 |
| 34 | i | 1376 | C | N1-C1'-C2' | 6.48 | 122.43 | 114.00 |
| 34 | i | 310 | G | C4'-C3'-O3' | 6.48 | 125.96 | 113.00 |
| 34 | i | 1202 | G | C1'-O4'-C4' | -6.48 | 104.72 | 109.90 |
| 34 | i | 79 | A | O5'-C5'-C4' | 6.48 | 124.01 | 111.70 |
| 34 | i | 903 | G | C1'-O4'-C4' | -6.48 | 104.72 | 109.90 |
| 34 | i | 1284 | U | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 34 | i | 1513 | C | P-O3'-C3' | -6.48 | 111.93 | 119.70 |
| 34 | i | 277 | U | P-O3'-C3' | 6.48 | 127.47 | 119.70 |
| 34 | i | 837 | G | C5'-C4'-O4' | 6.48 | 116.87 | 109.10 |
| 21 | U | 70 | CYS | O-C-N | -6.47 | 112.19 | 123.20 |
| 24 | X | 91 | LEU | N-CA-C | -6.47 | 93.52 | 111.00 |
| 26 | Z | 107 | VAL | CA-CB-CG2 | 6.47 | 120.61 | 110.90 |
| 26 | Z | 112 | ASN | N-CA-CB | -6.47 | 98.95 | 110.60 |
| 34 | i | 840 | U | P-O3'-C3' | -6.47 | 111.94 | 119.70 |
| 34 | i | 837 | G | C2'-C3'-O3' | -6.47 | 95.27 | 109.50 |
| 11 | K | 46 | MET | N-CA-CB | 6.47 | 122.24 | 110.60 |
| 34 | i | 10 | G | P-O3'-C3' | -6.47 | 111.94 | 119.70 |
| 34 | i | 947 | C | N1-C1'-C2' | 6.47 | 122.41 | 114.00 |
| 34 | i | 1537 | C | O5'-C5'-C4' | 6.46 | 123.98 | 111.70 |
| 3 | C | 157 | ASN | N-CA-C | 6.46 | 128.45 | 111.00 |
| 34 | i | 1339 | U | C3'-C2'-C1' | 6.46 | 106.67 | 101.50 |
| 34 | i | 1837 | G | O4'-C1'-C2' | 6.46 | 113.42 | 107.60 |
| 34 | i | 870 | G | O4'-C1'-N9 | 6.46 | 113.36 | 108.20 |
| 5 | E | 263 | GLY | CA-C-O | -6.45 | 108.98 | 120.60 |
| 9 | I | 119 | LEU | C-N-CD | -6.45 | 106.40 | 120.60 |
| 34 | i | 814 | A | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 34 | i | 1297 | A | P-O3'-C3' | 6.45 | 127.44 | 119.70 |
| 34 | i | 305 | U | P-O3'-C3' | -6.45 | 111.96 | 119.70 |
| 34 | i | 1089 | A | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 2 | B | 77 | ASP | N-CA-C | 6.45 | 128.40 | 111.00 |
| 34 | i | 882 | A | P-O3'-C3' | 6.44 | 127.43 | 119.70 |
| 34 | i | 211 | U | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 34 | i | 437 | A | C1'-O4'-C4' | 6.44 | 115.05 | 109.90 |
| 34 | i | 1254 | A | O4'-C1'-N9 | 6.44 | 113.35 | 108.20 |
| 34 | i | 147 | A | O4'-C1'-C2' | -6.44 | 99.36 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 29 | c | 7 | GLN | C-N-CD | -6.44 | 106.43 | 120.60 |
| 34 | i | 577 | A | P-O3'-C3' | -6.44 | 111.97 | 119.70 |
| 34 | i | 1202 | G | N9-C1'-C2' | 6.44 | 122.37 | 114.00 |
| 34 | i | 155 | G | C5'-C4'-C3' | 6.44 | 126.30 | 116.00 |
| 34 | i | 1467 | C | C3'-C2'-C1' | 6.43 | 106.65 | 101.50 |
| 34 | i | 236 | C | O4'-C1'-N1 | 6.43 | 113.34 | 108.20 |
| 34 | i | 1405 | A | C1'-O4'-C4' | 6.43 | 115.04 | 109.90 |
| 34 | i | 1702 | U | N1-C1'-C2' | 6.42 | 122.35 | 114.00 |
| 34 | i | 1436 | C | N1-C1'-C2' | 6.42 | 122.35 | 114.00 |
| 34 | i | 1384 | A | O4'-C1'-N9 | 6.42 | 113.34 | 108.20 |
| 10 | J | 188 | GLY | CA-C-O | -6.42 | 109.05 | 120.60 |
| 34 | i | 1785 | A | O4'-C1'-C2' | -6.42 | 99.38 | 105.80 |
| 34 | i | 1135 | C | O4'-C1'-N1 | 6.42 | 113.33 | 108.20 |
| 34 | i | 372 | C | P-O3'-C3' | -6.42 | 112.00 | 119.70 |
| 34 | i | 1232 | G | P-O3'-C3' | 6.41 | 127.39 | 119.70 |
| 2 | B | 233 | GLY | CA-C-O | -6.41 | 109.06 | 120.60 |
| 34 | i | 9 | U | O4'-C1'-N1 | 6.41 | 113.33 | 108.20 |
| 34 | i | 1502 | A | P-O3'-C3' | 6.41 | 127.39 | 119.70 |
| 33 | g | 284 | PRO | N-CA-C | -6.41 | 95.44 | 112.10 |
| 34 | i | 192 | U | O4'-C1'-N1 | 6.41 | 113.32 | 108.20 |
| 34 | i | 1361 | G | C4'-C3'-O3' | -6.40 | 95.95 | 109.40 |
| 34 | i | 1141 | A | O4'-C1'-N9 | 6.40 | 113.32 | 108.20 |
| 18 | R | 99 | ASP | C-N-CD | -6.40 | 106.52 | 120.60 |
| 27 | a | 96 | THR | O-C-N | 6.40 | 133.26 | 121.10 |
| 34 | i | 1284 | U | N1-C1'-C2' | 6.40 | 122.32 | 114.00 |
| 34 | i | 1801 | C | N1-C1'-C2' | 6.40 | 122.31 | 114.00 |
| 34 | i | 1151 | U | P-O5'-C5' | 6.39 | 131.13 | 120.90 |
| 34 | i | 1510 | G | N9-C1'-C2' | -6.39 | 104.97 | 112.00 |
| 34 | i | 38 | A | C1'-O4'-C4' | 6.39 | 115.01 | 109.90 |
| 34 | i | 794 | G | C3'-C2'-C1' | 6.39 | 106.61 | 101.50 |
| 3 | C | 83 | LEU | C-N-CA | -6.39 | 108.88 | 122.30 |
| 34 | i | 994 | A | C1'-O4'-C4' | 6.39 | 115.01 | 109.90 |
| 34 | i | 1122 | G | C1'-O4'-C4' | -6.39 | 104.79 | 109.90 |
| 34 | i | 1158 | C | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 34 | i | 1377 | G | N9-C1'-C2' | -6.39 | 104.97 | 112.00 |
| 34 | i | 1411 | C | O4'-C1'-N1 | 6.39 | 113.31 | 108.20 |
| 31 | e | 120 | VAL | C-N-CD | -6.38 | 106.55 | 120.60 |
| 34 | i | 523 | A | C2'-C3'-O3' | 6.38 | 123.92 | 113.70 |
| 34 | i | 1422 | U | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 34 | i | 70 | G | N9-C1'-C2' | -6.38 | 104.98 | 112.00 |
| 16 | P | 18 | ARG | N-CA-CB | 6.38 | 122.08 | 110.60 |
| 34 | i | 840 | U | O4'-C1'-C2' | -6.38 | 99.42 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1360 | U | P-O3'-C3' | -6.38 | 112.04 | 119.70 |
| 34 | i | 1353 | A | O4'-C1'-N9 | 6.38 | 113.30 | 108.20 |
| 34 | i | 1858 | U | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 34 | i | 150 | A | O4'-C1'-C2' | -6.37 | 99.43 | 105.80 |
| 34 | i | 1227 | C | C3'-C2'-C1' | 6.37 | 106.59 | 101.50 |
| 22 | V | 47 | ASN | N-CA-C | -6.36 | 93.82 | 111.00 |
| 34 | i | 639 | U | O4'-C1'-N1 | 6.36 | 113.29 | 108.20 |
| 19 | S | 49 | ASP | O-C-N | -6.36 | 112.53 | 122.70 |
| 34 | i | 205 | G | O4'-C1'-N9 | 6.36 | 113.29 | 108.20 |
| 34 | i | 1790 | G | O4'-C1'-N9 | 6.36 | 113.29 | 108.20 |
| 34 | i | 176 | U | N1-C1'-C2' | 6.36 | 122.27 | 114.00 |
| 5 | E | 258 | ALA | C-N-CA | -6.35 | 105.82 | 121.70 |
| 34 | i | 634 | G | O4'-C1'-N9 | 6.35 | 113.28 | 108.20 |
| 34 | i | 1534 | U | C1'-O4'-C4' | 6.35 | 114.98 | 109.90 |
| 34 | i | 190 | A | C5'-C4'-C3' | -6.35 | 105.84 | 116.00 |
| 28 | b | 53 | VAL | N-CA-C | -6.34 | 93.88 | 111.00 |
| 34 | i | 1207 | G | N9-C1'-C2' | 6.34 | 122.24 | 114.00 |
| 34 | i | 568 | C | C3'-C2'-C1' | 6.34 | 106.57 | 101.50 |
| 34 | i | 1167 | G | C3'-C2'-C1' | -6.34 | 96.43 | 101.50 |
| 34 | i | 1545 | G | O4'-C1'-N9 | 6.34 | 113.27 | 108.20 |
| 10 | J | 162 | ARG | N-CA-C | 6.33 | 128.09 | 111.00 |
| 16 | P | 37 | TYR | CB-CA-C | 6.33 | 123.06 | 110.40 |
| 34 | i | 174 | C | O4'-C1'-C2' | -6.33 | 99.47 | 105.80 |
| 34 | i | 635 | C | O4'-C1'-C2' | -6.33 | 99.47 | 105.80 |
| 34 | i | 1196 | A | O4'-C1'-N9 | 6.33 | 113.26 | 108.20 |
| 16 | P | 18 | ARG | NE-CZ-NH1 | 6.32 | 123.46 | 120.30 |
| 34 | i | 1076 | A | P-O3'-C3' | 6.32 | 127.29 | 119.70 |
| 34 | i | 8 | U | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 8 | H | 106 | ARG | CD-NE-CZ | 6.32 | 132.45 | 123.60 |
| 34 | i | 1202 | G | C3'-C2'-C1' | -6.32 | 96.44 | 101.50 |
| 34 | i | 1425 | G | O3'-P-O5' | -6.32 | 91.99 | 104.00 |
| 34 | i | 831 | C | P-O3'-C3' | 6.32 | 127.28 | 119.70 |
| 2 | B | 76 | ASN | N-CA-C | 6.31 | 128.05 | 111.00 |
| 34 | i | 582 | C | N1-C1'-C2' | -6.31 | 105.06 | 112.00 |
| 34 | i | 1495 | U | O4'-C1'-N1 | 6.31 | 113.25 | 108.20 |
| 34 | i | 1015 | C | C3'-C2'-C1' | 6.31 | 106.55 | 101.50 |
| 34 | i | 1348 | G | C3'-C2'-C1' | -6.31 | 96.45 | 101.50 |
| 34 | i | 1540 | A | C5'-C4'-O4' | 6.31 | 116.67 | 109.10 |
| 34 | i | 1390 | G | C1'-O4'-C4' | -6.30 | 104.86 | 109.90 |
| 34 | i | 1480 | A | P-O3'-C3' | 6.30 | 127.27 | 119.70 |
| 7 | G | 128 | THR | N-CA-CB | -6.30 | 98.33 | 110.30 |
| 16 | P | 68 | PRO | C-N-CD | -6.30 | 106.73 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 597 | U | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 34 | i | 806 | A | C3'-C2'-C1' | 6.30 | 106.54 | 101.50 |
| 34 | i | 626 | C | O4'-C1'-C2' | -6.30 | 99.50 | 105.80 |
| 34 | i | 796 | U | C5'-C4'-C3' | -6.30 | 105.92 | 116.00 |
| 34 | i | 522 | C | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 34 | i | 730 | C | C3'-C2'-C1' | 6.30 | 106.54 | 101.50 |
| 34 | i | 1256 | A | N9-C1'-C2' | 6.29 | 122.18 | 114.00 |
| 16 | P | 18 | ARG | CB-CG-CD | 6.29 | 127.96 | 111.60 |
| 9 | I | 55 | TYR | CB-CG-CD1 | 6.29 | 124.77 | 121.00 |
| 19 | S | 92 | ASP | N-CA-C | 6.29 | 127.98 | 111.00 |
| 34 | i | 486 | C | O4'-C1'-N1 | 6.29 | 113.23 | 108.20 |
| 34 | i | 509 | A | N9-C1'-C2' | -6.29 | 105.08 | 112.00 |
| 34 | i | 794 | G | N9-C1'-C2' | 6.29 | 122.17 | 114.00 |
| 34 | i | 837 | G | P-O3'-C3' | 6.29 | 127.24 | 119.70 |
| 34 | i | 1415 | C | O4'-C1'-C2' | -6.29 | 99.51 | 105.80 |
| 34 | i | 110 | U | P-O3'-C3' | -6.28 | 112.17 | 119.70 |
| 34 | i | 493 | C | O4'-C1'-C2' | -6.28 | 99.52 | 105.80 |
| 34 | i | 1774 | G | N9-C1'-C2' | 6.28 | 122.16 | 114.00 |
| 34 | i | 887 | G | N9-C1'-C2' | 6.28 | 122.16 | 114.00 |
| 34 | i | 424 | G | C2'-C3'-O3' | 6.27 | 123.74 | 113.70 |
| 34 | i | 1111 | U | O4'-C1'-C2' | 6.27 | 113.25 | 107.60 |
| 34 | i | 1415 | C | C3'-C2'-C1' | 6.27 | 106.52 | 101.50 |
| 34 | i | 1594 | U | P-O5'-C5' | 6.27 | 130.94 | 120.90 |
| 34 | i | 733 | G | O4'-C1'-C2' | -6.27 | 99.53 | 105.80 |
| 34 | i | 1337 | C | O4'-C1'-C2' | -6.27 | 99.53 | 105.80 |
| 7 | G | 173 | ALA | C-N-CD | -6.27 | 106.81 | 120.60 |
| 34 | i | 1084 | U | O4'-C1'-N1 | 6.27 | 113.21 | 108.20 |
| 34 | i | 1337 | C | C3'-C2'-C1' | 6.27 | 106.51 | 101.50 |
| 34 | i | 62 | G | N9-C1'-C2' | 6.26 | 122.14 | 114.00 |
| 34 | i | 1304 | U | P-O3'-C3' | 6.26 | 127.22 | 119.70 |
| 15 | O | 102 | GLY | C-N-CA | -6.26 | 106.05 | 121.70 |
| 34 | i | 341 | G | N9-C1'-C2' | -6.26 | 105.12 | 112.00 |
| 31 | e | 120 | VAL | CB-CA-C | -6.25 | 99.52 | 111.40 |
| 34 | i | 356 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 34 | i | 973 | C | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 34 | i | 1486 | G | C3'-C2'-C1' | -6.25 | 96.50 | 101.50 |
| 34 | i | 1487 | G | O4'-C1'-N9 | 6.25 | 113.20 | 108.20 |
| 1 | A | 186 | ARG | C-N-CA | 6.25 | 135.42 | 122.30 |
| 34 | i | 109 | U | C4'-C3'-O3' | -6.25 | 96.28 | 109.40 |
| 34 | i | 1807 | A | C1'-O4'-C4' | -6.24 | 104.91 | 109.90 |
| 34 | i | 74 | G | C4'-C3'-C2' | -6.24 | 96.36 | 102.60 |
| 34 | i | 1404 | U | P-O3'-C3' | 6.24 | 127.19 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 33 | g | 47 | ARG | N-CA-C | -6.24 | 94.16 | 111.00 |
| 9 | I | 6 | ASP | N-CA-CB | -6.24 | 99.38 | 110.60 |
| 34 | i | 341 | G | O4'-C1'-N9 | 6.24 | 113.19 | 108.20 |
| 10 | J | 164 | PRO | N-CD-CG | -6.23 | 93.85 | 103.20 |
| 34 | i | 605 | C | C1'-O4'-C4' | -6.23 | 104.91 | 109.90 |
| 34 | i | 1515 | G | O4'-C1'-N9 | 6.23 | 113.19 | 108.20 |
| 34 | i | 1658 | A | C3'-C2'-C1' | 6.23 | 106.48 | 101.50 |
| 19 | S | 82 | TRP | CB-CA-C | -6.23 | 97.94 | 110.40 |
| 34 | i | 279 | G | P-O5'-C5' | 6.23 | 130.86 | 120.90 |
| 34 | i | 1214 | C | C3'-C2'-C1' | 6.23 | 106.48 | 101.50 |
| 34 | i | 295 | C | O3'-P-O5' | 6.23 | 115.83 | 104.00 |
| 6 | F | 130 | ARG | N-CA-CB | 6.22 | 121.81 | 110.60 |
| 12 | L | 152 | LYS | CA-C-O | -6.22 | 107.04 | 120.10 |
| 34 | i | 1445 | G | P-O3'-C3' | 6.22 | 127.17 | 119.70 |
| 34 | i | 1636 | A | C3'-C2'-C1' | 6.22 | 106.48 | 101.50 |
| 34 | i | 825 | C | P-O3'-C3' | 6.22 | 127.16 | 119.70 |
| 34 | i | 220 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 34 | i | 1300 | U | C1'-O4'-C4' | -6.21 | 104.93 | 109.90 |
| 34 | i | 1514 | U | N1-C1'-C2' | -6.21 | 105.17 | 112.00 |
| 34 | i | 1654 | U | O3'-P-O5' | 6.21 | 115.80 | 104.00 |
| 19 | S | 6 | PRO | CA-C-O | -6.21 | 105.30 | 120.20 |
| 34 | i | 313 | C | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 34 | i | 445 | A | C3'-C2'-C1' | 6.21 | 106.46 | 101.50 |
| 9 | I | 178 | ARG | CD-NE-CZ | 6.20 | 132.28 | 123.60 |
| 34 | i | 544 | A | C1'-O4'-C4' | -6.20 | 104.94 | 109.90 |
| 34 | i | 1784 | A | N9-C1'-C2' | 6.20 | 122.06 | 114.00 |
| 34 | i | 1563 | C | C1'-O4'-C4' | -6.20 | 104.94 | 109.90 |
| 34 | i | 1855 | G | C1'-O4'-C4' | -6.19 | 104.94 | 109.90 |
| 10 | J | 145 | PRO | N-CA-C | -6.19 | 96.00 | 112.10 |
| 34 | i | 678 | U | P-O3'-C3' | 6.19 | 127.13 | 119.70 |
| 26 | Z | 104 | ARG | CA-C-N | -6.19 | 103.58 | 117.20 |
| 34 | i | 1489 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 34 | i | 424 | G | O3'-P-O5' | -6.19 | 92.24 | 104.00 |
| 34 | i | 1036 | G | C3'-C2'-C1' | -6.19 | 96.55 | 101.50 |
| 33 | g | 50 | THR | CB-CA-C | 6.19 | 128.30 | 111.60 |
| 34 | i | 1030 | A | C1'-O4'-C4' | 6.19 | 114.85 | 109.90 |
| 34 | i | 1395 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 34 | i | 1519 | G | O4'-C4'-C3' | -6.19 | 97.81 | 104.00 |
| 6 | F | 46 | ALA | C-N-CA | -6.18 | 106.24 | 121.70 |
| 34 | i | 1214 | C | C1'-O4'-C4' | -6.18 | 104.95 | 109.90 |
| 34 | i | 1587 | C | C1'-O4'-C4' | -6.18 | 104.95 | 109.90 |
| 34 | i | 1521 | G | N9-C1'-C2' | -6.18 | 105.20 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1562 | G | P-O3'-C3' | -6.18 | 112.28 | 119.70 |
| 34 | i | 1623 | C | C1'-O4'-C4' | -6.18 | 104.96 | 109.90 |
| 3 | C | 258 | LEU | CA-CB-CG | 6.18 | 129.51 | 115.30 |
| 34 | i | 1135 | C | P-O5'-C5' | -6.18 | 111.02 | 120.90 |
| 34 | i | 958 | A | N9-C1'-C2' | -6.17 | 105.21 | 112.00 |
| 34 | i | 1723 | U | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 34 | i | 1729 | G | C3'-C2'-C1' | 6.17 | 106.44 | 101.50 |
| 12 | L | 102 | PHE | N-CA-C | -6.17 | 94.34 | 111.00 |
| 34 | i | 1293 | U | C1'-O4'-C4' | 6.16 | 114.83 | 109.90 |
| 34 | i | 456 | G | O4'-C1'-C2' | 6.16 | 113.14 | 107.60 |
| 34 | i | 792 | G | C1'-O4'-C4' | -6.16 | 104.97 | 109.90 |
| 10 | J | 93 | LYS | O-C-N | -6.16 | 112.85 | 122.70 |
| 34 | i | 210 | G | P-O3'-C3' | -6.16 | 112.31 | 119.70 |
| 34 | i | 542 | G | C1'-O4'-C4' | -6.16 | 104.97 | 109.90 |
| 6 | F | 41 | VAL | N-CA-C | -6.15 | 94.39 | 111.00 |
| 13 | M | 116 | LYS | N-CA-C | 6.15 | 127.62 | 111.00 |
| 34 | i | 2 | A | O4'-C1'-N9 | 6.15 | 113.12 | 108.20 |
| 34 | i | 1364 | U | O4'-C1'-N1 | 6.15 | 113.12 | 108.20 |
| 34 | i | 343 | C | C4'-C3'-C2' | 6.15 | 108.75 | 102.60 |
| 34 | i | 1663 | U | C3'-C2'-C1' | -6.15 | 96.58 | 101.50 |
| 4 | D | 4 | GLN | CA-C-O | 6.15 | 133.01 | 120.10 |
| 34 | i | 924 | G | O4'-C1'-N9 | 6.15 | 113.12 | 108.20 |
| 34 | i | 1395 | C | C5'-C4'-C3' | -6.15 | 106.16 | 116.00 |
| 34 | i | 1514 | U | O4'-C1'-C2' | -6.15 | 99.65 | 105.80 |
| 34 | i | 549 | G | N9-C1'-C2' | 6.15 | 121.99 | 114.00 |
| 34 | i | 1570 | G | C4'-C3'-C2' | -6.14 | 96.46 | 102.60 |
| 10 | J | 180 | LYS | N-CA-C | 6.14 | 127.58 | 111.00 |
| 34 | i | 126 | G | O3'-P-O5' | 6.14 | 115.67 | 104.00 |
| 34 | i | 1238 | U | C1'-O4'-C4' | -6.14 | 104.99 | 109.90 |
| 34 | i | 272 | C | O5'-P-OP1 | -6.14 | 100.17 | 105.70 |
| 34 | i | 795 | U | C1'-O4'-C4' | -6.14 | 104.99 | 109.90 |
| 19 | S | 9 | PHE | C-N-CA | -6.14 | 106.35 | 121.70 |
| 34 | i | 824 | G | C1'-O4'-C4' | -6.14 | 104.99 | 109.90 |
| 34 | i | 954 | G | C3'-C2'-C1' | -6.14 | 96.59 | 101.50 |
| 34 | i | 1255 | A | C1'-O4'-C4' | -6.14 | 104.99 | 109.90 |
| 34 | i | 1489 | C | N1-C1'-C2' | -6.13 | 105.26 | 112.00 |
| 34 | i | 1657 | U | O4'-C1'-N1 | 6.13 | 113.10 | 108.20 |
| 15 | O | 143 | LYS | CB-CA-C | -6.13 | 98.15 | 110.40 |
| 34 | i | 395 | G | C1'-O4'-C4' | -6.12 | 105.00 | 109.90 |
| 34 | i | 489 | G | C1'-O4'-C4' | -6.12 | 105.00 | 109.90 |
| 34 | i | 1644 | U | P-O3'-C3' | -6.12 | 112.35 | 119.70 |
| 34 | i | 903 | G | C3'-C2'-C1' | -6.12 | 96.60 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 205 | G | C1'-O4'-C4' | -6.12 | 105.00 | 109.90 |
| 34 | i | 1361 | G | P-O5'-C5' | 6.12 | 130.69 | 120.90 |
| 34 | i | 1186 | A | C3'-C2'-C1' | 6.12 | 106.39 | 101.50 |
| 34 | i | 1776 | G | O4'-C4'-C3' | -6.11 | 97.89 | 104.00 |
| 34 | i | 973 | C | O4'-C1'-C2' | -6.11 | 99.69 | 105.80 |
| 34 | i | 201 | G | O4'-C1'-C2' | -6.11 | 99.69 | 105.80 |
| 34 | i | 685 | G | C5'-C4'-C3' | 6.11 | 125.77 | 116.00 |
| 34 | i | 1543 | G | C3'-C2'-C1' | -6.11 | 96.61 | 101.50 |
| 34 | i | 986 | A | C1'-O4'-C4' | -6.11 | 105.02 | 109.90 |
| 34 | i | 1050 | G | C1'-O4'-C4' | -6.11 | 105.02 | 109.90 |
| 34 | i | 1849 | G | O4'-C1'-C2' | 6.11 | 113.09 | 107.60 |
| 34 | i | 193 | C | C3'-C2'-C1' | 6.10 | 106.38 | 101.50 |
| 34 | i | 880 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 34 | i | 1796 | C | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 31 | e | 121 | PRO | CA-N-CD | -6.10 | 102.96 | 111.50 |
| 34 | i | 1535 | G | O4'-C1'-N9 | 6.10 | 113.08 | 108.20 |
| 19 | S | 10 | GLN | C-N-CA | 6.10 | 136.94 | 121.70 |
| 34 | i | 906 | G | O4'-C1'-C2' | 6.10 | 113.09 | 107.60 |
| 34 | i | 1533 | C | P-O5'-C5' | -6.10 | 111.15 | 120.90 |
| 34 | i | 209 | C | P-O5'-C5' | 6.09 | 130.65 | 120.90 |
| 34 | i | 1181 | C | N1-C1'-C2' | 6.09 | 121.92 | 114.00 |
| 34 | i | 1400 | U | N1-C1'-C2' | 6.09 | 121.92 | 114.00 |
| 34 | i | 1610 | U | C1'-O4'-C4' | -6.09 | 105.03 | 109.90 |
| 34 | i | 1678 | C | C3'-C2'-C1' | 6.09 | 106.37 | 101.50 |
| 11 | K | 89 | ILE | CA-CB-CG2 | 6.09 | 123.08 | 110.90 |
| 34 | i | 327 | C | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 34 | i | 940 | A | C3'-C2'-C1' | 6.08 | 106.37 | 101.50 |
| 34 | i | 1066 | A | N9-C1'-C2' | 6.08 | 121.91 | 114.00 |
| 34 | i | 1462 | G | O4'-C1'-N9 | 6.08 | 113.07 | 108.20 |
| 34 | i | 741 | C | O4'-C1'-C2' | -6.08 | 99.72 | 105.80 |
| 34 | i | 854 | A | C3'-C2'-C1' | 6.08 | 106.36 | 101.50 |
| 34 | i | 872 | C | C3'-C2'-C1' | 6.08 | 106.36 | 101.50 |
| 34 | i | 64 | A | C3'-C2'-C1' | -6.08 | 96.64 | 101.50 |
| 12 | L | 151 | THR | C-N-CA | 6.08 | 136.89 | 121.70 |
| 34 | i | 352 | C | N1-C1'-C2' | 6.08 | 121.90 | 114.00 |
| 34 | i | 584 | A | P-O3'-C3' | 6.08 | 126.99 | 119.70 |
| 34 | i | 1433 | C | N1-C1'-C2' | 6.07 | 121.89 | 114.00 |
| 25 | Y | 96 | LEU | N-CA-CB | 6.07 | 122.54 | 110.40 |
| 34 | i | 1118 | A | C4'-C3'-C2' | -6.07 | 96.53 | 102.60 |
| 34 | i | 1431 | C | C3'-C2'-C1' | 6.07 | 106.36 | 101.50 |
| 34 | i | 1701 | G | O4'-C1'-N9 | 6.07 | 113.05 | 108.20 |
| 34 | i | 1702 | U | O4'-C1'-N1 | 6.07 | 113.05 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1774 | G | C3'-C2'-C1' | -6.07 | 96.65 | 101.50 |
| 34 | i | 4 | C | C1'-O4'-C4' | -6.06 | 105.05 | 109.90 |
| 34 | i | 460 | G | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 34 | i | 1486 | G | O4'-C1'-C2' | 6.06 | 113.06 | 107.60 |
| 34 | i | 1698 | C | O4'-C1'-C2' | -6.06 | 99.74 | 105.80 |
| 34 | i | 1705 | C | C3'-C2'-C1' | 6.06 | 106.35 | 101.50 |
| 16 | P | 49 | LEU | C-N-CA | -6.06 | 106.55 | 121.70 |
| 21 | U | 117 | ALA | O-C-N | 6.06 | 132.40 | 122.70 |
| 32 | f | 134 | SER | O-C-N | 6.06 | 132.40 | 122.70 |
| 2 | B | 151 | ARG | C-N-CA | -6.06 | 106.56 | 121.70 |
| 34 | i | 410 | G | O4'-C1'-C2' | 6.06 | 113.05 | 107.60 |
| 34 | i | 1845 | A | C1'-O4'-C4' | 6.06 | 114.75 | 109.90 |
| 34 | i | 1102 | C | O4'-C1'-C2' | -6.06 | 99.74 | 105.80 |
| 25 | Y | 64 | PHE | N-CA-CB | -6.05 | 99.70 | 110.60 |
| 16 | P | 17 | TYR | N-CA-CB | 6.05 | 121.49 | 110.60 |
| 34 | i | 1425 | G | OP1-P-O3' | 6.05 | 118.51 | 105.20 |
| 34 | i | 1571 | G | C1'-O4'-C4' | -6.05 | 105.06 | 109.90 |
| 12 | L | 150 | GLY | N-CA-C | -6.05 | 97.98 | 113.10 |
| 29 | c | 6 | VAL | N-CA-C | 6.05 | 127.33 | 111.00 |
| 34 | i | 960 | A | N9-C1'-C2' | -6.05 | 105.35 | 112.00 |
| 34 | i | 1112 | C | O4'-C1'-C2' | 6.05 | 113.05 | 107.60 |
| 34 | i | 1187 | C | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 11 | K | 40 | VAL | C-N-CD | -6.04 | 107.30 | 120.60 |
| 34 | i | 1588 | C | O4'-C1'-N1 | 6.04 | 113.04 | 108.20 |
| 34 | i | 1558 | G | C1'-O4'-C4' | -6.04 | 105.06 | 109.90 |
| 33 | g | 213 | ASP | CB-CG-OD2 | -6.04 | 112.86 | 118.30 |
| 34 | i | 1394 | G | P-O3'-C3' | -6.04 | 112.45 | 119.70 |
| 34 | i | 1172 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 34 | i | 1440 | U | O4'-C1'-N1 | 6.03 | 113.03 | 108.20 |
| 3 | C | 262 | HIS | CB-CA-C | -6.03 | 98.34 | 110.40 |
| 18 | R | 88 | VAL | C-N-CA | -6.03 | 106.62 | 121.70 |
| 27 | a | 107 | ALA | C-N-CD | 6.03 | 141.06 | 128.40 |
| 34 | i | 410 | G | O4'-C1'-N9 | 6.03 | 113.02 | 108.20 |
| 34 | i | 1431 | C | C5'-C4'-C3' | 6.02 | 125.64 | 116.00 |
| 6 | F | 135 | ARG | CB-CA-C | 6.02 | 122.44 | 110.40 |
| 33 | g | 15 | ASN | C-N-CA | -6.02 | 109.66 | 122.30 |
| 34 | i | 1549 | C | C2'-C3'-O3' | -6.02 | 96.26 | 109.50 |
| 32 | f | 88 | PRO | N-CA-C | -6.02 | 96.46 | 112.10 |
| 34 | i | 623 | C | N1-C1'-C2' | 6.02 | 121.82 | 114.00 |
| 34 | i | 952 | G | O4'-C1'-N9 | 6.02 | 113.01 | 108.20 |
| 34 | i | 1742 | C | C5'-C4'-O4' | 6.02 | 116.32 | 109.10 |
| 34 | i | 1355 | U | O4'-C1'-C2' | -6.02 | 99.78 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1698 | C | C3'-C2'-C1' | 6.02 | 106.31 | 101.50 |
| 34 | i | 1743 | G | O5'-C5'-C4' | 6.02 | 123.13 | 111.70 |
| 34 | i | 1367 | U | C3'-C2'-C1' | 6.01 | 106.31 | 101.50 |
| 21 | U | 109 | GLY | N-CA-C | -6.01 | 98.07 | 113.10 |
| 11 | K | 38 | LYS | N-CA-C | -6.01 | 94.78 | 111.00 |
| 34 | i | 1391 | C | O4'-C1'-N1 | 6.01 | 113.01 | 108.20 |
| 34 | i | 1441 | U | C4'-C3'-O3' | -6.01 | 96.78 | 109.40 |
| 26 | Z | 112 | ASN | N-CA-C | 6.00 | 127.22 | 111.00 |
| 34 | i | 1547 | G | P-O5'-C5' | 6.00 | 130.50 | 120.90 |
| 34 | i | 1393 | U | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |
| 34 | i | 946 | C | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |
| 7 | G | 173 | ALA | O-C-N | -5.99 | 109.71 | 121.10 |
| 9 | I | 29 | LEU | C-N-CA | 5.99 | 134.88 | 122.30 |
| 34 | i | 204 | G | O4'-C1'-C2' | -5.99 | 99.81 | 105.80 |
| 34 | i | 1663 | U | P-O3'-C3' | 5.99 | 126.89 | 119.70 |
| 34 | i | 1219 | A | O4'-C1'-C2' | -5.99 | 99.81 | 105.80 |
| 34 | i | 7 | G | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 34 | i | 1403 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 34 | i | 1367 | U | O4'-C1'-N1 | 5.98 | 112.99 | 108.20 |
| 34 | i | 430 | G | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 34 | i | 1740 | A | C4'-C3'-C2' | -5.98 | 96.62 | 102.60 |
| 9 | I | 132 | GLU | CA-C-N | 5.98 | 130.35 | 117.20 |
| 34 | i | 844 | U | C1'-O4'-C4' | -5.98 | 105.12 | 109.90 |
| 34 | i | 848 | G | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 1 | A | 193 | HIS | C-N-CD | -5.97 | 107.46 | 120.60 |
| 34 | i | 1348 | G | O4'-C1'-N9 | 5.97 | 112.98 | 108.20 |
| 34 | i | 1441 | U | P-O3'-C3' | -5.97 | 112.53 | 119.70 |
| 34 | i | 1752 | G | C1'-O4'-C4' | -5.97 | 105.12 | 109.90 |
| 34 | i | 849 | C | O4'-C1'-N1 | 5.97 | 112.98 | 108.20 |
| 34 | i | 959 | A | P-O5'-C5' | -5.97 | 111.35 | 120.90 |
| 34 | i | 563 | U | N1-C1'-C2' | 5.96 | 121.75 | 114.00 |
| 34 | i | 610 | G | C1'-O4'-C4' | 5.96 | 114.67 | 109.90 |
| 34 | i | 1535 | G | C1'-O4'-C4' | -5.96 | 105.13 | 109.90 |
| 34 | i | 1091 | U | C1'-O4'-C4' | -5.96 | 105.13 | 109.90 |
| 22 | V | 66 | ASP | C-N-CA | -5.96 | 106.80 | 121.70 |
| 34 | i | 194 | C | O4'-C1'-N1 | 5.96 | 112.97 | 108.20 |
| 34 | i | 1343 | U | O4'-C1'-C2' | -5.96 | 99.84 | 105.80 |
| 21 | U | 69 | PRO | N-CA-C | -5.96 | 96.62 | 112.10 |
| 25 | Y | 86 | GLU | CA-C-N | 5.96 | 133.77 | 117.10 |
| 6 | F | 38 | TYR | C-N-CA | -5.95 | 106.82 | 121.70 |
| 34 | i | 558 | C | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 34 | i | 1547 | G | O4'-C1'-C2' | -5.95 | 99.85 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 223 | A | O4'-C1'-C2' | -5.95 | 99.85 | 105.80 |
| 11 | K | 41 | PRO | N-CA-C | -5.95 | 96.63 | 112.10 |
| 22 | V | 32 | ILE | C-N-CD | 5.95 | 140.90 | 128.40 |
| 21 | U | 68 | THR | N-CA-CB | -5.95 | 99.00 | 110.30 |
| 34 | i | 743 | U | O3'-P-O5' | -5.95 | 92.70 | 104.00 |
| 34 | i | 727 | G | C5'-C4'-O4' | -5.95 | 101.97 | 109.10 |
| 34 | i | 853 | U | P-O5'-C5' | -5.95 | 111.39 | 120.90 |
| 34 | i | 1485 | A | P-O3'-C3' | 5.95 | 126.84 | 119.70 |
| 34 | i | 272 | C | O5'-P-OP2 | -5.94 | 100.35 | 105.70 |
| 34 | i | 623 | C | C3'-C2'-C1' | 5.94 | 106.25 | 101.50 |
| 34 | i | 1646 | A | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 11 | K | 90 | VAL | N-CA-C | 5.94 | 127.05 | 111.00 |
| 34 | i | 621 | U | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 34 | i | 1497 | C | P-O3'-C3' | 5.94 | 126.83 | 119.70 |
| 34 | i | 373 | G | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 34 | i | 970 | C | C1'-O4'-C4' | -5.94 | 105.15 | 109.90 |
| 34 | i | 1019 | A | O4'-C1'-C2' | -5.94 | 99.86 | 105.80 |
| 8 | H | 16 | PRO | O-C-N | -5.93 | 113.20 | 122.70 |
| 34 | i | 793 | C | P-O5'-C5' | 5.93 | 130.39 | 120.90 |
| 34 | i | 1534 | U | C3'-C2'-C1' | 5.93 | 106.25 | 101.50 |
| 34 | i | 1087 | C | O4'-C1'-C2' | -5.93 | 99.87 | 105.80 |
| 34 | i | 1834 | U | O4'-C1'-N1 | 5.93 | 112.94 | 108.20 |
| 34 | i | 1459 | U | P-O3'-C3' | -5.93 | 112.58 | 119.70 |
| 16 | P | 121 | ILE | O-C-N | -5.93 | 113.22 | 122.70 |
| 34 | i | 1138 | G | C3'-C2'-C1' | -5.93 | 96.76 | 101.50 |
| 34 | i | 541 | U | P-O3'-C3' | 5.93 | 126.81 | 119.70 |
| 34 | i | 1426 | C | C1'-O4'-C4' | 5.93 | 114.64 | 109.90 |
| 16 | P | 130 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 34 | i | 1022 | C | O4'-C1'-C2' | -5.92 | 99.88 | 105.80 |
| 34 | i | 1058 | A | C3'-C2'-C1' | 5.92 | 106.23 | 101.50 |
| 34 | i | 1127 | G | C5'-C4'-C3' | -5.92 | 106.53 | 116.00 |
| 34 | i | 1408 | C | C4'-C3'-O3' | 5.92 | 124.83 | 113.00 |
| 34 | i | 858 | A | C1'-O4'-C4' | -5.91 | 105.17 | 109.90 |
| 34 | i | 1694 | A | P-O3'-C3' | -5.91 | 112.61 | 119.70 |
| 34 | i | 603 | C | C1'-O4'-C4' | 5.91 | 114.63 | 109.90 |
| 34 | i | 1621 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 34 | i | 24 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 34 | i | 278 | U | P-O5'-C5' | 5.91 | 130.35 | 120.90 |
| 34 | i | 1121 | C | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 34 | i | 1547 | G | C1'-O4'-C4' | 5.91 | 114.63 | 109.90 |
| 34 | i | 1733 | C | C3'-C2'-C1' | 5.90 | 106.22 | 101.50 |
| 34 | i | 419 | C | C3'-C2'-C1' | 5.90 | 106.22 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1148 | U | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 34 | i | 581 | U | N1-C1'-C2' | 5.90 | 121.67 | 114.00 |
| 34 | i | 1051 | A | C3'-C2'-C1' | 5.90 | 106.22 | 101.50 |
| 34 | i | 1300 | U | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 34 | i | 684 | A | P-O5'-C5' | 5.89 | 130.33 | 120.90 |
| 34 | i | 788 | C | N1-C1'-C2' | 5.89 | 121.66 | 114.00 |
| 34 | i | 1846 | C | N1-C1'-C2' | 5.89 | 121.66 | 114.00 |
| 34 | i | 1114 | C | C3'-C2'-C1' | -5.89 | 96.79 | 101.50 |
| 34 | i | 1349 | A | O3'-P-O5' | -5.89 | 92.80 | 104.00 |
| 34 | i | 1413 | C | OP1-P-OP2 | -5.89 | 110.76 | 119.60 |
| 34 | i | 1732 | G | C1'-O4'-C4' | -5.89 | 105.19 | 109.90 |
| 34 | i | 1527 | C | N1-C1'-C2' | 5.89 | 121.66 | 114.00 |
| 29 | c | 5 | ARG | N-CA-C | 5.89 | 126.89 | 111.00 |
| 34 | i | 21 | U | O4'-C1'-C2' | -5.88 | 99.92 | 105.80 |
| 34 | i | 1134 | C | C4'-C3'-O3' | -5.88 | 97.04 | 109.40 |
| 34 | i | 1571 | G | N9-C1'-C2' | 5.88 | 121.65 | 114.00 |
| 34 | i | 1230 | C | C1'-O4'-C4' | -5.88 | 105.20 | 109.90 |
| 34 | i | 163 | U | O4'-C4'-C3' | -5.88 | 98.12 | 104.00 |
| 34 | i | 292 | A | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 34 | i | 1318 | G | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 34 | i | 1434 | A | C3'-C2'-C1' | 5.88 | 106.20 | 101.50 |
| 34 | i | 1577 | C | N1-C1'-C2' | 5.88 | 121.64 | 114.00 |
| 34 | i | 617 | U | O4'-C1'-C2' | -5.87 | 99.93 | 105.80 |
| 34 | i | 826 | A | O4'-C1'-C2' | 5.87 | 112.88 | 107.60 |
| 34 | i | 119 | U | O4'-C1'-N1 | 5.87 | 112.89 | 108.20 |
| 34 | i | 172 | U | O4'-C1'-C2' | -5.87 | 99.93 | 105.80 |
| 34 | i | 1380 | C | O4'-C1'-N1 | 5.87 | 112.89 | 108.20 |
| 34 | i | 1800 | A | N9-C1'-C2' | 5.87 | 121.63 | 114.00 |
| 34 | i | 830 | C | C3'-C2'-C1' | -5.87 | 96.81 | 101.50 |
| 34 | i | 1416 | G | N9-C1'-C2' | 5.86 | 121.62 | 114.00 |
| 33 | g | 159 | ASN | O-C-N | -5.86 | 113.32 | 122.70 |
| 34 | i | 1605 | G | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 34 | i | 192 | U | O5'-C5'-C4' | -5.86 | 100.57 | 111.70 |
| 34 | i | 213 | C | C3'-C2'-C1' | 5.86 | 106.18 | 101.50 |
| 20 | T | 30 | VAL | N-CA-C | 5.85 | 126.80 | 111.00 |
| 28 | b | 53 | VAL | C-N-CA | -5.85 | 107.07 | 121.70 |
| 34 | i | 103 | A | O4'-C1'-C2' | 5.85 | 112.87 | 107.60 |
| 34 | i | 1013 | U | C1'-O4'-C4' | 5.85 | 114.58 | 109.90 |
| 34 | i | 1552 | C | C2'-C3'-O3' | 5.85 | 123.06 | 113.70 |
| 34 | i | 1199 | G | C3'-C2'-C1' | -5.85 | 96.82 | 101.50 |
| 34 | i | 1274 | A | P-O5'-C5' | 5.85 | 130.26 | 120.90 |
| 34 | i | 1417 | A | O4'-C1'-N9 | 5.85 | 112.88 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 10 | MET | N-CA-C | 5.85 | 126.78 | 111.00 |
| 34 | i | 875 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 34 | i | 98 | C | N1-C1'-C2' | -5.84 | 105.57 | 112.00 |
| 34 | i | 368 | U | N1-C1'-C2' | 5.84 | 121.60 | 114.00 |
| 17 | Q | 17 | LYS | O-C-N | -5.84 | 113.35 | 122.70 |
| 27 | a | 96 | THR | CA-C-N | -5.84 | 100.74 | 117.10 |
| 34 | i | 1065 | U | P-O5'-C5' | -5.84 | 111.56 | 120.90 |
| 34 | i | 332 | C | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 34 | i | 392 | C | O4'-C1'-C2' | -5.84 | 99.96 | 105.80 |
| 34 | i | 633 | A | O4'-C1'-C2' | -5.84 | 99.96 | 105.80 |
| 34 | i | 1204 | A | C1'-O4'-C4' | 5.84 | 114.57 | 109.90 |
| 8 | H | 192 | PHE | N-CA-C | 5.83 | 126.75 | 111.00 |
| 34 | i | 115 | U | O4'-C1'-N1 | 5.83 | 112.87 | 108.20 |
| 34 | i | 1779 | C | O4'-C1'-N1 | 5.83 | 112.87 | 108.20 |
| 34 | i | 114 | G | C1'-O4'-C4' | 5.83 | 114.57 | 109.90 |
| 34 | i | 314 | U | C3'-C2'-C1' | -5.83 | 96.83 | 101.50 |
| 34 | i | 730 | C | N1-C1'-C2' | 5.83 | 121.58 | 114.00 |
| 34 | i | 190 | A | O5'-P-OP2 | -5.83 | 100.46 | 105.70 |
| 34 | i | 376 | C | C1'-O4'-C4' | -5.82 | 105.24 | 109.90 |
| 34 | i | 546 | U | C5'-C4'-C3' | 5.82 | 125.32 | 116.00 |
| 34 | i | 730 | C | O3'-P-O5' | 5.82 | 115.07 | 104.00 |
| 34 | i | 528 | U | C3'-C2'-C1' | 5.82 | 106.16 | 101.50 |
| 34 | i | 1282 | G | C4'-C3'-O3' | -5.82 | 97.18 | 109.40 |
| 33 | g | 12 | LYS | C-N-CA | 5.82 | 134.51 | 122.30 |
| 34 | i | 544 | A | O4'-C1'-C2' | 5.82 | 112.83 | 107.60 |
| 34 | i | 611 | C | C1'-O4'-C4' | -5.81 | 105.25 | 109.90 |
| 34 | i | 1602 | A | O4'-C1'-C2' | 5.81 | 112.83 | 107.60 |
| 3 | C | 241 | TRP | C-N-CA | -5.81 | 107.17 | 121.70 |
| 34 | i | 1118 | A | C3'-C2'-C1' | 5.81 | 106.15 | 101.50 |
| 34 | i | 1303 | U | N1-C1'-C2' | -5.81 | 105.61 | 112.00 |
| 11 | K | 40 | VAL | CB-CA-C | -5.81 | 100.36 | 111.40 |
| 13 | M | 99 | LYS | N-CA-C | 5.81 | 126.67 | 111.00 |
| 34 | i | 1227 | C | O4'-C1'-N1 | -5.81 | 103.56 | 108.20 |
| 34 | i | 1428 | U | N1-C1'-C2' | 5.81 | 121.55 | 114.00 |
| 34 | i | 1532 | A | C3'-C2'-C1' | 5.81 | 106.14 | 101.50 |
| 34 | i | 998 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 34 | i | 1790 | G | C5'-C4'-O4' | 5.80 | 116.06 | 109.10 |
| 34 | i | 1450 | A | O4'-C1'-C2' | -5.80 | 100.00 | 105.80 |
| 34 | i | 54 | A | N9-C1'-C2' | 5.80 | 121.53 | 114.00 |
| 34 | i | 726 | C | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 34 | i | 914 | U | C1'-O4'-C4' | -5.80 | 105.26 | 109.90 |
| 34 | i | 367 | G | O4'-C1'-N9 | 5.79 | 112.84 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | U | 108 | PRO | CA-N-CD | -5.79 | 103.39 | 111.50 |
| 34 | i | 77 | A | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 34 | i | 1633 | G | O4'-C1'-N9 | -5.79 | 103.57 | 108.20 |
| 34 | i | 1414 | C | N1-C1'-C2' | 5.79 | 121.53 | 114.00 |
| 34 | i | 839 | C | C3'-C2'-C1' | 5.79 | 106.13 | 101.50 |
| 34 | i | 884 | U | P-O5'-C5' | 5.79 | 130.16 | 120.90 |
| 6 | F | 131 | ALA | N-CA-C | 5.78 | 126.61 | 111.00 |
| 34 | i | 55 | U | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 34 | i | 402 | G | C3'-C2'-C1' | 5.78 | 106.13 | 101.50 |
| 34 | i | 1110 | U | C1'-O4'-C4' | 5.78 | 114.53 | 109.90 |
| 34 | i | 90 | G | O4'-C1'-N9 | 5.78 | 112.82 | 108.20 |
| 34 | i | 277 | U | N1-C1'-C2' | 5.78 | 121.51 | 114.00 |
| 34 | i | 1020 | A | O4'-C1'-N9 | 5.78 | 112.82 | 108.20 |
| 34 | i | 1047 | G | C3'-C2'-C1' | -5.78 | 96.88 | 101.50 |
| 5 | E | 170 | THR | C-N-CA | 5.78 | 136.14 | 121.70 |
| 11 | K | 41 | PRO | CA-N-CD | -5.78 | 103.41 | 111.50 |
| 34 | i | 461 | G | C5'-C4'-O4' | 5.78 | 116.03 | 109.10 |
| 34 | i | 876 | G | N9-C1'-C2' | -5.77 | 105.65 | 112.00 |
| 34 | i | 516 | A | C3'-C2'-C1' | -5.77 | 96.89 | 101.50 |
| 34 | i | 832 | G | C1'-O4'-C4' | 5.77 | 114.52 | 109.90 |
| 34 | i | 1501 | U | C1'-O4'-C4' | 5.77 | 114.51 | 109.90 |
| 34 | i | 206 | A | O3'-P-O5' | 5.76 | 114.95 | 104.00 |
| 34 | i | 1801 | C | C1'-O4'-C4' | -5.76 | 105.29 | 109.90 |
| 12 | L | 4 | ILE | N-CA-C | -5.76 | 95.44 | 111.00 |
| 34 | i | 139 | C | C1'-O4'-C4' | 5.76 | 114.51 | 109.90 |
| 34 | i | 1142 | C | C1'-O4'-C4' | -5.76 | 105.29 | 109.90 |
| 17 | Q | 146 | ARG | CA-CB-CG | 5.76 | 126.07 | 113.40 |
| 34 | i | 962 | U | C5'-C4'-O4' | 5.76 | 116.01 | 109.10 |
| 34 | i | 970 | C | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 34 | i | 1138 | G | N9-C1'-C2' | -5.76 | 105.67 | 112.00 |
| 7 | G | 131 | ARG | CG-CD-NE | 5.76 | 123.89 | 111.80 |
| 34 | i | 188 | U | C1'-O4'-C4' | -5.76 | 105.29 | 109.90 |
| 34 | i | 1168 | U | N1-C1'-C2' | -5.76 | 105.67 | 112.00 |
| 34 | i | 871 | A | O4'-C1'-C2' | -5.75 | 100.05 | 105.80 |
| 34 | i | 1251 | G | C3'-C2'-C1' | -5.75 | 96.90 | 101.50 |
| 8 | H | 40 | LEU | CA-CB-CG | -5.75 | 102.07 | 115.30 |
| 34 | i | 958 | A | O4'-C1'-C2' | -5.75 | 100.05 | 105.80 |
| 34 | i | 1706 | U | N1-C1'-C2' | 5.75 | 121.48 | 114.00 |
| 34 | i | 652 | G | C1'-O4'-C4' | -5.75 | 105.30 | 109.90 |
| 7 | G | 155 | GLN | C-N-CA | -5.75 | 107.33 | 121.70 |
| 26 | Z | 104 | ARG | N-CA-C | 5.75 | 126.52 | 111.00 |
| 34 | i | 148 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1135 | C | C4'-C3'-O3' | -5.75 | 97.33 | 109.40 |
| 34 | i | 1100 | G | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 34 | i | 1842 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 34 | i | 923 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 12 | L | 151 | THR | CB-CA-C | 5.74 | 127.11 | 111.60 |
| 34 | i | 386 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 34 | i | 215 | U | C1'-O4'-C4' | -5.74 | 105.31 | 109.90 |
| 5 | E | 151 | ASP | CB-CA-C | 5.74 | 121.87 | 110.40 |
| 34 | i | 1057 | U | O4'-C1'-N1 | 5.74 | 112.79 | 108.20 |
| 34 | i | 1345 | G | N9-C1'-C2' | 5.74 | 121.46 | 114.00 |
| 34 | i | 1494 | A | O4'-C1'-C2' | 5.74 | 112.76 | 107.60 |
| 34 | i | 1327 | C | C1'-O4'-C4' | -5.74 | 105.31 | 109.90 |
| 34 | i | 1771 | G | P-O3'-C3' | -5.74 | 112.82 | 119.70 |
| 22 | V | 42 | VAL | CB-CA-C | -5.73 | 100.51 | 111.40 |
| 34 | i | 495 | G | P-O3'-C3' | -5.73 | 112.82 | 119.70 |
| 34 | i | 1471 | G | O4'-C1'-N9 | 5.73 | 112.79 | 108.20 |
| 11 | K | 29 | MET | C-N-CD | -5.73 | 107.99 | 120.60 |
| 20 | T | 4 | VAL | O-C-N | -5.73 | 113.53 | 122.70 |
| 34 | i | 163 | U | O4'-C1'-N1 | 5.73 | 112.78 | 108.20 |
| 34 | i | 331 | C | P-O3'-C3' | -5.73 | 112.83 | 119.70 |
| 34 | i | 1501 | U | O4'-C1'-C2' | -5.73 | 100.07 | 105.80 |
| 34 | i | 1309 | A | O4'-C1'-C2' | -5.73 | 100.07 | 105.80 |
| 34 | i | 1532 | A | C5'-C4'-C3' | -5.72 | 106.84 | 116.00 |
| 34 | i | 86 | C | C3'-C2'-C1' | 5.72 | 106.08 | 101.50 |
| 34 | i | 190 | A | C5'-C4'-O4' | 5.72 | 115.97 | 109.10 |
| 34 | i | 969 | C | C3'-C2'-C1' | 5.72 | 106.08 | 101.50 |
| 34 | i | 1774 | G | O4'-C1'-N9 | 5.72 | 112.78 | 108.20 |
| 24 | X | 98 | ASP | N-CA-C | 5.72 | 126.44 | 111.00 |
| 34 | i | 1262 | C | N1-C1'-C2' | 5.72 | 121.44 | 114.00 |
| 34 | i | 1366 | A | C1'-O4'-C4' | 5.72 | 114.47 | 109.90 |
| 34 | i | 79 | A | O3'-P-O5' | -5.71 | 93.14 | 104.00 |
| 34 | i | 1407 | G | N9-C1'-C2' | 5.71 | 121.43 | 114.00 |
| 20 | T | 51 | ASN | C-N-CA | 5.71 | 135.98 | 121.70 |
| 34 | i | 864 | G | O4'-C1'-N9 | -5.71 | 103.63 | 108.20 |
| 34 | i | 504 | U | N1-C1'-C2' | 5.71 | 121.43 | 114.00 |
| 34 | i | 1390 | G | C2'-C3'-O3' | 5.71 | 122.84 | 113.70 |
| 34 | i | 1859 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 4 | D | 96 | LEU | O-C-N | -5.71 | 113.56 | 122.70 |
| 34 | i | 897 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 26 | Z | 107 | VAL | C-N-CA | 5.71 | 135.97 | 121.70 |
| 34 | i | 645 | A | C5'-C4'-O4' | 5.70 | 115.94 | 109.10 |
| 34 | i | 1045 | A | P-O3'-C3' | 5.70 | 126.54 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1437 | U | O4'-C1'-C2' | -5.70 | 100.10 | 105.80 |
| 19 | S | 53 | THR | CA-C-N | 5.70 | 129.74 | 117.20 |
| 34 | i | 734 | C | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 34 | i | 965 | U | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 34 | i | 1271 | G | C5'-C4'-C3' | 5.70 | 125.12 | 116.00 |
| 16 | P | 49 | LEU | O-C-N | -5.70 | 113.58 | 122.70 |
| 34 | i | 171 | A | C1'-O4'-C4' | 5.70 | 114.46 | 109.90 |
| 34 | i | 441 | G | P-O5'-C5' | 5.69 | 130.01 | 120.90 |
| 34 | i | 1446 | G | C3'-C2'-C1' | -5.69 | 96.94 | 101.50 |
| 34 | i | 141 | A | C2'-C3'-O3' | 5.69 | 122.81 | 113.70 |
| 34 | i | 827 | G | O4'-C1'-C2' | 5.69 | 112.72 | 107.60 |
| 34 | i | 895 | U | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 34 | i | 895 | U | O4'-C1'-C2' | -5.69 | 100.11 | 105.80 |
| 34 | i | 78 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 34 | i | 1779 | C | N1-C1'-C2' | -5.69 | 105.74 | 112.00 |
| 34 | i | 274 | G | N9-C1'-C2' | 5.69 | 121.39 | 114.00 |
| 34 | i | 290 | A | N9-C1'-C2' | -5.68 | 105.75 | 112.00 |
| 34 | i | 625 | G | C5'-C4'-C3' | 5.68 | 125.09 | 116.00 |
| 34 | i | 856 | G | N9-C1'-C2' | 5.68 | 121.39 | 114.00 |
| 34 | i | 569 | C | O4'-C1'-C2' | -5.68 | 100.12 | 105.80 |
| 34 | i | 597 | U | C3'-C2'-C1' | 5.68 | 106.04 | 101.50 |
| 34 | i | 1821 | U | O4'-C1'-N1 | 5.68 | 112.75 | 108.20 |
| 8 | H | 111 | LYS | CA-CB-CG | 5.68 | 125.89 | 113.40 |
| 34 | i | 1407 | G | C3'-C2'-C1' | -5.67 | 96.96 | 101.50 |
| 11 | K | 42 | ASN | N-CA-C | -5.67 | 95.69 | 111.00 |
| 34 | i | 340 | C | C1'-O4'-C4' | 5.67 | 114.44 | 109.90 |
| 34 | i | 820 | C | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 34 | i | 1144 | A | C3'-C2'-C1' | -5.67 | 96.97 | 101.50 |
| 31 | e | 100 | LYS | N-CA-C | -5.66 | 95.72 | 111.00 |
| 34 | i | 1323 | G | C1'-O4'-C4' | -5.66 | 105.37 | 109.90 |
| 34 | i | 1826 | A | P-O5'-C5' | 5.66 | 129.96 | 120.90 |
| 34 | i | 818 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 12 | L | 98 | LYS | N-CA-C | -5.66 | 95.73 | 111.00 |
| 34 | i | 1646 | A | O4'-C1'-C2' | -5.66 | 100.14 | 105.80 |
| 34 | i | 1781 | G | C3'-C2'-C1' | -5.66 | 96.97 | 101.50 |
| 34 | i | 1467 | C | O4'-C1'-C2' | -5.65 | 100.15 | 105.80 |
| 34 | i | 1608 | G | C3'-C2'-C1' | -5.65 | 96.98 | 101.50 |
| 34 | i | 927 | C | C5'-C4'-O4' | 5.65 | 115.88 | 109.10 |
| 34 | i | 1753 | G | C3'-C2'-C1' | -5.65 | 96.98 | 101.50 |
| 34 | i | 741 | C | C5'-C4'-C3' | 5.64 | 125.03 | 116.00 |
| 34 | i | 1515 | G | C5'-C4'-C3' | 5.64 | 125.03 | 116.00 |
| 34 | i | 597 | U | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1174 | U | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 34 | i | 397 | G | P-O3'-C3' | 5.64 | 126.47 | 119.70 |
| 34 | i | 1518 | C | P-O5'-C5' | -5.64 | 111.88 | 120.90 |
| 34 | i | 1589 | A | C5'-C4'-C3' | 5.63 | 125.01 | 116.00 |
| 34 | i | 225 | C | C2'-C3'-O3' | 5.63 | 122.71 | 113.70 |
| 34 | i | 1705 | C | O4'-C1'-C2' | -5.63 | 100.17 | 105.80 |
| 34 | i | 789 | G | C4'-C3'-C2' | -5.63 | 96.97 | 102.60 |
| 34 | i | 1181 | C | C3'-C2'-C1' | 5.63 | 106.00 | 101.50 |
| 34 | i | 374 | U | C1'-O4'-C4' | -5.62 | 105.40 | 109.90 |
| 34 | i | 1018 | U | C1'-O4'-C4' | -5.62 | 105.40 | 109.90 |
| 20 | T | 45 | LEU | O-C-N | -5.62 | 113.70 | 122.70 |
| 24 | X | 58 | GLU | N-CA-C | 5.62 | 126.18 | 111.00 |
| 21 | U | 70 | CYS | CA-C-N | 5.62 | 127.44 | 116.20 |
| 34 | i | 341 | G | C4'-C3'-C2' | -5.62 | 96.98 | 102.60 |
| 34 | i | 1219 | A | C3'-C2'-C1' | 5.62 | 105.99 | 101.50 |
| 34 | i | 1390 | G | N9-C1'-C2' | 5.62 | 121.30 | 114.00 |
| 34 | i | 1044 | G | P-O5'-C5' | 5.62 | 129.89 | 120.90 |
| 19 | S | 10 | GLN | N-CA-C | 5.62 | 126.16 | 111.00 |
| 34 | i | 1413 | C | C5'-C4'-C3' | 5.62 | 124.99 | 116.00 |
| 34 | i | 1542 | C | N1-C1'-C2' | 5.62 | 121.30 | 114.00 |
| 34 | i | 278 | U | C3'-C2'-C1' | 5.61 | 105.99 | 101.50 |
| 8 | H | 105 | THR | CB-CA-C | 5.61 | 126.75 | 111.60 |
| 34 | i | 1423 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 34 | i | 1460 | C | C3'-C2'-C1' | 5.61 | 105.99 | 101.50 |
| 34 | i | 819 | U | O4'-C1'-C2' | 5.61 | 112.65 | 107.60 |
| 34 | i | 3 | C | C1'-O4'-C4' | 5.61 | 114.39 | 109.90 |
| 34 | i | 323 | G | C1'-O4'-C4' | -5.61 | 105.41 | 109.90 |
| 34 | i | 346 | C | O4'-C1'-C2' | 5.61 | 112.65 | 107.60 |
| 34 | i | 434 | G | C3'-C2'-C1' | -5.61 | 97.01 | 101.50 |
| 34 | i | 619 | A | C1'-O4'-C4' | 5.61 | 114.39 | 109.90 |
| 34 | i | 1411 | C | O4'-C1'-C2' | -5.61 | 100.19 | 105.80 |
| 34 | i | 1817 | A | C5'-C4'-O4' | -5.61 | 102.37 | 109.10 |
| 34 | i | 86 | C | O4'-C1'-N1 | 5.61 | 112.68 | 108.20 |
| 34 | i | 151 | C | C3'-C2'-C1' | 5.61 | 105.98 | 101.50 |
| 34 | i | 235 | C | O4'-C1'-C2' | -5.61 | 100.19 | 105.80 |
| 34 | i | 1561 | G | N9-C1'-C2' | -5.61 | 105.83 | 112.00 |
| 27 | a | 70 | LYS | CD-CE-NZ | 5.60 | 124.59 | 111.70 |
| 34 | i | 1819 | A | C2'-C3'-O3' | 5.60 | 122.67 | 113.70 |
| 34 | i | 176 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 34 | i | 667 | G | C1'-O4'-C4' | -5.60 | 105.42 | 109.90 |
| 34 | i | 817 | G | C2'-C3'-O3' | 5.60 | 122.66 | 113.70 |
| 34 | i | 874 | G | C1'-O4'-C4' | -5.60 | 105.42 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1160 | G | N9-C1'-C2' | 5.60 | 121.28 | 114.00 |
| 34 | i | 1407 | G | O4'-C1'-C2' | 5.60 | 112.64 | 107.60 |
| 34 | i | 1448 | A | O4'-C1'-C2' | -5.60 | 100.20 | 105.80 |
| 34 | i | 143 | U | C1'-O4'-C4' | -5.60 | 105.42 | 109.90 |
| 34 | i | 742 | C | C4'-C3'-C2' | -5.60 | 97.00 | 102.60 |
| 34 | i | 1439 | C | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 21 | U | 68 | THR | CB-CA-C | 5.60 | 126.71 | 111.60 |
| 34 | i | 93 | U | N1-C1'-C2' | -5.60 | 105.84 | 112.00 |
| 34 | i | 1220 | G | N9-C1'-C2' | 5.60 | 121.28 | 114.00 |
| 34 | i | 1037 | G | C3'-C2'-C1' | -5.59 | 97.03 | 101.50 |
| 34 | i | 1639 | C | C1'-O4'-C4' | -5.59 | 105.42 | 109.90 |
| 16 | P | 53 | GLN | CB-CA-C | 5.59 | 121.58 | 110.40 |
| 34 | i | 1587 | C | C3'-C2'-C1' | 5.59 | 105.97 | 101.50 |
| 32 | f | 125 | GLU | CB-CA-C | 5.59 | 121.58 | 110.40 |
| 33 | g | 294 | ASP | N-CA-CB | -5.59 | 100.54 | 110.60 |
| 34 | i | 1152 | U | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 34 | i | 1409 | G | P-O3'-C3' | -5.59 | 112.99 | 119.70 |
| 34 | i | 1042 | U | O4'-C1'-C2' | -5.58 | 100.22 | 105.80 |
| 34 | i | 1471 | G | C4'-C3'-C2' | -5.58 | 97.02 | 102.60 |
| 34 | i | 224 | U | P-O5'-C5' | 5.58 | 129.83 | 120.90 |
| 34 | i | 648 | U | O4'-C1'-N1 | 5.58 | 112.66 | 108.20 |
| 34 | i | 804 | A | N9-C1'-C2' | 5.58 | 121.25 | 114.00 |
| 34 | i | 1672 | U | C1'-O4'-C4' | 5.58 | 114.36 | 109.90 |
| 34 | i | 91 | A | C1'-O4'-C4' | 5.58 | 114.36 | 109.90 |
| 34 | i | 49 | C | C1'-O4'-C4' | -5.58 | 105.44 | 109.90 |
| 34 | i | 125 | C | C4'-C3'-O3' | 5.57 | 124.15 | 113.00 |
| 34 | i | 225 | C | C1'-O4'-C4' | -5.57 | 105.44 | 109.90 |
| 34 | i | 1587 | C | N1-C1'-C2' | 5.57 | 121.25 | 114.00 |
| 34 | i | 1361 | G | P-O3'-C3' | -5.57 | 113.01 | 119.70 |
| 34 | i | 230 | C | O4'-C1'-C2' | -5.57 | 100.23 | 105.80 |
| 34 | i | 508 | G | O4'-C1'-N9 | 5.57 | 112.66 | 108.20 |
| 34 | i | 1079 | A | C3'-C2'-C1' | 5.57 | 105.96 | 101.50 |
| 24 | X | 37 | LYS | N-CA-C | 5.57 | 126.04 | 111.00 |
| 33 | g | 143 | GLN | N-CA-C | -5.57 | 95.96 | 111.00 |
| 34 | i | 314 | U | O4'-C1'-C2' | 5.57 | 112.61 | 107.60 |
| 34 | i | 549 | G | C3'-C2'-C1' | -5.57 | 97.05 | 101.50 |
| 34 | i | 1078 | A | C3'-C2'-C1' | 5.57 | 105.95 | 101.50 |
| 34 | i | 1411 | C | C3'-C2'-C1' | 5.57 | 105.95 | 101.50 |
| 34 | i | 1618 | A | N9-C1'-C2' | -5.57 | 105.88 | 112.00 |
| 34 | i | 539 | C | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 34 | i | 656 | U | C3'-C2'-C1' | 5.57 | 105.95 | 101.50 |
| 34 | i | 1283 | A | N9-C1'-C2' | -5.57 | 105.88 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 1557 | C | C3'-C2'-C1' | 5.57 | 105.95 | 101.50 |
| 9 | I | 105 | ASP | CB-CA-C | 5.56 | 121.53 | 110.40 |
| 34 | i | 1198 | U | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 34 | i | 1661 | C | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 29 | c | 60 | GLU | N-CA-C | -5.56 | 95.98 | 111.00 |
| 34 | i | 226 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 1 | A | 159 | ILE | CA-CB-CG1 | -5.56 | 100.44 | 111.00 |
| 32 | f | 148 | TYR | C-N-CA | 5.56 | 135.59 | 121.70 |
| 34 | i | 658 | A | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 34 | i | 996 | C | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 34 | i | 1070 | C | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 34 | i | 1692 | A | N9-C1'-C2' | -5.56 | 105.89 | 112.00 |
| 4 | D | 142 | LEU | CB-CG-CD1 | 5.55 | 120.44 | 111.00 |
| 34 | i | 1143 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 34 | i | 1246 | A | C1'-O4'-C4' | 5.55 | 114.34 | 109.90 |
| 34 | i | 1538 | U | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 34 | i | 987 | G | C3'-C2'-C1' | -5.55 | 97.06 | 101.50 |
| 34 | i | 1240 | U | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 34 | i | 1639 | C | C3'-C2'-C1' | 5.55 | 105.94 | 101.50 |
| 34 | i | 1708 | C | N1-C1'-C2' | 5.55 | 121.21 | 114.00 |
| 34 | i | 1814 | G | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 34 | i | 676 | U | P-O3'-C3' | -5.54 | 113.05 | 119.70 |
| 34 | i | 994 | A | O4'-C1'-C2' | -5.54 | 100.26 | 105.80 |
| 34 | i | 1432 | C | O4'-C1'-C2' | -5.54 | 100.26 | 105.80 |
| 17 | Q | 6 | PRO | CB-CA-C | -5.54 | 98.16 | 112.00 |
| 34 | i | 286 | C | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 34 | i | 1063 | C | C1'-O4'-C4' | -5.54 | 105.47 | 109.90 |
| 17 | Q | 145 | TYR | C-N-CA | 5.54 | 135.54 | 121.70 |
| 34 | i | 40 | A | N9-C1'-C2' | -5.54 | 105.91 | 112.00 |
| 34 | i | 308 | C | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 34 | i | 1274 | A | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 34 | i | 1854 | A | P-O3'-C3' | -5.54 | 113.06 | 119.70 |
| 34 | i | 58 | C | C1'-O4'-C4' | 5.53 | 114.33 | 109.90 |
| 34 | i | 329 | A | P-O3'-C3' | -5.53 | 113.06 | 119.70 |
| 34 | i | 398 | A | O4'-C1'-C2' | -5.53 | 100.27 | 105.80 |
| 34 | i | 1343 | U | O4'-C1'-N1 | 5.53 | 112.63 | 108.20 |
| 9 | I | 5 | ARG | CA-C-N | 5.53 | 129.36 | 117.20 |
| 34 | i | 116 | U | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 34 | i | 805 | A | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 34 | i | 1259 | U | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 34 | i | 1638 | U | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 34 | i | 13 | C | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 949 | C | P-O3'-C3' | -5.52 | 113.07 | 119.70 |
| 34 | i | 964 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 6 | F | 47 | LYS | CD-CE-NZ | -5.52 | 99.00 | 111.70 |
| 34 | i | 388 | A | C1'-O4'-C4' | 5.52 | 114.31 | 109.90 |
| 34 | i | 675 | A | O4'-C1'-N9 | 5.52 | 112.61 | 108.20 |
| 34 | i | 38 | A | C5'-C4'-C3' | -5.51 | 107.18 | 116.00 |
| 34 | i | 376 | C | P-O5'-C5' | -5.51 | 112.08 | 120.90 |
| 16 | P | 36 | LEU | C-N-CA | 5.51 | 135.48 | 121.70 |
| 34 | i | 1795 | A | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 34 | i | 489 | G | P-O5'-C5' | -5.51 | 112.08 | 120.90 |
| 34 | i | 536 | G | O4'-C1'-C2' | -5.51 | 100.29 | 105.80 |
| 34 | i | 642 | U | C1'-O4'-C4' | 5.51 | 114.31 | 109.90 |
| 22 | V | 67 | ASP | N-CA-CB | -5.50 | 100.69 | 110.60 |
| 34 | i | 522 | C | C4'-C3'-C2' | -5.50 | 97.09 | 102.60 |
| 4 | D | 3 | VAL | C-N-CA | 5.50 | 135.46 | 121.70 |
| 15 | O | 103 | ASN | N-CA-CB | 5.50 | 120.51 | 110.60 |
| 34 | i | 282 | G | C1'-O4'-C4' | -5.50 | 105.50 | 109.90 |
| 34 | i | 1370 | C | N1-C1'-C2' | 5.50 | 121.15 | 114.00 |
| 34 | i | 1837 | G | P-O3'-C3' | -5.50 | 113.10 | 119.70 |
| 16 | P | 130 | ARG | NE-CZ-NH2 | -5.50 | 117.55 | 120.30 |
| 34 | i | 462 | C | P-O3'-C3' | 5.50 | 126.30 | 119.70 |
| 34 | i | 1123 | C | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 34 | i | 503 | G | C1'-O4'-C4' | -5.50 | 105.50 | 109.90 |
| 34 | i | 241 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 34 | i | 516 | A | C5'-C4'-C3' | 5.49 | 124.79 | 116.00 |
| 34 | i | 1106 | G | O4'-C1'-C2' | -5.49 | 100.31 | 105.80 |
| 34 | i | 350 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 34 | i | 1280 | A | C5'-C4'-O4' | 5.49 | 115.69 | 109.10 |
| 34 | i | 400 | G | N9-C1'-C2' | -5.49 | 105.97 | 112.00 |
| 34 | i | 459 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 34 | i | 1382 | A | O4'-C1'-C2' | -5.49 | 100.31 | 105.80 |
| 34 | i | 1013 | U | O4'-C1'-C2' | -5.48 | 100.32 | 105.80 |
| 18 | R | 89 | SER | CA-C-O | -5.48 | 108.59 | 120.10 |
| 34 | i | 919 | G | O4'-C1'-N9 | 5.48 | 112.59 | 108.20 |
| 34 | i | 1705 | C | O4'-C1'-N1 | 5.48 | 112.59 | 108.20 |
| 34 | i | 469 | C | C3'-C2'-C1' | 5.48 | 105.88 | 101.50 |
| 34 | i | 1035 | C | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 34 | i | 1191 | A | N9-C1'-C2' | -5.48 | 105.97 | 112.00 |
| 34 | i | 614 | C | C5'-C4'-C3' | -5.48 | 107.23 | 116.00 |
| 34 | i | 1271 | G | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 34 | i | 1691 | C | C3'-C2'-C1' | 5.48 | 105.88 | 101.50 |
| 4 | D | 167 | TYR | CA-CB-CG | -5.48 | 103.00 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 101 | U | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 34 | i | 391 | A | C3'-C2'-C1' | 5.47 | 105.88 | 101.50 |
| 34 | i | 80 | G | O4'-C1'-N9 | 5.47 | 112.58 | 108.20 |
| 34 | i | 355 | C | C3'-C2'-C1' | 5.47 | 105.88 | 101.50 |
| 34 | i | 456 | G | C3'-C2'-C1' | -5.47 | 97.12 | 101.50 |
| 34 | i | 1221 | U | O4'-C1'-N1 | 5.47 | 112.58 | 108.20 |
| 34 | i | 1344 | G | P-O3'-C3' | 5.47 | 126.27 | 119.70 |
| 34 | i | 560 | C | C5'-C4'-O4' | 5.47 | 115.66 | 109.10 |
| 34 | i | 822 | A | P-O3'-C3' | -5.47 | 113.14 | 119.70 |
| 34 | i | 564 | A | N9-C1'-C2' | 5.47 | 121.11 | 114.00 |
| 34 | i | 889 | U | C1'-O4'-C4' | 5.47 | 114.27 | 109.90 |
| 34 | i | 1556 | A | O4'-C1'-C2' | -5.47 | 100.33 | 105.80 |
| 34 | i | 15 | U | O4'-C1'-C2' | -5.46 | 100.33 | 105.80 |
| 34 | i | 1716 | U | O3'-P-O5' | 5.46 | 114.38 | 104.00 |
| 34 | i | 859 | U | O4'-C1'-C2' | 5.46 | 112.52 | 107.60 |
| 34 | i | 440 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 3 | C | 241 | TRP | O-C-N | -5.46 | 113.97 | 122.70 |
| 34 | i | 71 | G | C4'-C3'-O3' | 5.46 | 123.91 | 113.00 |
| 34 | i | 1595 | G | P-O3'-C3' | -5.46 | 113.15 | 119.70 |
| 19 | S | 89 | ASP | CB-CA-C | -5.45 | 99.49 | 110.40 |
| 34 | i | 929 | G | C3'-C2'-C1' | -5.45 | 97.14 | 101.50 |
| 34 | i | 396 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 34 | i | 586 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 34 | i | 57 | U | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 34 | i | 292 | A | O4'-C1'-C2' | -5.45 | 100.35 | 105.80 |
| 34 | i | 790 | A | O4'-C1'-C2' | -5.45 | 100.35 | 105.80 |
| 34 | i | 606 | A | C1'-O4'-C4' | -5.45 | 105.54 | 109.90 |
| 34 | i | 540 | C | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 34 | i | 1823 | G | O4'-C1'-C2' | -5.45 | 100.35 | 105.80 |
| 34 | i | 509 | A | C1'-O4'-C4' | 5.44 | 114.25 | 109.90 |
| 34 | i | 640 | A | O4'-C1'-C2' | -5.44 | 100.36 | 105.80 |
| 34 | i | 1848 | U | N1-C1'-C2' | -5.44 | 106.01 | 112.00 |
| 17 | Q | 18 | THR | C-N-CA | 5.44 | 135.30 | 121.70 |
| 34 | i | 1279 | C | C1'-O4'-C4' | -5.44 | 105.55 | 109.90 |
| 34 | i | 882 | A | O3'-P-O5' | 5.44 | 114.33 | 104.00 |
| 9 | I | 55 | TYR | CB-CG-CD2 | -5.44 | 117.74 | 121.00 |
| 34 | i | 396 | U | N1-C1'-C2' | 5.44 | 121.07 | 114.00 |
| 34 | i | 1458 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 34 | i | 1740 | A | C3'-C2'-C1' | -5.44 | 97.15 | 101.50 |
| 19 | S | 81 | ASP | CB-CG-OD2 | 5.43 | 123.19 | 118.30 |
| 34 | i | 101 | U | O4'-C1'-C2' | -5.43 | 100.36 | 105.80 |
| 34 | i | 911 | G | O4'-C1'-C2' | 5.43 | 112.49 | 107.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 536 | G | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 1 | A | 205 | ARG | NE-CZ-NH1 | 5.43 | 123.01 | 120.30 |
| 34 | i | 560 | C | N1-C1'-C2' | 5.42 | 121.05 | 114.00 |
| 34 | i | 1053 | C | P-O3'-C3' | -5.42 | 113.19 | 119.70 |
| 34 | i | 1528 | A | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 2 | B | 63 | LYS | N-CA-C | 5.42 | 125.64 | 111.00 |
| 10 | J | 100 | LEU | N-CA-C | 5.42 | 125.64 | 111.00 |
| 34 | i | 378 | U | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 34 | i | 462 | C | C3'-C2'-C1' | 5.42 | 105.83 | 101.50 |
| 34 | i | 682 | G | C1'-O4'-C4' | -5.42 | 105.56 | 109.90 |
| 34 | i | 1166 | A | C3'-C2'-C1' | -5.42 | 97.17 | 101.50 |
| 34 | i | 218 | A | C3'-C2'-C1' | -5.42 | 97.17 | 101.50 |
| 34 | i | 67 | C | N1-C1'-C2' | -5.42 | 106.04 | 112.00 |
| 34 | i | 1227 | C | C1'-O4'-C4' | -5.42 | 105.57 | 109.90 |
| 34 | i | 404 | A | O4'-C1'-C2' | -5.41 | 100.39 | 105.80 |
| 34 | i | 868 | A | O4'-C1'-C2' | 5.41 | 112.47 | 107.60 |
| 34 | i | 1625 | A | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 34 | i | 1819 | A | C5'-C4'-O4' | 5.41 | 115.60 | 109.10 |
| 21 | U | 118 | ASP | N-CA-C | -5.41 | 96.39 | 111.00 |
| 34 | i | 1058 | A | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 34 | i | 1164 | G | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 1 | A | 14 | ASP | CB-CG-OD2 | 5.41 | 123.17 | 118.30 |
| 29 | c | 36 | ASP | CB-CG-OD2 | 5.41 | 123.17 | 118.30 |
| 34 | i | 1165 | G | C1'-O4'-C4' | -5.41 | 105.57 | 109.90 |
| 34 | i | 1374 | A | O4'-C1'-C2' | -5.41 | 100.39 | 105.80 |
| 34 | i | 1618 | A | C1'-O4'-C4' | 5.41 | 114.23 | 109.90 |
| 8 | H | 16 | PRO | CA-N-CD | -5.41 | 103.93 | 111.50 |
| 34 | i | 870 | G | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 34 | i | 1027 | A | C5'-C4'-O4' | 5.40 | 115.58 | 109.10 |
| 9 | I | 132 | GLU | CA-C-O | -5.40 | 108.76 | 120.10 |
| 23 | W | 54 | ASP | CB-CG-OD2 | 5.40 | 123.16 | 118.30 |
| 29 | c | 54 | ASP | CB-CG-OD2 | 5.40 | 123.16 | 118.30 |
| 34 | i | 1127 | G | O4'-C1'-C2' | -5.40 | 100.40 | 105.80 |
| 34 | i | 852 | C | C1'-O4'-C4' | -5.39 | 105.58 | 109.90 |
| 34 | i | 1122 | G | O4'-C1'-N9 | 5.39 | 112.52 | 108.20 |
| 34 | i | 1384 | A | P-O3'-C3' | -5.39 | 113.23 | 119.70 |
| 34 | i | 1608 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 10 | J | 35 | TYR | C-N-CA | 5.39 | 133.62 | 122.30 |
| 34 | i | 613 | G | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 34 | i | 1424 | G | C3'-C2'-C1' | -5.39 | 97.19 | 101.50 |
| 15 | O | 39 | ASP | CB-CG-OD2 | 5.39 | 123.15 | 118.30 |
| 34 | i | 25 | A | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | V | 28 | ASP | CB-CG-OD2 | 5.39 | 123.15 | 118.30 |
| 22 | V | 82 | ASN | CB-CA-C | -5.39 | 99.63 | 110.40 |
| 34 | i | 188 | U | P-O3'-C3' | -5.39 | 113.24 | 119.70 |
| 34 | i | 550 | A | O5'-C5'-C4' | 5.39 | 121.93 | 111.70 |
| 34 | i | 1437 | U | C1'-O4'-C4' | 5.39 | 114.21 | 109.90 |
| 34 | i | 918 | A | N9-C1'-C2' | -5.38 | 106.08 | 112.00 |
| 34 | i | 1003 | C | O4'-C1'-C2' | -5.38 | 100.42 | 105.80 |
| 25 | Y | 62 | THR | C-N-CA | -5.38 | 108.24 | 121.70 |
| 34 | i | 1356 | U | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 6 | F | 21 | GLY | N-CA-C | -5.38 | 99.65 | 113.10 |
| 34 | i | 297 | C | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 34 | i | 427 | G | N9-C1'-C2' | 5.38 | 120.99 | 114.00 |
| 34 | i | 1341 | G | O4'-C1'-C2' | -5.38 | 100.42 | 105.80 |
| 34 | i | 1851 | G | O4'-C1'-C2' | 5.38 | 112.44 | 107.60 |
| 11 | K | 98 | ARG | CA-C-O | -5.38 | 108.81 | 120.10 |
| 34 | i | 139 | C | O4'-C1'-N1 | 5.38 | 112.50 | 108.20 |
| 34 | i | 276 | U | P-O5'-C5' | -5.38 | 112.30 | 120.90 |
| 2 | B | 108 | ASP | CB-CG-OD2 | 5.37 | 123.14 | 118.30 |
| 34 | i | 375 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 16 | P | 71 | GLU | CA-C-N | -5.37 | 105.38 | 117.20 |
| 34 | i | 502 | A | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 33 | g | 14 | HIS | C-N-CA | -5.37 | 108.28 | 121.70 |
| 34 | i | 462 | C | N1-C1'-C2' | 5.37 | 120.98 | 114.00 |
| 34 | i | 1208 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 34 | i | 1491 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 34 | i | 69 | C | O4'-C1'-N1 | 5.37 | 112.49 | 108.20 |
| 3 | C | 216 | ALA | O-C-N | -5.37 | 114.11 | 122.70 |
| 34 | i | 94 | G | N9-C1'-C2' | 5.37 | 120.97 | 114.00 |
| 34 | i | 1370 | C | O4'-C1'-N1 | 5.37 | 112.49 | 108.20 |
| 34 | i | 461 | G | N9-C1'-C2' | -5.36 | 106.10 | 112.00 |
| 34 | i | 1823 | G | C5'-C4'-O4' | 5.36 | 115.54 | 109.10 |
| 11 | K | 43 | LEU | CB-CG-CD1 | 5.36 | 120.11 | 111.00 |
| 34 | i | 139 | C | C3'-C2'-C1' | 5.36 | 105.79 | 101.50 |
| 34 | i | 229 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 34 | i | 1318 | G | C1'-O4'-C4' | 5.36 | 114.19 | 109.90 |
| 34 | i | 1739 | G | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 34 | i | 146 | G | O4'-C1'-C2' | -5.36 | 100.44 | 105.80 |
| 34 | i | 346 | C | C3'-C2'-C1' | -5.36 | 97.22 | 101.50 |
| 34 | i | 1201 | C | O4'-C1'-N1 | 5.36 | 112.48 | 108.20 |
| 34 | i | 906 | G | O5'-P-OP1 | -5.35 | 100.88 | 105.70 |
| 34 | i | 1357 | G | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 31 | e | 95 | LYS | C-N-CA | 5.35 | 135.08 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 76 | U | N1-C1'-C2' | 5.35 | 120.96 | 114.00 |
| 34 | i | 1037 | G | N9-C1'-C2' | 5.35 | 120.96 | 114.00 |
| 34 | i | 727 | G | N9-C1'-C2' | 5.35 | 120.96 | 114.00 |
| 14 | N | 151 | ALA | CA-C-O | -5.35 | 108.86 | 120.10 |
| 34 | i | 235 | C | N1-C1'-C2' | 5.35 | 120.95 | 114.00 |
| 15 | O | 129 | ILE | CG1-CB-CG2 | 5.35 | 123.16 | 111.40 |
| 34 | i | 437 | A | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 34 | i | 109 | U | C2'-C3'-O3' | 5.34 | 122.25 | 113.70 |
| 34 | i | 685 | G | C1'-O4'-C4' | 5.34 | 114.17 | 109.90 |
| 1 | A | 53 | ARG | CD-NE-CZ | -5.34 | 116.12 | 123.60 |
| 24 | X | 142 | ARG | CA-C-O | -5.34 | 108.88 | 120.10 |
| 34 | i | 102 | A | C1'-O4'-C4' | -5.34 | 105.63 | 109.90 |
| 34 | i | 1313 | U | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 10 | J | 104 | ASP | CB-CG-OD2 | 5.34 | 123.11 | 118.30 |
| 14 | N | 6 | ALA | C-N-CD | 5.34 | 139.61 | 128.40 |
| 34 | i | 443 | C | N1-C1'-C2' | 5.34 | 120.94 | 114.00 |
| 34 | i | 988 | A | C1'-O4'-C4' | -5.34 | 105.63 | 109.90 |
| 34 | i | 1129 | A | O5'-C5'-C4' | -5.34 | 101.56 | 111.70 |
| 34 | i | 1300 | U | N1-C1'-C2' | 5.34 | 120.94 | 114.00 |
| 34 | i | 1717 | G | C5'-C4'-C3' | -5.34 | 107.46 | 116.00 |
| 8 | H | 16 | PRO | C-N-CA | 5.34 | 135.04 | 121.70 |
| 34 | i | 370 | G | C1'-O4'-C4' | 5.34 | 114.17 | 109.90 |
| 7 | G | 170 | ARG | CA-C-N | -5.34 | 105.46 | 117.20 |
| 34 | i | 820 | C | N1-C1'-C2' | 5.34 | 120.94 | 114.00 |
| 34 | i | 1846 | C | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 34 | i | 1150 | U | C4'-C3'-C2' | -5.33 | 97.27 | 102.60 |
| 34 | i | 1535 | G | P-O5'-C5' | -5.33 | 112.36 | 120.90 |
| 34 | i | 1158 | C | O4'-C1'-C2' | -5.33 | 100.47 | 105.80 |
| 34 | i | 1667 | U | C1'-O4'-C4' | -5.33 | 105.63 | 109.90 |
| 34 | i | 1703 | C | C3'-C2'-C1' | 5.33 | 105.77 | 101.50 |
| 34 | i | 1832 | U | O4'-C1'-N1 | 5.33 | 112.47 | 108.20 |
| 18 | R | 101 | ASP | CB-CG-OD2 | 5.33 | 123.10 | 118.30 |
| 34 | i | 1229 | G | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 34 | i | 1255 | A | C5'-C4'-O4' | 5.33 | 115.50 | 109.10 |
| 34 | i | 1301 | C | N1-C1'-C2' | 5.33 | 120.93 | 114.00 |
| 3 | C | 233 | TYR | CA-CB-CG | -5.33 | 103.28 | 113.40 |
| 34 | i | 835 | C | O3'-P-O5' | -5.33 | 93.88 | 104.00 |
| 34 | i | 1018 | U | P-O3'-C3' | 5.33 | 126.09 | 119.70 |
| 34 | i | 1635 | A | C3'-C2'-C1' | 5.33 | 105.76 | 101.50 |
| 34 | i | 313 | C | C2'-C3'-O3' | 5.33 | 122.22 | 113.70 |
| 34 | i | 795 | U | C4'-C3'-C2' | -5.33 | 97.27 | 102.60 |
| 34 | i | 1024 | A | C4'-C3'-O3' | -5.33 | 98.22 | 109.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3 | C | 244 | THR | N-CA-C | 5.32 | 125.37 | 111.00 |
| 24 | X | 88 | ASP | CB-CG-OD2 | 5.32 | 123.09 | 118.30 |
| 4 | D | 227 | LYS | CA-C-O | -5.32 | 108.93 | 120.10 |
| 6 | F | 46 | ALA | O-C-N | -5.32 | 114.19 | 122.70 |
| 1 | A | 209 | GLU | CA-C-O | -5.32 | 108.93 | 120.10 |
| 4 | D | 193 | ASP | C-N-CA | -5.32 | 99.67 | 122.00 |
| 34 | i | 33 | G | C5'-C4'-O4' | 5.32 | 115.48 | 109.10 |
| 34 | i | 332 | C | O4'-C1'-C2' | -5.32 | 100.48 | 105.80 |
| 34 | i | 729 | C | C4'-C3'-C2' | -5.32 | 97.28 | 102.60 |
| 34 | i | 1110 | U | O4'-C1'-C2' | -5.32 | 100.48 | 105.80 |
| 34 | i | 1479 | A | C4'-C3'-C2' | -5.32 | 97.28 | 102.60 |
| 34 | i | 1557 | C | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 25 | Y | 53 | ASP | CB-CG-OD2 | 5.32 | 123.08 | 118.30 |
| 34 | i | 1607 | G | C3'-C2'-C1' | -5.32 | 97.25 | 101.50 |
| 22 | V | 24 | ILE | CB-CA-C | -5.31 | 100.97 | 111.60 |
| 34 | i | 1267 | C | N1-C1'-C2' | 5.31 | 120.91 | 114.00 |
| 3 | C | 263 | THR | CA-C-O | -5.31 | 108.95 | 120.10 |
| 34 | i | 103 | A | P-O3'-C3' | 5.31 | 126.07 | 119.70 |
| 23 | W | 130 | PHE | CA-C-O | -5.31 | 108.96 | 120.10 |
| 34 | i | 66 | G | O4'-C1'-C2' | 5.31 | 112.38 | 107.60 |
| 34 | i | 901 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 34 | i | 1737 | C | N1-C1'-C2' | 5.31 | 120.90 | 114.00 |
| 34 | i | 1602 | A | C1'-O4'-C4' | -5.31 | 105.66 | 109.90 |
| 34 | i | 1833 | U | C5'-C4'-O4' | 5.31 | 115.47 | 109.10 |
| 10 | J | 95 | ASP | CB-CG-OD2 | 5.30 | 123.07 | 118.30 |
| 34 | i | 1234 | U | C3'-C2'-C1' | -5.30 | 97.26 | 101.50 |
| 34 | i | 1423 | C | C3'-C2'-C1' | 5.30 | 105.74 | 101.50 |
| 17 | Q | 110 | ASP | CB-CG-OD2 | 5.30 | 123.07 | 118.30 |
| 34 | i | 540 | C | O4'-C1'-C2' | -5.30 | 100.50 | 105.80 |
| 34 | i | 1256 | A | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 34 | i | 1624 | C | O4'-C4'-C3' | -5.30 | 98.70 | 104.00 |
| 34 | i | 911 | G | C3'-C2'-C1' | -5.30 | 97.26 | 101.50 |
| 34 | i | 1683 | C | C5'-C4'-O4' | 5.30 | 115.46 | 109.10 |
| 7 | G | 39 | ASP | CB-CG-OD2 | 5.30 | 123.07 | 118.30 |
| 34 | i | 65 | C | O4'-C1'-C2' | -5.30 | 100.50 | 105.80 |
| 34 | i | 960 | A | O4'-C1'-C2' | -5.30 | 100.50 | 105.80 |
| 5 | E | 88 | ASP | CB-CG-OD2 | 5.30 | 123.07 | 118.30 |
| 14 | N | 87 | ASP | CB-CG-OD2 | 5.29 | 123.06 | 118.30 |
| 34 | i | 1807 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 1 | A | 53 | ARG | N-CA-CB | -5.29 | 101.09 | 110.60 |
| 34 | i | 77 | A | C5'-C4'-C3' | 5.29 | 124.46 | 116.00 |
| 10 | J | 137 | VAL | C-N-CA | 5.28 | 134.91 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 994 | A | N9-C1'-C2' | -5.28 | 106.19 | 112.00 |
| 6 | F | 43 | GLU | N-CA-C | -5.28 | 96.74 | 111.00 |
| 8 | H | 118 | ARG | CB-CA-C | -5.28 | 99.84 | 110.40 |
| 30 | d | 56 | ASP | CA-C-O | -5.28 | 109.01 | 120.10 |
| 33 | g | 314 | ILE | CA-C-O | -5.28 | 109.01 | 120.10 |
| 34 | i | 516 | A | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 34 | i | 1486 | G | C1'-O4'-C4' | -5.28 | 105.67 | 109.90 |
| 5 | E | 59 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 27 | a | 52 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 29 | c | 68 | LEU | CA-C-O | -5.28 | 109.01 | 120.10 |
| 34 | i | 742 | C | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 34 | i | 1695 | C | N1-C1'-C2' | -5.28 | 106.19 | 112.00 |
| 18 | R | 94 | GLU | N-CA-C | -5.28 | 96.75 | 111.00 |
| 34 | i | 189 | G | O5'-C5'-C4' | 5.28 | 121.73 | 111.70 |
| 34 | i | 1539 | C | O4'-C1'-C2' | -5.28 | 100.52 | 105.80 |
| 34 | i | 1820 | G | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 34 | i | 1298 | G | C2'-C3'-O3' | -5.27 | 97.90 | 109.50 |
| 34 | i | 201 | G | C1'-O4'-C4' | 5.27 | 114.12 | 109.90 |
| 34 | i | 554 | A | N9-C1'-C2' | -5.27 | 106.20 | 112.00 |
| 34 | i | 84 | A | C5'-C4'-O4' | 5.27 | 115.42 | 109.10 |
| 34 | i | 109 | U | P-O3'-C3' | -5.27 | 113.38 | 119.70 |
| 28 | b | 52 | THR | O-C-N | 5.27 | 131.13 | 122.70 |
| 34 | i | 534 | G | O4'-C1'-C2' | -5.27 | 100.53 | 105.80 |
| 34 | i | 551 | A | C2'-C3'-O3' | 5.27 | 122.13 | 113.70 |
| 4 | D | 93 | THR | C-N-CA | 5.27 | 134.87 | 121.70 |
| 5 | E | 170 | THR | O-C-N | 5.27 | 131.13 | 122.70 |
| 15 | O | 80 | ASP | CB-CG-OD2 | 5.27 | 123.04 | 118.30 |
| 34 | i | 895 | U | P-O5'-C5' | 5.27 | 129.33 | 120.90 |
| 14 | N | 110 | ASP | CB-CG-OD2 | 5.26 | 123.04 | 118.30 |
| 34 | i | 84 | A | P-O5'-C5' | -5.26 | 112.48 | 120.90 |
| 34 | i | 209 | C | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |
| 34 | i | 378 | U | N1-C1'-C2' | 5.26 | 120.84 | 114.00 |
| 34 | i | 416 | A | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |
| 5 | E | 73 | ASP | CB-CG-OD2 | 5.26 | 123.04 | 118.30 |
| 8 | H | 56 | GLY | N-CA-C | 5.26 | 126.26 | 113.10 |
| 34 | i | 1209 | C | N1-C1'-C2' | 5.26 | 120.84 | 114.00 |
| 34 | i | 1408 | C | O5'-P-OP1 | 5.26 | 117.01 | 110.70 |
| 10 | J | 26 | ASP | CB-CG-OD2 | 5.26 | 123.03 | 118.30 |
| 12 | L | 158 | PHE | CA-C-O | -5.26 | 109.06 | 120.10 |
| 31 | e | 133 | SER | CA-C-O | -5.26 | 109.05 | 120.10 |
| 34 | i | 1397 | A | N9-C1'-C2' | -5.26 | 106.22 | 112.00 |
| 34 | i | 1695 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 655 | G | N9-C1'-C2' | 5.26 | 120.83 | 114.00 |
| 34 | i | 660 | A | C1'-O4'-C4' | 5.26 | 114.11 | 109.90 |
| 34 | i | 1036 | G | O4'-C1'-C2' | 5.26 | 112.33 | 107.60 |
| 34 | i | 516 | A | C1'-O4'-C4' | -5.25 | 105.70 | 109.90 |
| 10 | J | 124 | HIS | N-CA-C | -5.25 | 96.81 | 111.00 |
| 34 | i | 1280 | A | N9-C1'-C2' | 5.25 | 120.83 | 114.00 |
| 34 | i | 1473 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 10 | J | 91 | LYS | CA-C-N | 5.25 | 128.75 | 117.20 |
| 21 | U | 27 | ARG | O-C-N | -5.25 | 114.30 | 122.70 |
| 34 | i | 1094 | C | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 34 | i | 1283 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 9 | I | 191 | GLU | CB-CA-C | -5.25 | 99.90 | 110.40 |
| 34 | i | 459 | A | C1'-O4'-C4' | 5.25 | 114.10 | 109.90 |
| 34 | i | 1130 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 34 | i | 1419 | C | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 28 | b | 3 | LEU | CB-CG-CD2 | 5.25 | 119.92 | 111.00 |
| 34 | i | 1580 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 14 | N | 133 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 34 | i | 235 | C | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 34 | i | 1137 | G | O4'-C1'-C2' | 5.25 | 112.32 | 107.60 |
| 34 | i | 1473 | U | C1'-O4'-C4' | -5.25 | 105.70 | 109.90 |
| 34 | i | 306 | C | P-O5'-C5' | -5.25 | 112.51 | 120.90 |
| 34 | i | 458 | A | P-O5'-C5' | -5.25 | 112.51 | 120.90 |
| 34 | i | 1331 | G | N9-C1'-C2' | 5.24 | 120.82 | 114.00 |
| 34 | i | 165 | G | N9-C1'-C2' | -5.24 | 106.23 | 112.00 |
| 34 | i | 1130 | G | C5'-C4'-O4' | 5.24 | 115.39 | 109.10 |
| 34 | i | 1361 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 15 | O | 46 | ASP | CB-CG-OD2 | 5.24 | 123.02 | 118.30 |
| 34 | i | 895 | U | C3'-C2'-C1' | 5.24 | 105.69 | 101.50 |
| 23 | W | 80 | ASP | CB-CG-OD2 | 5.24 | 123.02 | 118.30 |
| 34 | i | 1051 | A | C1'-O4'-C4' | 5.24 | 114.09 | 109.90 |
| 34 | i | 1635 | A | N9-C1'-C2' | -5.24 | 106.24 | 112.00 |
| 34 | i | 382 | A | C5'-C4'-O4' | 5.24 | 115.38 | 109.10 |
| 5 | E | 104 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 28 | b | 84 | HIS | CA-C-O | -5.23 | 109.11 | 120.10 |
| 34 | i | 624 | A | C3'-C2'-C1' | 5.23 | 105.69 | 101.50 |
| 34 | i | 725 | C | C1'-O4'-C4' | 5.23 | 114.08 | 109.90 |
| 34 | i | 1262 | C | C1'-O4'-C4' | -5.23 | 105.72 | 109.90 |
| 34 | i | 1645 | A | O4'-C1'-C2' | -5.23 | 100.57 | 105.80 |
| 17 | Q | 67 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 18 | R | 25 | GLY | O-C-N | 5.23 | 131.07 | 122.70 |
| 28 | b | 34 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 621 | U | N1-C1'-C2' | 5.23 | 120.80 | 114.00 |
| 7 | G | 57 | ASP | CB-CG-OD2 | 5.23 | 123.00 | 118.30 |
| 34 | i | 923 | C | C3'-C2'-C1' | 5.23 | 105.68 | 101.50 |
| 34 | i | 1119 | C | O4'-C1'-N1 | 5.23 | 112.38 | 108.20 |
| 34 | i | 207 | U | N1-C1'-C2' | 5.22 | 120.79 | 114.00 |
| 8 | H | 194 | LEU | CA-C-O | -5.22 | 109.13 | 120.10 |
| 9 | I | 133 | GLU | CA-C-N | 5.22 | 128.69 | 117.20 |
| 24 | X | 138 | LYS | O-C-N | -5.22 | 114.34 | 122.70 |
| 34 | i | 1560 | C | O4'-C1'-N1 | 5.22 | 112.38 | 108.20 |
| 34 | i | 1645 | A | P-O5'-C5' | -5.22 | 112.55 | 120.90 |
| 34 | i | 88 | G | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 5 | E | 253 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |
| 34 | i | 1186 | A | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 34 | i | 107 | A | C1'-O4'-C4' | 5.22 | 114.08 | 109.90 |
| 13 | M | 132 | LYS | CA-C-O | -5.22 | 109.15 | 120.10 |
| 34 | i | 1161 | G | C5'-C4'-O4' | 5.22 | 115.36 | 109.10 |
| 34 | i | 178 | C | N1-C1'-C2' | 5.21 | 120.78 | 114.00 |
| 34 | i | 1416 | G | O4'-C1'-C2' | 5.21 | 112.29 | 107.60 |
| 12 | L | 18 | GLN | C-N-CA | -5.21 | 108.67 | 121.70 |
| 23 | W | 9 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 34 | i | 1455 | G | C3'-C2'-C1' | -5.21 | 97.33 | 101.50 |
| 34 | i | 906 | G | C3'-C2'-C1' | -5.21 | 97.33 | 101.50 |
| 34 | i | 1137 | G | P-O5'-C5' | 5.21 | 129.24 | 120.90 |
| 34 | i | 682 | G | O4'-C1'-C2' | 5.21 | 112.29 | 107.60 |
| 34 | i | 1340 | A | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 34 | i | 1348 | G | N9-C1'-C2' | 5.21 | 120.77 | 114.00 |
| 34 | i | 1513 | C | O4'-C4'-C3' | -5.21 | 98.79 | 104.00 |
| 19 | S | 104 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 25 | Y | 80 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 21 | U | 90 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 26 | Z | 52 | LYS | N-CA-C | -5.20 | 96.95 | 111.00 |
| 34 | i | 832 | G | N9-C1'-C2' | -5.20 | 106.28 | 112.00 |
| 6 | F | 204 | ARG | CA-C-O | -5.20 | 109.18 | 120.10 |
| 34 | i | 916 | A | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 34 | i | 1006 | G | N9-C1'-C2' | -5.20 | 106.28 | 112.00 |
| 34 | i | 1078 | A | O4'-C1'-C2' | -5.20 | 100.60 | 105.80 |
| 34 | i | 1482 | A | O5'-C5'-C4' | -5.20 | 101.82 | 111.70 |
| 15 | O | 131 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 34 | i | 370 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 2 | B | 104 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 24 | X | 114 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 34 | i | 317 | G | C5'-C4'-O4' | 5.20 | 115.33 | 109.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 516 | A | O4'-C1'-C2' | 5.20 | 112.28 | 107.60 |
| 34 | i | 1675 | G | C3'-C2'-C1' | 5.20 | 105.66 | 101.50 |
| 34 | i | 1688 | G | O4'-C1'-C2' | 5.20 | 112.28 | 107.60 |
| 34 | i | 599 | U | O4'-C1'-C2' | -5.19 | 100.61 | 105.80 |
| 34 | i | 984 | C | O4'-C1'-N1 | -5.19 | 104.05 | 108.20 |
| 34 | i | 1400 | U | C3'-C2'-C1' | 5.19 | 105.65 | 101.50 |
| 34 | i | 1658 | A | O4'-C1'-C2' | -5.19 | 100.61 | 105.80 |
| 1 | A | 126 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 34 | i | 125 | C | C5'-C4'-O4' | -5.19 | 102.87 | 109.10 |
| 34 | i | 652 | G | C3'-C2'-C1' | 5.19 | 105.65 | 101.50 |
| 34 | i | 78 | C | C1'-O4'-C4' | -5.19 | 105.75 | 109.90 |
| 14 | N | 32 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 23 | W | 55 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 34 | i | 530 | U | N1-C1'-C2' | -5.19 | 106.29 | 112.00 |
| 34 | i | 549 | G | O4'-C4'-C3' | -5.19 | 98.81 | 104.00 |
| 10 | J | 152 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 32 | f | 152 | LYS | CA-C-O | -5.19 | 109.21 | 120.10 |
| 34 | i | 1629 | A | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 34 | i | 1862 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 10 | J | 158 | ASP | CB-CG-OD2 | 5.18 | 122.97 | 118.30 |
| 34 | i | 480 | C | O4'-C1'-C2' | -5.18 | 100.62 | 105.80 |
| 34 | i | 1328 | A | C4'-C3'-C2' | -5.18 | 97.42 | 102.60 |
| 34 | i | 1501 | U | C3'-C2'-C1' | 5.18 | 105.65 | 101.50 |
| 34 | i | 1742 | C | C5'-C4'-C3' | 5.18 | 124.29 | 116.00 |
| 34 | i | 120 | U | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 16 | P | 71 | GLU | C-N-CA | 5.18 | 134.65 | 121.70 |
| 24 | X | 139 | GLU | CB-CA-C | 5.18 | 120.76 | 110.40 |
| 34 | i | 1048 | A | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 34 | i | 1335 | U | C5'-C4'-O4' | 5.18 | 115.32 | 109.10 |
| 16 | P | 82 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 12 | L | 24 | LEU | C-N-CA | 5.18 | 134.64 | 121.70 |
| 34 | i | 71 | G | C2'-C3'-O3' | -5.18 | 98.11 | 109.50 |
| 34 | i | 142 | C | O4'-C1'-C2' | 5.17 | 112.26 | 107.60 |
| 34 | i | 1558 | G | O4'-C1'-C2' | 5.17 | 112.26 | 107.60 |
| 34 | i | 1603 | U | N1-C1'-C2' | 5.17 | 120.73 | 114.00 |
| 5 | E | 158 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 34 | i | 74 | G | C1'-O4'-C4' | -5.17 | 105.76 | 109.90 |
| 34 | i | 539 | C | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 2 | B | 60 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 26 | Z | 104 | ARG | CB-CA-C | -5.17 | 100.06 | 110.40 |
| 34 | i | 136 | C | C5'-C4'-C3' | 5.17 | 124.27 | 116.00 |
| 34 | i | 279 | G | C1'-O4'-C4' | 5.17 | 114.03 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 850 | A | P-O3'-C3' | 5.17 | 125.90 | 119.70 |
| 34 | i | 1323 | G | N9-C1'-C2' | 5.17 | 120.72 | 114.00 |
| 34 | i | 1858 | U | C5'-C4'-O4' | 5.17 | 115.30 | 109.10 |
| 33 | g | 213 | ASP | CB-CG-OD1 | 5.17 | 122.95 | 118.30 |
| 34 | i | 271 | G | OP1-P-O3' | 5.17 | 116.57 | 105.20 |
| 34 | i | 1275 | C | C3'-C2'-C1' | 5.17 | 105.63 | 101.50 |
| 34 | i | 1544 | U | N1-C1'-C2' | 5.17 | 120.72 | 114.00 |
| 34 | i | 1714 | A | C3'-C2'-C1' | 5.17 | 105.63 | 101.50 |
| 34 | i | 1019 | A | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 5 | E | 258 | ALA | O-C-N | -5.16 | 114.44 | 122.70 |
| 34 | i | 72 | C | P-O5'-C5' | 5.16 | 129.16 | 120.90 |
| 34 | i | 1090 | C | N1-C1'-C2' | 5.16 | 120.71 | 114.00 |
| 34 | i | 1555 | U | C4'-C3'-C2' | -5.16 | 97.44 | 102.60 |
| 32 | f | 148 | TYR | CB-CG-CD1 | -5.16 | 117.90 | 121.00 |
| 34 | i | 1233 | C | C4'-C3'-C2' | -5.16 | 97.44 | 102.60 |
| 34 | i | 1453 | U | P-O3'-C3' | -5.16 | 113.51 | 119.70 |
| 34 | i | 971 | G | O4'-C4'-C3' | -5.16 | 98.84 | 104.00 |
| 34 | i | 932 | G | O4'-C1'-N9 | 5.16 | 112.32 | 108.20 |
| 34 | i | 1039 | G | O4'-C1'-N9 | 5.16 | 112.32 | 108.20 |
| 34 | i | 1461 | A | C3'-C2'-C1' | 5.16 | 105.62 | 101.50 |
| 34 | i | 1611 | U | C3'-C2'-C1' | 5.16 | 105.62 | 101.50 |
| 5 | E | 164 | LEU | C-N-CA | -5.15 | 108.81 | 121.70 |
| 16 | P | 37 | TYR | CA-CB-CG | 5.15 | 123.19 | 113.40 |
| 34 | i | 231 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 34 | i | 1302 | U | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 19 | S | 16 | LEU | CA-C-N | -5.15 | 105.87 | 117.20 |
| 33 | g | 12 | LYS | CB-CA-C | -5.15 | 100.10 | 110.40 |
| 34 | i | 629 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 34 | i | 1651 | G | C3'-C2'-C1' | -5.15 | 97.38 | 101.50 |
| 34 | i | 550 | A | C1'-O4'-C4' | -5.15 | 105.78 | 109.90 |
| 34 | i | 1238 | U | O4'-C1'-N1 | -5.15 | 104.08 | 108.20 |
| 34 | i | 1338 | U | C3'-C2'-C1' | 5.15 | 105.62 | 101.50 |
| 34 | i | 455 | A | O3'-P-O5' | -5.15 | 94.22 | 104.00 |
| 34 | i | 542 | G | O4'-C1'-C2' | 5.15 | 112.23 | 107.60 |
| 34 | i | 1575 | A | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 26 | Z | 50 | PHE | CB-CA-C | -5.14 | 100.11 | 110.40 |
| 34 | i | 1217 | G | C3'-C2'-C1' | -5.14 | 97.38 | 101.50 |
| 16 | P | 51 | ARG | N-CA-C | 5.14 | 124.88 | 111.00 |
| 34 | i | 32 | U | C5'-C4'-O4' | 5.14 | 115.27 | 109.10 |
| 34 | i | 308 | C | O4'-C1'-C2' | -5.14 | 100.66 | 105.80 |
| 34 | i | 410 | G | P-O3'-C3' | -5.14 | 113.53 | 119.70 |
| 34 | i | 740 | G | O3'-P-O5' | -5.14 | 94.23 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 799 | C | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 34 | i | 323 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 34 | i | 411 | G | O4'-C1'-C2' | 5.14 | 112.22 | 107.60 |
| 34 | i | 1267 | C | O4'-C1'-C2' | -5.14 | 100.66 | 105.80 |
| 24 | X | 126 | ALA | N-CA-C | -5.14 | 97.13 | 111.00 |
| 34 | i | 1308 | G | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 16 | P | 21 | ASP | CB-CG-OD2 | 5.13 | 122.92 | 118.30 |
| 34 | i | 520 | U | C4'-C3'-C2' | -5.13 | 97.47 | 102.60 |
| 34 | i | 1106 | G | C1'-O4'-C4' | 5.13 | 114.01 | 109.90 |
| 1 | A | 53 | ARG | CB-CG-CD | -5.13 | 98.26 | 111.60 |
| 24 | X | 115 | ILE | C-N-CD | -5.13 | 109.31 | 120.60 |
| 34 | i | 1568 | G | C4'-C3'-C2' | -5.13 | 97.47 | 102.60 |
| 34 | i | 1788 | C | C3'-C2'-C1' | 5.13 | 105.61 | 101.50 |
| 34 | i | 608 | C | C1'-O4'-C4' | 5.13 | 114.00 | 109.90 |
| 13 | M | 43 | ASP | CB-CG-OD2 | 5.13 | 122.92 | 118.30 |
| 20 | T | 144 | LYS | CA-C-O | -5.13 | 109.33 | 120.10 |
| 34 | i | 1275 | C | C1'-O4'-C4' | 5.13 | 114.00 | 109.90 |
| 11 | K | 43 | LEU | N-CA-C | -5.13 | 97.16 | 111.00 |
| 34 | i | 638 | A | C1'-O4'-C4' | -5.13 | 105.80 | 109.90 |
| 34 | i | 1235 | U | O3'-P-O5' | 5.13 | 113.74 | 104.00 |
| 34 | i | 1280 | A | C5'-C4'-C3' | -5.13 | 107.80 | 116.00 |
| 1 | A | 151 | ASP | CB-CG-OD2 | 5.12 | 122.91 | 118.30 |
| 7 | G | 103 | ASP | CB-CG-OD2 | 5.12 | 122.91 | 118.30 |
| 34 | i | 1157 | U | N1-C1'-C2' | -5.12 | 106.36 | 112.00 |
| 34 | i | 1375 | A | C5'-C4'-C3' | -5.12 | 107.80 | 116.00 |
| 22 | V | 66 | ASP | CB-CG-OD2 | 5.12 | 122.91 | 118.30 |
| 34 | i | 1298 | G | C5'-C4'-O4' | 5.12 | 115.25 | 109.10 |
| 2 | B | 196 | ASP | CB-CG-OD2 | 5.12 | 122.91 | 118.30 |
| 5 | E | 21 | ASP | CB-CG-OD2 | 5.12 | 122.91 | 118.30 |
| 34 | i | 78 | C | O4'-C1'-C2' | -5.12 | 100.68 | 105.80 |
| 2 | B | 191 | ASP | CB-CG-OD2 | 5.12 | 122.91 | 118.30 |
| 23 | W | 2 | VAL | O-C-N | -5.12 | 114.51 | 122.70 |
| 34 | i | 1320 | G | C3'-C2'-C1' | 5.12 | 105.59 | 101.50 |
| 34 | i | 1452 | G | N9-C1'-C2' | 5.12 | 120.65 | 114.00 |
| 34 | i | 1551 | A | C5'-C4'-C3' | -5.12 | 107.81 | 116.00 |
| 34 | i | 1645 | A | C1'-O4'-C4' | 5.12 | 113.99 | 109.90 |
| 34 | i | 1753 | G | C1'-O4'-C4' | -5.12 | 105.81 | 109.90 |
| 34 | i | 1784 | A | C1'-O4'-C4' | -5.12 | 105.81 | 109.90 |
| 32 | f | 124 | ASP | CB-CG-OD2 | 5.12 | 122.90 | 118.30 |
| 34 | i | 22 | A | C1'-O4'-C4' | 5.12 | 113.99 | 109.90 |
| 34 | i | 830 | C | O4'-C1'-N1 | 5.12 | 112.29 | 108.20 |
| 34 | i | 1562 | G | O4'-C4'-C3' | -5.12 | 98.88 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7 | G | 180 | VAL | N-CA-CB | -5.11 | 100.25 | 111.50 |
| 10 | J | 89 | GLU | N-CA-CB | -5.11 | 101.39 | 110.60 |
| 19 | S | 110 | ASP | CB-CG-OD2 | 5.11 | 122.90 | 118.30 |
| 23 | W | 85 | ASP | CB-CG-OD2 | 5.11 | 122.90 | 118.30 |
| 34 | i | 1308 | G | N9-C1'-C2' | 5.11 | 120.65 | 114.00 |
| 34 | i | 1021 | U | C1'-O4'-C4' | 5.11 | 113.99 | 109.90 |
| 15 | O | 67 | ASP | CB-CG-OD2 | 5.11 | 122.90 | 118.30 |
| 21 | U | 48 | LEU | CB-CG-CD2 | -5.11 | 102.32 | 111.00 |
| 34 | i | 503 | G | O4'-C1'-C2' | 5.11 | 112.20 | 107.60 |
| 9 | I | 8 | TRP | CE3-CZ3-CH2 | 5.11 | 126.82 | 121.20 |
| 34 | i | 13 | C | C3'-C2'-C1' | 5.11 | 105.58 | 101.50 |
| 34 | i | 309 | A | O4'-C1'-N9 | 5.11 | 112.28 | 108.20 |
| 34 | i | 1776 | G | O5'-C5'-C4' | 5.10 | 121.40 | 111.70 |
| 14 | N | 108 | ASP | CB-CG-OD2 | 5.10 | 122.89 | 118.30 |
| 34 | i | 581 | U | O4'-C1'-C2' | 5.10 | 112.19 | 107.60 |
| 34 | i | 819 | U | C3'-C2'-C1' | -5.10 | 97.42 | 101.50 |
| 29 | c | 37 | ASP | CB-CG-OD2 | 5.10 | 122.89 | 118.30 |
| 34 | i | 689 | G | N9-C1'-C2' | 5.10 | 120.63 | 114.00 |
| 34 | i | 729 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 34 | i | 896 | C | P-O5'-C5' | 5.10 | 129.06 | 120.90 |
| 34 | i | 1135 | C | C2-N1-C1' | 5.10 | 124.41 | 118.80 |
| 34 | i | 1490 | U | C3'-C2'-C1' | -5.10 | 97.42 | 101.50 |
| 16 | P | 28 | MET | CA-C-N | -5.10 | 105.99 | 117.20 |
| 34 | i | 1326 | G | O4'-C1'-C2' | 5.10 | 112.19 | 107.60 |
| 34 | i | 1477 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 16 | P | 27 | ASP | CB-CG-OD2 | 5.09 | 122.89 | 118.30 |
| 34 | i | 871 | A | C3'-C2'-C1' | 5.09 | 105.58 | 101.50 |
| 34 | i | 1483 | A | C4'-C3'-O3' | -5.09 | 98.70 | 109.40 |
| 2 | B | 152 | LYS | CB-CA-C | 5.09 | 120.58 | 110.40 |
| 31 | e | 118 | ASN | N-CA-C | 5.09 | 124.75 | 111.00 |
| 34 | i | 610 | G | O4'-C1'-C2' | -5.09 | 100.71 | 105.80 |
| 34 | i | 1313 | U | O4'-C1'-C2' | -5.09 | 100.71 | 105.80 |
| 34 | i | 1367 | U | O4'-C1'-C2' | -5.09 | 100.71 | 105.80 |
| 34 | i | 22 | A | O4'-C1'-C2' | -5.09 | 100.71 | 105.80 |
| 34 | i | 341 | G | O4'-C4'-C3' | -5.09 | 98.91 | 104.00 |
| 34 | i | 318 | U | C5'-C4'-C3' | 5.09 | 124.14 | 116.00 |
| 34 | i | 880 | C | C3'-C2'-C1' | 5.09 | 105.57 | 101.50 |
| 34 | i | 888 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 14 | N | 31 | ASP | CB-CG-OD2 | 5.09 | 122.88 | 118.30 |
| 18 | R | 110 | ASP | CB-CG-OD2 | 5.09 | 122.88 | 118.30 |
| 34 | i | 1272 | A | C1'-O4'-C4' | 5.09 | 113.97 | 109.90 |
| 34 | i | 1470 | A | O3'-P-O5' | 5.08 | 113.66 | 104.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32 | f | 106 | TYR | N-CA-C | -5.08 | 97.27 | 111.00 |
| 34 | i | 1813 | A | N9-C1'-C2' | 5.08 | 120.61 | 114.00 |
| 21 | U | 38 | ASP | CB-CG-OD2 | 5.08 | 122.87 | 118.30 |
| 34 | i | 1742 | C | C4'-C3'-O3' | -5.08 | 98.73 | 109.40 |
| 8 | H | 191 | GLU | C-N-CA | -5.08 | 109.00 | 121.70 |
| 25 | Y | 29 | HIS | C-N-CD | -5.08 | 109.43 | 120.60 |
| 34 | i | 660 | A | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 34 | i | 955 | G | C3'-C2'-C1' | 5.08 | 105.56 | 101.50 |
| 34 | i | 439 | A | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 34 | i | 1246 | A | O4'-C1'-C2' | -5.08 | 100.72 | 105.80 |
| 34 | i | 1614 | A | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 1 | A | 130 | ASP | CB-CG-OD2 | 5.07 | 122.86 | 118.30 |
| 34 | i | 1765 | G | P-O3'-C3' | 5.07 | 125.79 | 119.70 |
| 34 | i | 677 | C | N1-C1'-C2' | 5.07 | 120.59 | 114.00 |
| 7 | G | 151 | ASP | CB-CG-OD2 | 5.07 | 122.86 | 118.30 |
| 30 | d | 49 | ASP | CB-CG-OD2 | 5.07 | 122.86 | 118.30 |
| 34 | i | 216 | U | C3'-C2'-C1' | 5.07 | 105.56 | 101.50 |
| 34 | i | 292 | A | N9-C1'-C2' | -5.07 | 106.42 | 112.00 |
| 34 | i | 1427 | G | N9-C1'-C2' | 5.07 | 120.59 | 114.00 |
| 34 | i | 79 | A | C1'-O4'-C4' | 5.07 | 113.95 | 109.90 |
| 34 | i | 88 | G | O4'-C1'-C2' | 5.07 | 112.16 | 107.60 |
| 34 | i | 419 | C | N1-C1'-C2' | 5.07 | 120.59 | 114.00 |
| 4 | D | 52 | ALA | O-C-N | -5.07 | 114.60 | 122.70 |
| 34 | i | 1328 | A | N9-C1'-C2' | -5.07 | 106.43 | 112.00 |
| 5 | E | 237 | SER | N-CA-CB | -5.06 | 102.91 | 110.50 |
| 10 | J | 188 | GLY | N-CA-C | 5.06 | 125.75 | 113.10 |
| 34 | i | 586 | U | P-O3'-C3' | 5.06 | 125.77 | 119.70 |
| 1 | A | 193 | HIS | N-CA-C | 5.06 | 124.66 | 111.00 |
| 26 | Z | 56 | ASP | CB-CG-OD2 | 5.06 | 122.86 | 118.30 |
| 32 | f | 137 | ASP | CB-CG-OD2 | 5.06 | 122.86 | 118.30 |
| 34 | i | 1246 | A | N9-C1'-C2' | -5.06 | 106.43 | 112.00 |
| 32 | f | 134 | SER | CA-C-N | -5.06 | 106.07 | 117.20 |
| 33 | g | 143 | GLN | CB-CA-C | -5.06 | 100.29 | 110.40 |
| 34 | i | 1023 | A | O3'-P-O5' | 5.06 | 113.61 | 104.00 |
| 34 | i | 1493 | G | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 34 | i | 1663 | U | C4'-C3'-C2' | -5.06 | 97.54 | 102.60 |
| 2 | B | 155 | TYR | CB-CG-CD1 | -5.06 | 117.97 | 121.00 |
| 34 | i | 1413 | C | O4'-C4'-C3' | -5.06 | 98.94 | 104.00 |
| 5 | E | 93 | ASP | CB-CG-OD2 | 5.05 | 122.85 | 118.30 |
| 34 | i | 22 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 34 | i | 376 | C | C5'-C4'-C3' | -5.05 | 107.92 | 116.00 |
| 34 | i | 1656 | A | O4'-C1'-C2' | 5.05 | 112.15 | 107.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | E | 143 | ASP | CB-CG-OD2 | 5.05 | 122.84 | 118.30 |
| 34 | i | 1219 | A | C1'-O4'-C4' | 5.05 | 113.94 | 109.90 |
| 34 | i | 1730 | A | N9-C1'-C2' | 5.04 | 120.56 | 114.00 |
| 5 | E | 129 | ILE | CA-C-N | -5.04 | 106.10 | 117.20 |
| 10 | J | 85 | GLY | CA-C-N | -5.04 | 106.11 | 117.20 |
| 34 | i | 1426 | C | N1-C1'-C2' | -5.04 | 106.45 | 112.00 |
| 16 | P | 23 | ASP | CB-CG-OD2 | 5.04 | 122.84 | 118.30 |
| 34 | i | 410 | G | C4'-C3'-C2' | -5.04 | 97.56 | 102.60 |
| 24 | X | 19 | ASP | CB-CG-OD2 | 5.04 | 122.83 | 118.30 |
| 34 | i | 896 | C | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |
| 34 | i | 1541 | G | C3'-C2'-C1' | -5.04 | 97.47 | 101.50 |
| 17 | Q | 31 | LEU | C-N-CA | 5.03 | 134.28 | 121.70 |
| 34 | i | 1711 | C | N1-C1'-C2' | 5.03 | 120.54 | 114.00 |
| 25 | Y | 103 | SER | C-N-CA | 5.03 | 134.28 | 121.70 |
| 34 | i | 125 | C | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 34 | i | 1333 | C | C2'-C3'-O3' | 5.03 | 121.75 | 113.70 |
| 34 | i | 1573 | U | C5'-C4'-O4' | 5.03 | 115.14 | 109.10 |
| 34 | i | 1823 | G | C3'-C2'-C1' | 5.03 | 105.53 | 101.50 |
| 5 | E | 163 | ASP | CB-CG-OD2 | 5.03 | 122.83 | 118.30 |
| 21 | U | 52 | GLY | C-N-CD | -5.03 | 109.53 | 120.60 |
| 34 | i | 1410 | A | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 34 | i | 1609 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 34 | i | 160 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 34 | i | 577 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 34 | i | 625 | G | C3'-C2'-C1' | 5.03 | 105.52 | 101.50 |
| 34 | i | 1721 | G | C3'-C2'-C1' | -5.03 | 97.48 | 101.50 |
| 34 | i | 1133 | U | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 34 | i | 1385 | C | O5'-P-OP2 | -5.02 | 101.18 | 105.70 |
| 19 | S | 62 | ASP | CB-CG-OD2 | 5.02 | 122.81 | 118.30 |
| 25 | Y | 34 | THR | N-CA-C | 5.02 | 124.55 | 111.00 |
| 34 | i | 8 | U | O4'-C1'-C2' | -5.02 | 100.78 | 105.80 |
| 34 | i | 677 | C | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 34 | i | 850 | A | O5'-C5'-C4' | -5.02 | 102.17 | 111.70 |
| 34 | i | 994 | A | C3'-C2'-C1' | 5.02 | 105.52 | 101.50 |
| 34 | i | 1248 | C | P-O3'-C3' | -5.02 | 113.68 | 119.70 |
| 34 | i | 73 | C | P-O3'-C3' | -5.02 | 113.68 | 119.70 |
| 34 | i | 1240 | U | C4'-C3'-C2' | -5.01 | 97.58 | 102.60 |
| 34 | i | 1379 | A | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 34 | i | 1063 | C | N1-C1'-C2' | 5.01 | 120.52 | 114.00 |
| 34 | i | 1343 | U | C3'-C2'-C1' | 5.01 | 105.51 | 101.50 |
| 32 | f | 86 | THR | N-CA-C | -5.01 | 97.47 | 111.00 |
| 34 | i | 43 | U | C5'-C4'-O4' | 5.01 | 115.11 | 109.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | i | 859 | U | N1-C1'-C2' | 5.01 | 120.52 | 114.00 |
| 34 | i | 1386 | U | N1-C1'-C2' | 5.01 | 120.52 | 114.00 |
| 33 | g | 273 | GLU | C-N-CA | 5.01 | 134.22 | 121.70 |
| 2 | B | 32 | ASP | CB-CG-OD2 | 5.01 | 122.81 | 118.30 |
| 2 | B | 90 | ASP | CB-CG-OD2 | 5.01 | 122.81 | 118.30 |
| 34 | i | 1568 | G | O4'-C1'-N9 | 5.01 | 112.20 | 108.20 |
| 26 | Z | 51 | ASP | CB-CG-OD2 | 5.00 | 122.80 | 118.30 |
| 30 | d | 6 | LEU | N-CA-C | -5.00 | 97.49 | 111.00 |
| 34 | i | 15 | U | C1'-O4'-C4' | 5.00 | 113.90 | 109.90 |
| 34 | i | 1634 | G | O4'-C1'-C2' | -5.00 | 100.80 | 105.80 |
| 34 | i | 468 | G | P-O5'-C5' | 5.00 | 128.90 | 120.90 |
| 34 | i | 596 | G | P-O3'-C3' | 5.00 | 125.70 | 119.70 |

All (13) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 3 | C | 157 | ASN | CA |
| 5 | E | 171 | ASP | CA |
| 10 | J | 138 | ARG | CA |
| 18 | R | 3 | ARG | CA |
| 19 | S | 92 | ASP | CA |
| 20 | T | 93 | SER | CA |
| 25 | Y | 86 | GLU | CA |
| 34 | i | 544 | A | C1' |
| 34 | i | 794 | G | C4' |
| 34 | i | 835 | C | C1' |
| 34 | i | 1151 | U | C1' |
| 34 | i | 1414 | C | C1' |
| 34 | i | 1503 | G | C1' |

All (183) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | A | 146 | ALA | Mainchain |
| 1 | A | 185 | MET | Mainchain |
| 1 | A | 192 | GLU | Mainchain,Peptide |
| 1 | A | 199 | PRO | Mainchain |
| 1 | A | 206 | ASP | Mainchain,Peptide |
| 1 | A | 23 | THR | Mainchain |
| 1 | A | 4 | ALA | Peptide |
| 1 | A | 63 | ARG | Sidechain |
| 1 | A | 97 | THR | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 2 | B | 146 | CYS | Peptide |
| 2 | B | 56 | LYS | Mainchain |
| 2 | B | 75 | GLN | Peptide |
| 2 | B | 76 | ASN | Peptide |
| 3 | C | 157 | ASN | Peptide |
| 3 | C | 160 | GLY | Mainchain |
| 3 | C | 241 | TRP | Mainchain |
| 3 | C | 97 | VAL | Mainchain,Peptide |
| 4 | D | 144 | GLY | Peptide |
| 4 | D | 190 | LEU | Mainchain |
| 4 | D | 3 | VAL | Mainchain,Peptide |
| 4 | D | 96 | LEU | Mainchain |
| 5 | E | 1 | MET | Peptide |
| 5 | E | 129 | ILE | Peptide |
| 6 | F | 43 | GLU | Peptide |
| 6 | F | 44 | LYS | Peptide |
| 6 | F | 79 | HIS | Peptide |
| 7 | G | 155 | GLN | Mainchain |
| 8 | H | 105 | THR | Peptide |
| 8 | H | 108 | SER | Peptide |
| 8 | H | 109 | ARG | Sidechain |
| 8 | H | 113 | LYS | Mainchain |
| 8 | H | 118 | ARG | Sidechain |
| 8 | H | 16 | PRO | Peptide |
| 8 | H | 17 | ASP | Peptide |
| 8 | H | 190 | PRO | Peptide |
| 8 | H | 193 | GLN | Peptide |
| 8 | H | 53 | VAL | Peptide |
| 9 | I | 123 | ARG | Mainchain |
| 9 | I | 129 | LEU | Mainchain |
| 9 | I | 131 | PRO | Mainchain |
| 9 | I | 155 | ASN | Peptide |
| 9 | I | 190 | LEU | Mainchain |
| 9 | I | 2 | GLY | Mainchain |
| 9 | I | 3 | ILE | Peptide |
| 9 | I | 55 | TYR | Sidechain |
| 10 | J | 146 | SER | Mainchain |
| 10 | J | 16 | PRO | Peptide |
| 10 | J | 161 | LEU | Mainchain,Peptide |
| 10 | J | 162 | ARG | Peptide |
| 10 | J | 164 | PRO | Mainchain |
| 10 | J | 165 | TYR | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 10 | J | 85 | GLY | Mainchain |
| 10 | J | 90 | GLY | Peptide |
| 10 | J | 91 | LYS | Mainchain |
| 10 | J | 92 | MET | Peptide |
| 11 | K | 29 | MET | Peptide |
| 11 | K | 30 | PRO | Peptide |
| 11 | K | 37 | ASP | Peptide |
| 11 | K | 43 | LEU | Peptide |
| 11 | K | 55 | ARG | Sidechain |
| 11 | K | 70 | TYR | Sidechain |
| 11 | K | 86 | PRO | Peptide |
| 11 | K | 89 | ILE | Mainchain |
| 11 | K | 90 | VAL | Mainchain |
| 11 | K | 92 | ALA | Peptide |
| 11 | K | 97 | SER | Peptide |
| 12 | L | 147 | LYS | Peptide |
| 12 | L | 149 | ALA | Mainchain |
| 12 | L | 152 | LYS | Mainchain |
| 12 | L | 18 | GLN | Peptide |
| 12 | L | 26 | GLY | Peptide |
| 12 | L | 27 | GLU | Peptide |
| 12 | L | 97 | ARG | Peptide |
| 13 | M | 98 | GLY | Peptide |
| 14 | N | 13 | GLN | Peptide |
| 14 | N | 14 | SER | Peptide |
| 14 | N | 18 | TYR | Peptide |
| 14 | N | 82 | PRO | Peptide |
| 15 | O | 138 | ASP | Peptide |
| 16 | P | 17 | TYR | Sidechain,Peptide |
| 16 | P | 18 | ARG | Sidechain |
| 16 | P | 27 | ASP | Peptide |
| 16 | P | 36 | LEU | Peptide |
| 16 | P | 37 | TYR | Peptide |
| 16 | P | 38 | SER | Peptide |
| 16 | P | 48 | GLY | Mainchain,Peptide |
| 16 | P | 50 | ARG | Peptide |
| 17 | Q | 146 | ARG | Sidechain |
| 17 | Q | 31 | LEU | Peptide |
| 17 | Q | 43 | GLU | Peptide |
| 17 | Q | 47 | LEU | Peptide |
| 18 | R | 1 | MET | Mainchain |
| 18 | R | 122 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------------------|
| 18 | R | 88 | VAL | Mainchain,Peptide |
| 18 | R | 89 | SER | Peptide |
| 19 | S | 10 | GLN | Peptide |
| 19 | S | 141 | ARG | Mainchain |
| 19 | S | 15 | VAL | Peptide |
| 19 | S | 40 | TYR | Sidechain,Mainchain |
| 19 | S | 8 | LYS | Peptide |
| 19 | S | 87 | GLN | Mainchain |
| 19 | S | 9 | PHE | Peptide |
| 19 | S | 93 | GLY | Peptide |
| 19 | S | 94 | LYS | Peptide |
| 20 | T | 142 | LYS | Mainchain,Peptide |
| 20 | T | 4 | VAL | Mainchain,Peptide |
| 20 | T | 42 | HIS | Sidechain |
| 20 | T | 82 | ARG | Sidechain |
| 21 | U | 104 | ILE | Mainchain |
| 21 | U | 105 | SER | Mainchain |
| 21 | U | 108 | PRO | Peptide |
| 21 | U | 46 | LYS | Peptide |
| 21 | U | 50 | VAL | Peptide |
| 21 | U | 68 | THR | Peptide |
| 21 | U | 70 | CYS | Mainchain |
| 21 | U | 93 | SER | Mainchain |
| 22 | V | 25 | GLY | Peptide |
| 22 | V | 48 | GLY | Mainchain,Peptide |
| 22 | V | 49 | GLN | Peptide |
| 22 | V | 61 | ARG | Sidechain |
| 22 | V | 63 | GLY | Mainchain |
| 22 | V | 81 | GLN | Mainchain,Peptide |
| 22 | V | 9 | VAL | Peptide |
| 23 | W | 2 | VAL | Mainchain |
| 23 | W | 84 | LYS | Peptide |
| 24 | X | 1 | MET | Peptide |
| 24 | X | 127 | ASN | Peptide |
| 24 | X | 23 | HIS | Mainchain |
| 24 | X | 42 | GLY | Peptide |
| 25 | Y | 103 | SER | Peptide |
| 25 | Y | 32 | LYS | Peptide |
| 25 | Y | 33 | ALA | Peptide |
| 25 | Y | 34 | THR | Peptide |
| 25 | Y | 85 | ASN | Peptide |
| 25 | Y | 86 | GLU | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------------------|
| 26 | Z | 101 | SER | Mainchain |
| 26 | Z | 104 | ARG | Sidechain,Mainchain |
| 26 | Z | 41 | ARG | Peptide |
| 26 | Z | 93 | SER | Peptide |
| 26 | Z | 95 | GLY | Peptide |
| 27 | a | 96 | THR | Mainchain,Peptide |
| 28 | b | 2 | PRO | Mainchain |
| 28 | b | 36 | LYS | Peptide |
| 28 | b | 37 | CYS | Mainchain |
| 31 | e | 93 | VAL | Mainchain |
| 31 | e | 94 | ALA | Mainchain,Peptide |
| 31 | e | 96 | GLN | Mainchain |
| 31 | e | 97 | GLU | Peptide |
| 32 | f | 102 | VAL | Peptide |
| 32 | f | 105 | TYR | Peptide |
| 32 | f | 135 | HIS | Mainchain |
| 32 | f | 148 | TYR | Peptide |
| 32 | f | 84 | SER | Peptide |
| 32 | f | 90 | LYS | Peptide |
| 33 | g | 12 | LYS | Peptide |
| 33 | g | 142 | VAL | Mainchain |
| 33 | g | 148 | SER | Mainchain |
| 33 | g | 158 | PRO | Peptide |
| 33 | g | 159 | ASN | Mainchain,Peptide |
| 33 | g | 160 | SER | Peptide |
| 33 | g | 192 | THR | Peptide |
| 33 | g | 273 | GLU | Peptide |
| 33 | g | 283 | PRO | Peptide |
| 33 | g | 47 | ARG | Peptide |
| 33 | g | 59 | LEU | Mainchain |
| 33 | g | 60 | ARG | Peptide |

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1 | A | 206/295 (70%) | 156 (76%) | 23 (11%) | 27 (13%) | 0 | 4 |
| 2 | B | 213/264 (81%) | 174 (82%) | 24 (11%) | 15 (7%) | 1 | 14 |
| 3 | C | 224/278 (81%) | 199 (89%) | 14 (6%) | 11 (5%) | 2 | 20 |
| 4 | D | 225/243 (93%) | 180 (80%) | 23 (10%) | 22 (10%) | 0 | 9 |
| 5 | E | 261/263 (99%) | 210 (80%) | 27 (10%) | 24 (9%) | 1 | 11 |
| 6 | F | 189/204 (93%) | 162 (86%) | 15 (8%) | 12 (6%) | 1 | 17 |
| 7 | G | 235/249 (94%) | 201 (86%) | 19 (8%) | 15 (6%) | 1 | 16 |
| 8 | H | 188/194 (97%) | 146 (78%) | 11 (6%) | 31 (16%) | 0 | 3 |
| 9 | I | 204/208 (98%) | 169 (83%) | 13 (6%) | 22 (11%) | 0 | 8 |
| 10 | J | 180/194 (93%) | 138 (77%) | 18 (10%) | 24 (13%) | 0 | 4 |
| 11 | K | 96/165 (58%) | 67 (70%) | 11 (12%) | 18 (19%) | 0 | 2 |
| 12 | L | 156/158 (99%) | 132 (85%) | 10 (6%) | 14 (9%) | 1 | 11 |
| 13 | M | 122/132 (92%) | 85 (70%) | 16 (13%) | 21 (17%) | 0 | 3 |
| 14 | N | 148/151 (98%) | 123 (83%) | 19 (13%) | 6 (4%) | 3 | 22 |
| 15 | O | 134/151 (89%) | 101 (75%) | 14 (10%) | 19 (14%) | 0 | 4 |
| 16 | P | 125/145 (86%) | 92 (74%) | 16 (13%) | 17 (14%) | 0 | 4 |
| 17 | Q | 139/146 (95%) | 110 (79%) | 19 (14%) | 10 (7%) | 1 | 14 |
| 18 | R | 124/135 (92%) | 97 (78%) | 13 (10%) | 14 (11%) | 0 | 7 |
| 19 | S | 135/152 (89%) | 106 (78%) | 20 (15%) | 9 (7%) | 1 | 15 |
| 20 | T | 139/145 (96%) | 119 (86%) | 10 (7%) | 10 (7%) | 1 | 14 |
| 21 | U | 102/119 (86%) | 76 (74%) | 10 (10%) | 16 (16%) | 0 | 3 |
| 22 | V | 80/83 (96%) | 55 (69%) | 11 (14%) | 14 (18%) | 0 | 2 |
| 23 | W | 127/130 (98%) | 111 (87%) | 14 (11%) | 2 (2%) | 9 | 44 |
| 24 | X | 140/143 (98%) | 121 (86%) | 11 (8%) | 8 (6%) | 1 | 18 |
| 25 | Y | 124/133 (93%) | 91 (73%) | 15 (12%) | 18 (14%) | 0 | 4 |
| 26 | Z | 73/125 (58%) | 52 (71%) | 12 (16%) | 9 (12%) | 0 | 5 |
| 27 | a | 105/115 (91%) | 72 (69%) | 14 (13%) | 19 (18%) | 0 | 3 |
| 28 | b | 82/84 (98%) | 57 (70%) | 14 (17%) | 11 (13%) | 0 | 4 |
| 29 | c | 62/69 (90%) | 44 (71%) | 13 (21%) | 5 (8%) | 1 | 12 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 30 | d | 51/56 (91%) | 46 (90%) | 3 (6%) | 2 (4%) | 3 | 23 |
| 31 | e | 57/133 (43%) | 37 (65%) | 7 (12%) | 13 (23%) | 0 | 2 |
| 32 | f | 69/156 (44%) | 38 (55%) | 13 (19%) | 18 (26%) | 0 | 1 |
| 33 | g | 311/317 (98%) | 271 (87%) | 23 (7%) | 17 (6%) | 2 | 19 |
| 37 | n | 80/144 (56%) | 61 (76%) | 15 (19%) | 4 (5%) | 2 | 20 |
| All | All | 4906/5679 (86%) | 3899 (80%) | 510 (10%) | 497 (10%) | 0 | 9 |

All (497) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 9 | GLN |
| 1 | A | 31 | ASP |
| 1 | A | 45 | GLY |
| 1 | A | 103 | PHE |
| 1 | A | 164 | ASN |
| 1 | A | 165 | ASN |
| 1 | A | 188 | THR |
| 1 | A | 192 | GLU |
| 1 | A | 203 | PHE |
| 1 | A | 207 | PRO |
| 2 | B | 27 | LYS |
| 2 | B | 77 | ASP |
| 2 | B | 78 | GLU |
| 2 | B | 106 | THR |
| 2 | B | 154 | SER |
| 2 | B | 179 | ASN |
| 2 | B | 206 | PRO |
| 2 | B | 210 | VAL |
| 3 | C | 102 | GLN |
| 3 | C | 104 | GLY |
| 3 | C | 117 | ASP |
| 3 | C | 218 | LEU |
| 3 | C | 260 | LYS |
| 4 | D | 2 | ALA |
| 4 | D | 4 | GLN |
| 4 | D | 93 | THR |
| 4 | D | 98 | ALA |
| 4 | D | 202 | LYS |
| 4 | D | 205 | PRO |
| 4 | D | 213 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 214 | LYS |
| 4 | D | 216 | GLU |
| 4 | D | 220 | THR |
| 4 | D | 221 | THR |
| 4 | D | 222 | PRO |
| 4 | D | 223 | ILE |
| 4 | D | 226 | GLN |
| 5 | E | 12 | VAL |
| 5 | E | 24 | THR |
| 5 | E | 76 | VAL |
| 5 | E | 95 | THR |
| 5 | E | 163 | ASP |
| 5 | E | 196 | THR |
| 5 | E | 260 | GLN |
| 5 | E | 261 | SER |
| 6 | F | 43 | GLU |
| 6 | F | 44 | LYS |
| 6 | F | 202 | SER |
| 6 | F | 203 | ASN |
| 7 | G | 20 | ASP |
| 7 | G | 154 | ARG |
| 7 | G | 164 | LYS |
| 7 | G | 174 | PRO |
| 7 | G | 175 | LYS |
| 7 | G | 180 | VAL |
| 7 | G | 181 | THR |
| 8 | H | 15 | LYS |
| 8 | H | 16 | PRO |
| 8 | H | 33 | ASN |
| 8 | H | 35 | ASP |
| 8 | H | 66 | VAL |
| 8 | H | 88 | SER |
| 8 | H | 108 | SER |
| 8 | H | 109 | ARG |
| 8 | H | 110 | THR |
| 8 | H | 116 | ARG |
| 8 | H | 135 | PHE |
| 8 | H | 137 | SER |
| 8 | H | 138 | GLU |
| 8 | H | 160 | LYS |
| 8 | H | 190 | PRO |
| 9 | I | 8 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 120 | PRO |
| 9 | I | 124 | LYS |
| 9 | I | 131 | PRO |
| 9 | I | 133 | GLU |
| 9 | I | 139 | LYS |
| 9 | I | 140 | LYS |
| 9 | I | 142 | SER |
| 9 | I | 143 | LYS |
| 9 | I | 145 | ILE |
| 9 | I | 153 | LYS |
| 9 | I | 154 | LYS |
| 9 | I | 158 | ILE |
| 9 | I | 206 | LYS |
| 10 | J | 19 | PRO |
| 10 | J | 22 | LYS |
| 10 | J | 36 | GLY |
| 10 | J | 110 | LEU |
| 10 | J | 111 | GLN |
| 10 | J | 118 | GLY |
| 10 | J | 119 | LEU |
| 10 | J | 122 | SER |
| 10 | J | 138 | ARG |
| 10 | J | 161 | LEU |
| 10 | J | 163 | SER |
| 10 | J | 169 | ARG |
| 10 | J | 170 | PRO |
| 10 | J | 172 | ARG |
| 11 | K | 2 | LEU |
| 11 | K | 3 | MET |
| 11 | K | 30 | PRO |
| 11 | K | 35 | LEU |
| 11 | K | 39 | ASN |
| 11 | K | 40 | VAL |
| 11 | K | 41 | PRO |
| 11 | K | 44 | HIS |
| 11 | K | 63 | ALA |
| 11 | K | 88 | GLU |
| 11 | K | 89 | ILE |
| 12 | L | 5 | GLN |
| 12 | L | 6 | THR |
| 12 | L | 7 | GLU |
| 12 | L | 20 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 23 | VAL |
| 12 | L | 147 | LYS |
| 12 | L | 152 | LYS |
| 12 | L | 153 | LYS |
| 13 | M | 12 | MET |
| 13 | M | 15 | ASN |
| 13 | M | 44 | LYS |
| 13 | M | 72 | HIS |
| 13 | M | 77 | ILE |
| 13 | M | 78 | LYS |
| 13 | M | 79 | VAL |
| 13 | M | 81 | ASP |
| 13 | M | 89 | VAL |
| 13 | M | 96 | ARG |
| 13 | M | 100 | PRO |
| 13 | M | 116 | LYS |
| 13 | M | 117 | GLU |
| 14 | N | 22 | VAL |
| 15 | O | 23 | GLU |
| 15 | O | 52 | THR |
| 15 | O | 53 | ILE |
| 15 | O | 64 | ALA |
| 15 | O | 104 | ARG |
| 15 | O | 137 | SER |
| 15 | O | 138 | ASP |
| 15 | O | 139 | SER |
| 15 | O | 140 | THR |
| 16 | P | 6 | GLN |
| 16 | P | 11 | THR |
| 16 | P | 12 | PHE |
| 16 | P | 37 | TYR |
| 16 | P | 38 | SER |
| 16 | P | 68 | PRO |
| 16 | P | 69 | PRO |
| 16 | P | 71 | GLU |
| 16 | P | 73 | PRO |
| 16 | P | 75 | VAL |
| 16 | P | 125 | PRO |
| 16 | P | 126 | VAL |
| 16 | P | 127 | LYS |
| 17 | Q | 19 | ALA |
| 17 | Q | 61 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | Q | 62 | ARG |
| 17 | Q | 117 | ARG |
| 17 | Q | 119 | LEU |
| 17 | Q | 141 | TYR |
| 18 | R | 88 | VAL |
| 18 | R | 89 | SER |
| 18 | R | 100 | PRO |
| 18 | R | 101 | ASP |
| 18 | R | 121 | GLN |
| 18 | R | 123 | THR |
| 19 | S | 11 | HIS |
| 19 | S | 53 | THR |
| 19 | S | 59 | LEU |
| 19 | S | 90 | VAL |
| 20 | T | 5 | THR |
| 20 | T | 31 | PRO |
| 20 | T | 32 | GLU |
| 20 | T | 33 | TRP |
| 20 | T | 34 | VAL |
| 20 | T | 96 | SER |
| 20 | T | 143 | LYS |
| 21 | U | 51 | LYS |
| 21 | U | 94 | PRO |
| 21 | U | 95 | SER |
| 21 | U | 107 | GLU |
| 21 | U | 118 | ASP |
| 22 | V | 4 | ASN |
| 22 | V | 10 | ASP |
| 22 | V | 42 | VAL |
| 22 | V | 43 | THR |
| 22 | V | 44 | GLY |
| 22 | V | 50 | SER |
| 22 | V | 65 | SER |
| 22 | V | 78 | ILE |
| 24 | X | 3 | LYS |
| 24 | X | 4 | CYS |
| 25 | Y | 6 | THR |
| 25 | Y | 30 | PRO |
| 25 | Y | 34 | THR |
| 25 | Y | 86 | GLU |
| 25 | Y | 87 | PRO |
| 25 | Y | 100 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | Y | 104 | ARG |
| 25 | Y | 120 | THR |
| 26 | Z | 93 | SER |
| 26 | Z | 104 | ARG |
| 26 | Z | 108 | ILE |
| 26 | Z | 113 | THR |
| 27 | a | 28 | CYS |
| 27 | a | 46 | GLU |
| 27 | a | 47 | ALA |
| 27 | a | 58 | VAL |
| 27 | a | 59 | PHE |
| 27 | a | 61 | ALA |
| 27 | a | 63 | VAL |
| 27 | a | 64 | LEU |
| 27 | a | 98 | PRO |
| 27 | a | 99 | PRO |
| 27 | a | 103 | PRO |
| 28 | b | 62 | VAL |
| 28 | b | 63 | LEU |
| 28 | b | 64 | CYS |
| 29 | c | 8 | PRO |
| 29 | c | 67 | ARG |
| 30 | d | 8 | TRP |
| 31 | e | 76 | VAL |
| 31 | e | 78 | GLY |
| 31 | e | 81 | ALA |
| 31 | e | 98 | LYS |
| 31 | e | 119 | VAL |
| 31 | e | 121 | PRO |
| 31 | e | 126 | LYS |
| 32 | f | 84 | SER |
| 32 | f | 85 | TYR |
| 32 | f | 86 | THR |
| 32 | f | 91 | ASN |
| 32 | f | 102 | VAL |
| 32 | f | 106 | TYR |
| 32 | f | 110 | GLU |
| 32 | f | 128 | ALA |
| 33 | g | 3 | GLU |
| 33 | g | 48 | ASP |
| 33 | g | 52 | TYR |
| 33 | g | 96 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | g | 282 | GLU |
| 33 | g | 283 | PRO |
| 37 | n | 71 | ILE |
| 37 | n | 83 | ASP |
| 1 | A | 7 | VAL |
| 1 | A | 96 | ALA |
| 1 | A | 112 | ILE |
| 1 | A | 140 | VAL |
| 1 | A | 159 | ILE |
| 1 | A | 186 | ARG |
| 1 | A | 190 | SER |
| 1 | A | 191 | ARG |
| 2 | B | 93 | GLY |
| 2 | B | 209 | ASP |
| 3 | C | 43 | LYS |
| 3 | C | 246 | PHE |
| 4 | D | 78 | GLY |
| 4 | D | 194 | PRO |
| 4 | D | 201 | LYS |
| 4 | D | 208 | VAL |
| 5 | E | 104 | ASP |
| 5 | E | 164 | LEU |
| 6 | F | 21 | GLY |
| 6 | F | 32 | ASP |
| 6 | F | 41 | VAL |
| 6 | F | 54 | GLY |
| 6 | F | 79 | HIS |
| 7 | G | 26 | THR |
| 7 | G | 146 | ASN |
| 7 | G | 153 | VAL |
| 8 | H | 11 | PRO |
| 8 | H | 17 | ASP |
| 8 | H | 38 | ALA |
| 8 | H | 41 | ARG |
| 8 | H | 76 | GLN |
| 8 | H | 100 | ILE |
| 8 | H | 112 | ASN |
| 8 | H | 120 | ARG |
| 8 | H | 159 | ASP |
| 8 | H | 193 | GLN |
| 9 | I | 22 | HIS |
| 9 | I | 192 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 106 | LEU |
| 10 | J | 120 | ALA |
| 10 | J | 124 | HIS |
| 10 | J | 135 | ILE |
| 10 | J | 148 | ILE |
| 11 | K | 34 | GLU |
| 11 | K | 91 | PRO |
| 12 | L | 4 | ILE |
| 12 | L | 21 | LYS |
| 12 | L | 22 | ARG |
| 12 | L | 57 | ASP |
| 13 | M | 45 | ARG |
| 14 | N | 68 | GLY |
| 15 | O | 54 | CYS |
| 15 | O | 56 | VAL |
| 16 | P | 54 | HIS |
| 17 | Q | 32 | ILE |
| 17 | Q | 100 | VAL |
| 18 | R | 93 | GLN |
| 18 | R | 112 | GLY |
| 18 | R | 125 | GLY |
| 19 | S | 17 | ASN |
| 19 | S | 31 | THR |
| 19 | S | 140 | GLY |
| 20 | T | 142 | LYS |
| 21 | U | 74 | SER |
| 21 | U | 98 | VAL |
| 22 | V | 6 | GLY |
| 22 | V | 33 | PRO |
| 22 | V | 48 | GLY |
| 23 | W | 66 | THR |
| 24 | X | 59 | ALA |
| 25 | Y | 95 | GLY |
| 25 | Y | 99 | LYS |
| 25 | Y | 119 | GLY |
| 26 | Z | 53 | ALA |
| 27 | a | 35 | ALA |
| 28 | b | 2 | PRO |
| 28 | b | 38 | PRO |
| 28 | b | 81 | ARG |
| 31 | e | 77 | HIS |
| 31 | e | 104 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | e | 124 | GLY |
| 32 | f | 98 | VAL |
| 32 | f | 127 | GLY |
| 32 | f | 148 | TYR |
| 33 | g | 49 | GLU |
| 33 | g | 60 | ARG |
| 33 | g | 144 | ASP |
| 33 | g | 159 | ASN |
| 33 | g | 171 | ASP |
| 33 | g | 281 | ALA |
| 33 | g | 295 | GLY |
| 37 | n | 111 | GLU |
| 1 | A | 11 | LYS |
| 1 | A | 30 | LEU |
| 1 | A | 194 | PRO |
| 1 | A | 205 | ARG |
| 2 | B | 56 | LYS |
| 2 | B | 82 | ARG |
| 4 | D | 218 | LEU |
| 5 | E | 25 | SER |
| 5 | E | 168 | LYS |
| 5 | E | 194 | VAL |
| 5 | E | 205 | PHE |
| 7 | G | 69 | THR |
| 8 | H | 18 | GLU |
| 8 | H | 117 | PRO |
| 8 | H | 150 | GLY |
| 9 | I | 105 | ASP |
| 9 | I | 106 | SER |
| 9 | I | 144 | LYS |
| 10 | J | 91 | LYS |
| 11 | K | 28 | HIS |
| 11 | K | 87 | PRO |
| 13 | M | 91 | LEU |
| 14 | N | 28 | LEU |
| 15 | O | 32 | HIS |
| 16 | P | 17 | TYR |
| 16 | P | 39 | ALA |
| 18 | R | 86 | PRO |
| 18 | R | 122 | PRO |
| 20 | T | 29 | LYS |
| 21 | U | 70 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | U | 93 | SER |
| 21 | U | 110 | VAL |
| 24 | X | 92 | ASN |
| 25 | Y | 5 | VAL |
| 25 | Y | 53 | ASP |
| 25 | Y | 60 | PHE |
| 25 | Y | 63 | HIS |
| 27 | a | 13 | LYS |
| 27 | a | 97 | PRO |
| 27 | a | 102 | ARG |
| 27 | a | 107 | ALA |
| 28 | b | 7 | LEU |
| 29 | c | 65 | ALA |
| 31 | e | 127 | LYS |
| 31 | e | 129 | PRO |
| 32 | f | 137 | ASP |
| 32 | f | 138 | ARG |
| 33 | g | 84 | ASP |
| 33 | g | 255 | SER |
| 33 | g | 285 | GLN |
| 37 | n | 34 | GLU |
| 1 | A | 104 | THR |
| 2 | B | 224 | GLU |
| 3 | C | 244 | THR |
| 3 | C | 249 | SER |
| 5 | E | 30 | ARG |
| 5 | E | 119 | ALA |
| 5 | E | 189 | LEU |
| 6 | F | 37 | ASP |
| 7 | G | 33 | ALA |
| 7 | G | 122 | PRO |
| 10 | J | 151 | LEU |
| 10 | J | 162 | ARG |
| 11 | K | 67 | PHE |
| 11 | K | 95 | ARG |
| 12 | L | 119 | ASP |
| 13 | M | 29 | ASP |
| 13 | M | 94 | ILE |
| 13 | M | 113 | ASP |
| 15 | O | 17 | LEU |
| 15 | O | 83 | GLN |
| 16 | P | 50 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | R | 95 | ILE |
| 19 | S | 12 | ILE |
| 20 | T | 46 | ALA |
| 21 | U | 50 | VAL |
| 21 | U | 116 | ILE |
| 22 | V | 79 | VAL |
| 24 | X | 9 | THR |
| 24 | X | 129 | SER |
| 25 | Y | 102 | THR |
| 26 | Z | 111 | ARG |
| 26 | Z | 114 | LYS |
| 27 | a | 62 | TYR |
| 28 | b | 24 | LEU |
| 29 | c | 63 | ARG |
| 32 | f | 145 | CYS |
| 33 | g | 37 | ASP |
| 1 | A | 23 | THR |
| 3 | C | 164 | THR |
| 4 | D | 80 | PRO |
| 5 | E | 90 | ILE |
| 5 | E | 134 | LYS |
| 5 | E | 213 | ALA |
| 9 | I | 52 | ASN |
| 9 | I | 59 | ARG |
| 11 | K | 38 | LYS |
| 12 | L | 2 | ALA |
| 13 | M | 59 | PRO |
| 13 | M | 95 | ASP |
| 14 | N | 3 | ARG |
| 14 | N | 138 | ASN |
| 15 | O | 22 | ALA |
| 15 | O | 38 | ASN |
| 17 | Q | 43 | GLU |
| 18 | R | 99 | ASP |
| 19 | S | 7 | GLU |
| 21 | U | 26 | SER |
| 21 | U | 117 | ALA |
| 23 | W | 67 | GLY |
| 24 | X | 99 | GLU |
| 25 | Y | 51 | THR |
| 25 | Y | 121 | ALA |
| 26 | Z | 62 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | Z | 78 | LYS |
| 27 | a | 105 | GLY |
| 28 | b | 10 | PRO |
| 29 | c | 39 | SER |
| 31 | e | 97 | GLU |
| 32 | f | 93 | HIS |
| 32 | f | 94 | LYS |
| 32 | f | 147 | THR |
| 1 | A | 110 | ASN |
| 5 | E | 73 | ASP |
| 6 | F | 46 | ALA |
| 6 | F | 183 | GLY |
| 7 | G | 68 | LEU |
| 7 | G | 165 | GLU |
| 8 | H | 170 | VAL |
| 10 | J | 68 | PRO |
| 10 | J | 116 | LYS |
| 14 | N | 60 | VAL |
| 15 | O | 24 | GLY |
| 15 | O | 136 | PRO |
| 22 | V | 9 | VAL |
| 24 | X | 78 | GLY |
| 4 | D | 63 | GLY |
| 9 | I | 119 | LEU |
| 21 | U | 104 | ILE |
| 22 | V | 77 | GLY |
| 32 | f | 87 | THR |
| 5 | E | 152 | PRO |
| 8 | H | 10 | LYS |
| 1 | A | 95 | GLY |
| 1 | A | 98 | PRO |
| 2 | B | 24 | PRO |
| 3 | C | 161 | LYS |
| 5 | E | 195 | ILE |
| 5 | E | 231 | GLY |
| 15 | O | 62 | VAL |
| 17 | Q | 42 | ILE |
| 27 | a | 96 | THR |
| 28 | b | 37 | CYS |
| 30 | d | 11 | PRO |
| 2 | B | 21 | VAL |
| 8 | H | 93 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | M | 30 | GLY |
| 28 | b | 9 | HIS |
| 4 | D | 200 | PRO |
| 18 | R | 15 | VAL |
| 21 | U | 29 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 174/244 (71%) | 139 (80%) | 35 (20%) | 1 | 7 |
| 2 | B | 196/231 (85%) | 155 (79%) | 41 (21%) | 1 | 6 |
| 3 | C | 187/215 (87%) | 147 (79%) | 40 (21%) | 1 | 6 |
| 4 | D | 190/202 (94%) | 144 (76%) | 46 (24%) | 0 | 4 |
| 5 | E | 225/225 (100%) | 173 (77%) | 52 (23%) | 1 | 4 |
| 6 | F | 161/170 (95%) | 116 (72%) | 45 (28%) | 0 | 3 |
| 7 | G | 207/218 (95%) | 157 (76%) | 50 (24%) | 0 | 4 |
| 8 | H | 170/174 (98%) | 124 (73%) | 46 (27%) | 0 | 3 |
| 9 | I | 177/179 (99%) | 142 (80%) | 35 (20%) | 1 | 8 |
| 10 | J | 157/168 (94%) | 128 (82%) | 29 (18%) | 1 | 9 |
| 11 | K | 89/136 (65%) | 61 (68%) | 28 (32%) | 0 | 2 |
| 12 | L | 142/142 (100%) | 105 (74%) | 37 (26%) | 0 | 3 |
| 13 | M | 101/108 (94%) | 78 (77%) | 23 (23%) | 1 | 5 |
| 14 | N | 130/131 (99%) | 103 (79%) | 27 (21%) | 1 | 6 |
| 15 | O | 106/119 (89%) | 87 (82%) | 19 (18%) | 2 | 10 |
| 16 | P | 116/130 (89%) | 84 (72%) | 32 (28%) | 0 | 3 |
| 17 | Q | 117/121 (97%) | 89 (76%) | 28 (24%) | 0 | 4 |
| 18 | R | 114/121 (94%) | 90 (79%) | 24 (21%) | 1 | 6 |
| 19 | S | 119/132 (90%) | 95 (80%) | 24 (20%) | 1 | 7 |
| 20 | T | 113/116 (97%) | 87 (77%) | 26 (23%) | 1 | 4 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 21 | U | 94/107 (88%) | 74 (79%) | 20 (21%) | 1 | 6 |
| 22 | V | 67/68 (98%) | 50 (75%) | 17 (25%) | 0 | 3 |
| 23 | W | 112/113 (99%) | 98 (88%) | 14 (12%) | 4 | 19 |
| 24 | X | 114/115 (99%) | 91 (80%) | 23 (20%) | 1 | 7 |
| 25 | Y | 108/115 (94%) | 85 (79%) | 23 (21%) | 1 | 6 |
| 26 | Z | 66/103 (64%) | 53 (80%) | 13 (20%) | 1 | 8 |
| 27 | a | 91/99 (92%) | 76 (84%) | 15 (16%) | 2 | 12 |
| 28 | b | 76/76 (100%) | 63 (83%) | 13 (17%) | 2 | 11 |
| 29 | c | 57/62 (92%) | 46 (81%) | 11 (19%) | 1 | 8 |
| 30 | d | 47/49 (96%) | 35 (74%) | 12 (26%) | 0 | 3 |
| 31 | e | 49/106 (46%) | 26 (53%) | 23 (47%) | 0 | 0 |
| 32 | f | 64/140 (46%) | 43 (67%) | 21 (33%) | 0 | 2 |
| 33 | g | 272/275 (99%) | 224 (82%) | 48 (18%) | 2 | 11 |
| 37 | n | 66/123 (54%) | 48 (73%) | 18 (27%) | 0 | 3 |
| All | All | 4274/4833 (88%) | 3316 (78%) | 958 (22%) | 1 | 5 |

All (958) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 5 | LEU |
| 1 | A | 7 | VAL |
| 1 | A | 10 | MET |
| 1 | A | 12 | GLU |
| 1 | A | 13 | GLU |
| 1 | A | 17 | LYS |
| 1 | A | 19 | LEU |
| 1 | A | 25 | LEU |
| 1 | A | 36 | GLN |
| 1 | A | 40 | LYS |
| 1 | A | 42 | LYS |
| 1 | A | 44 | ASP |
| 1 | A | 52 | LYS |
| 1 | A | 58 | LEU |
| 1 | A | 63 | ARG |
| 1 | A | 73 | ASP |
| 1 | A | 88 | LEU |
| 1 | A | 89 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 102 | ARG |
| 1 | A | 117 | ARG |
| 1 | A | 128 | ARG |
| 1 | A | 139 | TYR |
| 1 | A | 147 | LEU |
| 1 | A | 155 | ARG |
| 1 | A | 159 | ILE |
| 1 | A | 169 | HIS |
| 1 | A | 181 | GLU |
| 1 | A | 186 | ARG |
| 1 | A | 188 | THR |
| 1 | A | 191 | ARG |
| 1 | A | 195 | TRP |
| 1 | A | 196 | GLU |
| 1 | A | 198 | MET |
| 1 | A | 204 | TYR |
| 1 | A | 207 | PRO |
| 2 | B | 19 | LYS |
| 2 | B | 20 | LYS |
| 2 | B | 21 | VAL |
| 2 | B | 22 | VAL |
| 2 | B | 34 | LYS |
| 2 | B | 41 | ILE |
| 2 | B | 48 | LEU |
| 2 | B | 52 | THR |
| 2 | B | 55 | THR |
| 2 | B | 56 | LYS |
| 2 | B | 75 | GLN |
| 2 | B | 78 | GLU |
| 2 | B | 82 | ARG |
| 2 | B | 83 | LYS |
| 2 | B | 89 | GLU |
| 2 | B | 94 | LYS |
| 2 | B | 115 | LYS |
| 2 | B | 116 | LYS |
| 2 | B | 131 | ASP |
| 2 | B | 138 | PHE |
| 2 | B | 144 | LYS |
| 2 | B | 148 | ASN |
| 2 | B | 150 | ILE |
| 2 | B | 151 | ARG |
| 2 | B | 158 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 162 | ARG |
| 2 | B | 165 | ARG |
| 2 | B | 166 | LYS |
| 2 | B | 172 | MET |
| 2 | B | 181 | LEU |
| 2 | B | 182 | LYS |
| 2 | B | 195 | LYS |
| 2 | B | 208 | HIS |
| 2 | B | 211 | PHE |
| 2 | B | 213 | ARG |
| 2 | B | 214 | LYS |
| 2 | B | 219 | LYS |
| 2 | B | 222 | LYS |
| 2 | B | 223 | PHE |
| 2 | B | 227 | LYS |
| 2 | B | 229 | MET |
| 3 | C | 43 | LYS |
| 3 | C | 48 | VAL |
| 3 | C | 49 | THR |
| 3 | C | 50 | LYS |
| 3 | C | 51 | LEU |
| 3 | C | 56 | LYS |
| 3 | C | 58 | MET |
| 3 | C | 59 | LYS |
| 3 | C | 61 | LYS |
| 3 | C | 79 | ILE |
| 3 | C | 89 | ASP |
| 3 | C | 95 | MET |
| 3 | C | 99 | LYS |
| 3 | C | 100 | GLN |
| 3 | C | 101 | THR |
| 3 | C | 105 | GLN |
| 3 | C | 119 | ASN |
| 3 | C | 127 | LYS |
| 3 | C | 131 | GLU |
| 3 | C | 145 | LEU |
| 3 | C | 151 | ARG |
| 3 | C | 152 | ARG |
| 3 | C | 157 | ASN |
| 3 | C | 158 | LYS |
| 3 | C | 168 | LYS |
| 3 | C | 169 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 196 | LYS |
| 3 | C | 197 | LYS |
| 3 | C | 201 | MET |
| 3 | C | 221 | PHE |
| 3 | C | 223 | LYS |
| 3 | C | 235 | TYR |
| 3 | C | 242 | LYS |
| 3 | C | 244 | THR |
| 3 | C | 246 | PHE |
| 3 | C | 247 | THR |
| 3 | C | 248 | LYS |
| 3 | C | 252 | GLN |
| 3 | C | 256 | ASP |
| 3 | C | 260 | LYS |
| 4 | D | 8 | LYS |
| 4 | D | 10 | LYS |
| 4 | D | 18 | LYS |
| 4 | D | 21 | LEU |
| 4 | D | 27 | ARG |
| 4 | D | 31 | GLU |
| 4 | D | 35 | SER |
| 4 | D | 44 | THR |
| 4 | D | 56 | GLN |
| 4 | D | 64 | ARG |
| 4 | D | 67 | ARG |
| 4 | D | 74 | GLN |
| 4 | D | 76 | ARG |
| 4 | D | 79 | PHE |
| 4 | D | 89 | GLU |
| 4 | D | 90 | LYS |
| 4 | D | 94 | ARG |
| 4 | D | 97 | CYS |
| 4 | D | 103 | GLU |
| 4 | D | 113 | LEU |
| 4 | D | 120 | TYR |
| 4 | D | 127 | MET |
| 4 | D | 129 | SER |
| 4 | D | 146 | ARG |
| 4 | D | 151 | LYS |
| 4 | D | 156 | LEU |
| 4 | D | 157 | MET |
| 4 | D | 158 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 176 | LEU |
| 4 | D | 177 | LEU |
| 4 | D | 178 | ARG |
| 4 | D | 187 | LYS |
| 4 | D | 190 | LEU |
| 4 | D | 192 | TRP |
| 4 | D | 198 | ILE |
| 4 | D | 202 | LYS |
| 4 | D | 206 | ASP |
| 4 | D | 207 | HIS |
| 4 | D | 211 | VAL |
| 4 | D | 212 | GLU |
| 4 | D | 214 | LYS |
| 4 | D | 215 | ASP |
| 4 | D | 216 | GLU |
| 4 | D | 218 | LEU |
| 4 | D | 220 | THR |
| 4 | D | 226 | GLN |
| 5 | E | 1 | MET |
| 5 | E | 6 | LYS |
| 5 | E | 7 | LYS |
| 5 | E | 9 | LEU |
| 5 | E | 10 | LYS |
| 5 | E | 38 | LEU |
| 5 | E | 39 | ARG |
| 5 | E | 48 | LEU |
| 5 | E | 49 | ARG |
| 5 | E | 56 | LEU |
| 5 | E | 65 | CYS |
| 5 | E | 67 | GLN |
| 5 | E | 68 | ARG |
| 5 | E | 77 | ARG |
| 5 | E | 94 | LYS |
| 5 | E | 97 | GLU |
| 5 | E | 106 | LYS |
| 5 | E | 118 | GLU |
| 5 | E | 120 | LYS |
| 5 | E | 122 | LYS |
| 5 | E | 123 | LEU |
| 5 | E | 125 | LYS |
| 5 | E | 128 | LYS |
| 5 | E | 130 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 133 | THR |
| 5 | E | 136 | ILE |
| 5 | E | 145 | ARG |
| 5 | E | 147 | ILE |
| 5 | E | 148 | ARG |
| 5 | E | 151 | ASP |
| 5 | E | 153 | LEU |
| 5 | E | 164 | LEU |
| 5 | E | 165 | GLU |
| 5 | E | 168 | LYS |
| 5 | E | 174 | LYS |
| 5 | E | 175 | PHE |
| 5 | E | 180 | LEU |
| 5 | E | 181 | CYS |
| 5 | E | 198 | ARG |
| 5 | E | 200 | ARG |
| 5 | E | 202 | PRO |
| 5 | E | 211 | LYS |
| 5 | E | 212 | ASP |
| 5 | E | 221 | ARG |
| 5 | E | 222 | LEU |
| 5 | E | 237 | SER |
| 5 | E | 240 | ARG |
| 5 | E | 242 | LYS |
| 5 | E | 245 | ARG |
| 5 | E | 246 | LEU |
| 5 | E | 259 | LYS |
| 5 | E | 260 | GLN |
| 6 | F | 15 | PRO |
| 6 | F | 18 | LYS |
| 6 | F | 29 | GLN |
| 6 | F | 36 | GLN |
| 6 | F | 37 | ASP |
| 6 | F | 38 | TYR |
| 6 | F | 41 | VAL |
| 6 | F | 42 | LYS |
| 6 | F | 43 | GLU |
| 6 | F | 44 | LYS |
| 6 | F | 47 | LYS |
| 6 | F | 49 | LEU |
| 6 | F | 60 | ARG |
| 6 | F | 62 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 63 | LYS |
| 6 | F | 65 | GLN |
| 6 | F | 71 | ARG |
| 6 | F | 76 | MET |
| 6 | F | 78 | MET |
| 6 | F | 85 | LYS |
| 6 | F | 88 | MET |
| 6 | F | 91 | ARG |
| 6 | F | 94 | LYS |
| 6 | F | 98 | GLU |
| 6 | F | 110 | GLN |
| 6 | F | 116 | ILE |
| 6 | F | 122 | ARG |
| 6 | F | 125 | SER |
| 6 | F | 127 | ARG |
| 6 | F | 128 | ILE |
| 6 | F | 130 | ARG |
| 6 | F | 136 | ARG |
| 6 | F | 145 | ARG |
| 6 | F | 164 | ARG |
| 6 | F | 167 | LYS |
| 6 | F | 173 | LEU |
| 6 | F | 175 | ASP |
| 6 | F | 177 | LEU |
| 6 | F | 182 | LYS |
| 6 | F | 186 | ASN |
| 6 | F | 190 | ILE |
| 6 | F | 192 | LYS |
| 6 | F | 195 | GLU |
| 6 | F | 202 | SER |
| 6 | F | 204 | ARG |
| 7 | G | 1 | MET |
| 7 | G | 2 | LYS |
| 7 | G | 13 | GLN |
| 7 | G | 17 | GLU |
| 7 | G | 19 | ASP |
| 7 | G | 29 | GLU |
| 7 | G | 30 | LYS |
| 7 | G | 31 | ARG |
| 7 | G | 32 | MET |
| 7 | G | 44 | GLU |
| 7 | G | 58 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 64 | LYS |
| 7 | G | 74 | ARG |
| 7 | G | 76 | LEU |
| 7 | G | 77 | LEU |
| 7 | G | 79 | LYS |
| 7 | G | 88 | ARG |
| 7 | G | 94 | ARG |
| 7 | G | 98 | ARG |
| 7 | G | 115 | LYS |
| 7 | G | 116 | LYS |
| 7 | G | 120 | ASP |
| 7 | G | 121 | ILE |
| 7 | G | 126 | ASP |
| 7 | G | 127 | THR |
| 7 | G | 128 | THR |
| 7 | G | 131 | ARG |
| 7 | G | 133 | LEU |
| 7 | G | 137 | ARG |
| 7 | G | 142 | ARG |
| 7 | G | 143 | LYS |
| 7 | G | 145 | PHE |
| 7 | G | 150 | GLU |
| 7 | G | 158 | VAL |
| 7 | G | 159 | ARG |
| 7 | G | 164 | LYS |
| 7 | G | 168 | LYS |
| 7 | G | 170 | ARG |
| 7 | G | 172 | LYS |
| 7 | G | 175 | LYS |
| 7 | G | 179 | LEU |
| 7 | G | 180 | VAL |
| 7 | G | 191 | ARG |
| 7 | G | 196 | LYS |
| 7 | G | 198 | ARG |
| 7 | G | 218 | LYS |
| 7 | G | 219 | GLU |
| 7 | G | 224 | ARG |
| 7 | G | 230 | LYS |
| 7 | G | 233 | ARG |
| 8 | H | 9 | VAL |
| 8 | H | 10 | LYS |
| 8 | H | 11 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | H | 14 | GLU |
| 8 | H | 15 | LYS |
| 8 | H | 16 | PRO |
| 8 | H | 17 | ASP |
| 8 | H | 23 | ILE |
| 8 | H | 32 | MET |
| 8 | H | 34 | SER |
| 8 | H | 36 | LEU |
| 8 | H | 37 | LYS |
| 8 | H | 40 | LEU |
| 8 | H | 57 | ARG |
| 8 | H | 58 | LYS |
| 8 | H | 61 | ILE |
| 8 | H | 69 | LEU |
| 8 | H | 72 | PHE |
| 8 | H | 74 | LYS |
| 8 | H | 78 | ARG |
| 8 | H | 81 | ARG |
| 8 | H | 82 | GLU |
| 8 | H | 85 | LYS |
| 8 | H | 87 | PHE |
| 8 | H | 93 | VAL |
| 8 | H | 99 | ARG |
| 8 | H | 105 | THR |
| 8 | H | 107 | LYS |
| 8 | H | 109 | ARG |
| 8 | H | 111 | LYS |
| 8 | H | 112 | ASN |
| 8 | H | 113 | LYS |
| 8 | H | 116 | ARG |
| 8 | H | 118 | ARG |
| 8 | H | 120 | ARG |
| 8 | H | 122 | LEU |
| 8 | H | 131 | GLU |
| 8 | H | 143 | ARG |
| 8 | H | 145 | ARG |
| 8 | H | 157 | HIS |
| 8 | H | 158 | LEU |
| 8 | H | 160 | LYS |
| 8 | H | 163 | GLN |
| 8 | H | 179 | LYS |
| 8 | H | 185 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | H | 193 | GLN |
| 9 | I | 3 | ILE |
| 9 | I | 5 | ARG |
| 9 | I | 6 | ASP |
| 9 | I | 13 | LYS |
| 9 | I | 19 | LYS |
| 9 | I | 23 | LYS |
| 9 | I | 25 | ARG |
| 9 | I | 37 | LYS |
| 9 | I | 41 | ARG |
| 9 | I | 49 | ARG |
| 9 | I | 56 | ARG |
| 9 | I | 70 | GLU |
| 9 | I | 74 | ARG |
| 9 | I | 100 | CYS |
| 9 | I | 110 | ARG |
| 9 | I | 117 | TYR |
| 9 | I | 119 | LEU |
| 9 | I | 123 | ARG |
| 9 | I | 124 | LYS |
| 9 | I | 125 | LYS |
| 9 | I | 140 | LYS |
| 9 | I | 141 | ARG |
| 9 | I | 143 | LYS |
| 9 | I | 144 | LYS |
| 9 | I | 148 | LYS |
| 9 | I | 150 | ASP |
| 9 | I | 154 | LYS |
| 9 | I | 155 | ASN |
| 9 | I | 158 | ILE |
| 9 | I | 161 | LEU |
| 9 | I | 167 | GLN |
| 9 | I | 191 | GLU |
| 9 | I | 202 | ILE |
| 9 | I | 205 | ARG |
| 9 | I | 206 | LYS |
| 10 | J | 8 | VAL |
| 10 | J | 10 | ARG |
| 10 | J | 17 | ARG |
| 10 | J | 18 | ARG |
| 10 | J | 29 | LEU |
| 10 | J | 38 | ARG |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 42 | GLU |
| 10 | J | 50 | LEU |
| 10 | J | 58 | ARG |
| 10 | J | 66 | LYS |
| 10 | J | 69 | ARG |
| 10 | J | 79 | ARG |
| 10 | J | 89 | GLU |
| 10 | J | 93 | LYS |
| 10 | J | 101 | LYS |
| 10 | J | 108 | ARG |
| 10 | J | 109 | ARG |
| 10 | J | 110 | LEU |
| 10 | J | 119 | LEU |
| 10 | J | 121 | LYS |
| 10 | J | 127 | ARG |
| 10 | J | 139 | LYS |
| 10 | J | 143 | ASN |
| 10 | J | 162 | ARG |
| 10 | J | 165 | TYR |
| 10 | J | 172 | ARG |
| 10 | J | 174 | LYS |
| 10 | J | 176 | LYS |
| 10 | J | 180 | LYS |
| 11 | K | 1 | MET |
| 11 | K | 2 | LEU |
| 11 | K | 3 | MET |
| 11 | K | 5 | LYS |
| 11 | K | 13 | GLU |
| 11 | K | 16 | PHE |
| 11 | K | 17 | LYS |
| 11 | K | 20 | VAL |
| 11 | K | 31 | LYS |
| 11 | K | 34 | GLU |
| 11 | K | 35 | LEU |
| 11 | K | 37 | ASP |
| 11 | K | 38 | LYS |
| 11 | K | 43 | LEU |
| 11 | K | 53 | LYS |
| 11 | K | 55 | ARG |
| 11 | K | 65 | ARG |
| 11 | K | 66 | HIS |
| 11 | K | 69 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | K | 74 | GLU |
| 11 | K | 84 | HIS |
| 11 | K | 85 | LEU |
| 11 | K | 89 | ILE |
| 11 | K | 93 | THR |
| 11 | K | 94 | LEU |
| 11 | K | 95 | ARG |
| 11 | K | 96 | ARG |
| 11 | K | 98 | ARG |
| 12 | L | 1 | MET |
| 12 | L | 4 | ILE |
| 12 | L | 7 | GLU |
| 12 | L | 8 | ARG |
| 12 | L | 12 | LYS |
| 12 | L | 15 | THR |
| 12 | L | 18 | GLN |
| 12 | L | 20 | LYS |
| 12 | L | 22 | ARG |
| 12 | L | 25 | LEU |
| 12 | L | 30 | LYS |
| 12 | L | 40 | ILE |
| 12 | L | 49 | GLU |
| 12 | L | 56 | ILE |
| 12 | L | 69 | ARG |
| 12 | L | 71 | ARG |
| 12 | L | 79 | LYS |
| 12 | L | 80 | MET |
| 12 | L | 82 | MET |
| 12 | L | 83 | GLN |
| 12 | L | 89 | ARG |
| 12 | L | 97 | ARG |
| 12 | L | 99 | TYR |
| 12 | L | 100 | ASN |
| 12 | L | 101 | ARG |
| 12 | L | 102 | PHE |
| 12 | L | 105 | ARG |
| 12 | L | 118 | ARG |
| 12 | L | 121 | GLN |
| 12 | L | 136 | LYS |
| 12 | L | 147 | LYS |
| 12 | L | 151 | THR |
| 12 | L | 153 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 155 | PHE |
| 12 | L | 156 | GLN |
| 12 | L | 157 | LYS |
| 12 | L | 158 | PHE |
| 13 | M | 12 | MET |
| 13 | M | 13 | ASP |
| 13 | M | 18 | LEU |
| 13 | M | 20 | GLU |
| 13 | M | 26 | LEU |
| 13 | M | 28 | HIS |
| 13 | M | 33 | ARG |
| 13 | M | 36 | ARG |
| 13 | M | 40 | LYS |
| 13 | M | 43 | ASP |
| 13 | M | 45 | ARG |
| 13 | M | 71 | GLU |
| 13 | M | 76 | LEU |
| 13 | M | 77 | ILE |
| 13 | M | 78 | LYS |
| 13 | M | 83 | LYS |
| 13 | M | 85 | LEU |
| 13 | M | 91 | LEU |
| 13 | M | 94 | ILE |
| 13 | M | 101 | ARG |
| 13 | M | 102 | LYS |
| 13 | M | 127 | TYR |
| 13 | M | 128 | PHE |
| 14 | N | 3 | ARG |
| 14 | N | 9 | LYS |
| 14 | N | 16 | LEU |
| 14 | N | 21 | SER |
| 14 | N | 27 | LYS |
| 14 | N | 49 | GLN |
| 14 | N | 50 | ILE |
| 14 | N | 53 | ILE |
| 14 | N | 56 | ASP |
| 14 | N | 64 | ARG |
| 14 | N | 73 | ARG |
| 14 | N | 76 | LYS |
| 14 | N | 78 | LYS |
| 14 | N | 80 | LEU |
| 14 | N | 94 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | N | 104 | ARG |
| 14 | N | 107 | LYS |
| 14 | N | 112 | LYS |
| 14 | N | 114 | ARG |
| 14 | N | 119 | GLU |
| 14 | N | 121 | ARG |
| 14 | N | 125 | LEU |
| 14 | N | 130 | LYS |
| 14 | N | 133 | ARG |
| 14 | N | 134 | VAL |
| 14 | N | 141 | TYR |
| 14 | N | 142 | GLU |
| 15 | O | 23 | GLU |
| 15 | O | 25 | GLU |
| 15 | O | 28 | PHE |
| 15 | O | 34 | PHE |
| 15 | O | 65 | ASP |
| 15 | O | 66 | ARG |
| 15 | O | 72 | TYR |
| 15 | O | 90 | ILE |
| 15 | O | 103 | ASN |
| 15 | O | 116 | LEU |
| 15 | O | 117 | ARG |
| 15 | O | 121 | ARG |
| 15 | O | 125 | LYS |
| 15 | O | 128 | ARG |
| 15 | O | 129 | ILE |
| 15 | O | 138 | ASP |
| 15 | O | 141 | ARG |
| 15 | O | 146 | ARG |
| 15 | O | 150 | ARG |
| 16 | P | 5 | GLU |
| 16 | P | 6 | GLN |
| 16 | P | 7 | LYS |
| 16 | P | 10 | ARG |
| 16 | P | 12 | PHE |
| 16 | P | 13 | ARG |
| 16 | P | 14 | LYS |
| 16 | P | 15 | PHE |
| 16 | P | 17 | TYR |
| 16 | P | 34 | MET |
| 16 | P | 40 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | P | 41 | GLN |
| 16 | P | 43 | ARG |
| 16 | P | 50 | ARG |
| 16 | P | 51 | ARG |
| 16 | P | 52 | LYS |
| 16 | P | 61 | ARG |
| 16 | P | 64 | LYS |
| 16 | P | 71 | GLU |
| 16 | P | 72 | LYS |
| 16 | P | 74 | GLU |
| 16 | P | 84 | ILE |
| 16 | P | 86 | LEU |
| 16 | P | 88 | GLU |
| 16 | P | 89 | MET |
| 16 | P | 100 | LYS |
| 16 | P | 104 | GLN |
| 16 | P | 110 | GLU |
| 16 | P | 111 | MET |
| 16 | P | 122 | THR |
| 16 | P | 124 | LYS |
| 16 | P | 127 | LYS |
| 17 | Q | 6 | PRO |
| 17 | Q | 7 | LEU |
| 17 | Q | 13 | PHE |
| 17 | Q | 17 | LYS |
| 17 | Q | 20 | THR |
| 17 | Q | 24 | HIS |
| 17 | Q | 26 | LYS |
| 17 | Q | 33 | LYS |
| 17 | Q | 37 | ARG |
| 17 | Q | 41 | MET |
| 17 | Q | 56 | LEU |
| 17 | Q | 62 | ARG |
| 17 | Q | 73 | LYS |
| 17 | Q | 101 | ASP |
| 17 | Q | 102 | GLU |
| 17 | Q | 105 | LYS |
| 17 | Q | 107 | GLU |
| 17 | Q | 115 | TYR |
| 17 | Q | 117 | ARG |
| 17 | Q | 120 | LEU |
| 17 | Q | 126 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | Q | 130 | LYS |
| 17 | Q | 131 | LYS |
| 17 | Q | 135 | PRO |
| 17 | Q | 140 | ARG |
| 17 | Q | 142 | GLN |
| 17 | Q | 145 | TYR |
| 17 | Q | 146 | ARG |
| 18 | R | 1 | MET |
| 18 | R | 8 | THR |
| 18 | R | 26 | ASN |
| 18 | R | 32 | LYS |
| 18 | R | 47 | ARG |
| 18 | R | 59 | LYS |
| 18 | R | 63 | ARG |
| 18 | R | 69 | ILE |
| 18 | R | 78 | ARG |
| 18 | R | 83 | ASN |
| 18 | R | 87 | GLU |
| 18 | R | 88 | VAL |
| 18 | R | 89 | SER |
| 18 | R | 91 | LEU |
| 18 | R | 93 | GLN |
| 18 | R | 94 | GLU |
| 18 | R | 95 | ILE |
| 18 | R | 103 | LYS |
| 18 | R | 105 | MET |
| 18 | R | 111 | PHE |
| 18 | R | 118 | GLN |
| 18 | R | 120 | THR |
| 18 | R | 121 | GLN |
| 18 | R | 123 | THR |
| 19 | S | 7 | GLU |
| 19 | S | 8 | LYS |
| 19 | S | 9 | PHE |
| 19 | S | 11 | HIS |
| 19 | S | 12 | ILE |
| 19 | S | 17 | ASN |
| 19 | S | 34 | LYS |
| 19 | S | 36 | VAL |
| 19 | S | 39 | ARG |
| 19 | S | 59 | LEU |
| 19 | S | 63 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | S | 71 | MET |
| 19 | S | 78 | LYS |
| 19 | S | 86 | ARG |
| 19 | S | 87 | GLN |
| 19 | S | 92 | ASP |
| 19 | S | 94 | LYS |
| 19 | S | 118 | ARG |
| 19 | S | 125 | HIS |
| 19 | S | 130 | ARG |
| 19 | S | 132 | ARG |
| 19 | S | 134 | GLN |
| 19 | S | 137 | LYS |
| 19 | S | 142 | ARG |
| 20 | T | 11 | GLN |
| 20 | T | 16 | ARG |
| 20 | T | 21 | PHE |
| 20 | T | 23 | LYS |
| 20 | T | 28 | LEU |
| 20 | T | 29 | LYS |
| 20 | T | 38 | LYS |
| 20 | T | 41 | LYS |
| 20 | T | 42 | HIS |
| 20 | T | 44 | GLU |
| 20 | T | 62 | ARG |
| 20 | T | 64 | LEU |
| 20 | T | 67 | ARG |
| 20 | T | 83 | GLN |
| 20 | T | 84 | ARG |
| 20 | T | 88 | MET |
| 20 | T | 91 | HIS |
| 20 | T | 93 | SER |
| 20 | T | 94 | ARG |
| 20 | T | 97 | LYS |
| 20 | T | 102 | ARG |
| 20 | T | 121 | ARG |
| 20 | T | 130 | ASP |
| 20 | T | 133 | ARG |
| 20 | T | 143 | LYS |
| 20 | T | 144 | LYS |
| 21 | U | 19 | ARG |
| 21 | U | 20 | ILE |
| 21 | U | 21 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | U | 24 | LEU |
| 21 | U | 33 | GLU |
| 21 | U | 44 | LYS |
| 21 | U | 47 | ASN |
| 21 | U | 48 | LEU |
| 21 | U | 49 | LYS |
| 21 | U | 51 | LYS |
| 21 | U | 62 | ARG |
| 21 | U | 68 | THR |
| 21 | U | 72 | GLU |
| 21 | U | 75 | LYS |
| 21 | U | 85 | HIS |
| 21 | U | 87 | ARG |
| 21 | U | 104 | ILE |
| 21 | U | 106 | ILE |
| 21 | U | 108 | PRO |
| 21 | U | 111 | GLU |
| 22 | V | 1 | MET |
| 22 | V | 7 | GLU |
| 22 | V | 16 | LYS |
| 22 | V | 24 | ILE |
| 22 | V | 31 | SER |
| 22 | V | 32 | ILE |
| 22 | V | 40 | ASP |
| 22 | V | 41 | LYS |
| 22 | V | 43 | THR |
| 22 | V | 45 | ARG |
| 22 | V | 49 | GLN |
| 22 | V | 51 | LYS |
| 22 | V | 52 | THR |
| 22 | V | 61 | ARG |
| 22 | V | 64 | GLU |
| 22 | V | 74 | LYS |
| 22 | V | 78 | ILE |
| 23 | W | 3 | ARG |
| 23 | W | 4 | MET |
| 23 | W | 18 | GLU |
| 23 | W | 20 | ARG |
| 23 | W | 23 | ARG |
| 23 | W | 52 | ILE |
| 23 | W | 64 | ASN |
| 23 | W | 84 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | W | 98 | GLN |
| 23 | W | 103 | VAL |
| 23 | W | 114 | GLU |
| 23 | W | 124 | LYS |
| 23 | W | 128 | PHE |
| 23 | W | 129 | PHE |
| 24 | X | 1 | MET |
| 24 | X | 3 | LYS |
| 24 | X | 5 | ARG |
| 24 | X | 7 | LEU |
| 24 | X | 12 | LYS |
| 24 | X | 21 | LYS |
| 24 | X | 29 | LYS |
| 24 | X | 37 | LYS |
| 24 | X | 67 | ARG |
| 24 | X | 68 | LYS |
| 24 | X | 71 | ARG |
| 24 | X | 75 | ILE |
| 24 | X | 80 | LYS |
| 24 | X | 91 | LEU |
| 24 | X | 98 | ASP |
| 24 | X | 101 | LEU |
| 24 | X | 107 | ARG |
| 24 | X | 108 | LYS |
| 24 | X | 110 | HIS |
| 24 | X | 115 | ILE |
| 24 | X | 135 | LYS |
| 24 | X | 141 | PRO |
| 24 | X | 142 | ARG |
| 25 | Y | 16 | ARG |
| 25 | Y | 20 | ARG |
| 25 | Y | 21 | LYS |
| 25 | Y | 23 | MET |
| 25 | Y | 29 | HIS |
| 25 | Y | 32 | LYS |
| 25 | Y | 35 | VAL |
| 25 | Y | 46 | LYS |
| 25 | Y | 58 | PHE |
| 25 | Y | 61 | ARG |
| 25 | Y | 64 | PHE |
| 25 | Y | 68 | LYS |
| 25 | Y | 93 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | Y | 96 | LEU |
| 25 | Y | 97 | TYR |
| 25 | Y | 98 | GLU |
| 25 | Y | 99 | LYS |
| 25 | Y | 100 | LYS |
| 25 | Y | 101 | LYS |
| 25 | Y | 102 | THR |
| 25 | Y | 111 | LYS |
| 25 | Y | 118 | ARG |
| 25 | Y | 122 | LYS |
| 26 | Z | 44 | LEU |
| 26 | Z | 50 | PHE |
| 26 | Z | 52 | LYS |
| 26 | Z | 65 | TYR |
| 26 | Z | 85 | ARG |
| 26 | Z | 91 | LEU |
| 26 | Z | 94 | LYS |
| 26 | Z | 102 | LYS |
| 26 | Z | 103 | HIS |
| 26 | Z | 104 | ARG |
| 26 | Z | 107 | VAL |
| 26 | Z | 112 | ASN |
| 26 | Z | 114 | LYS |
| 27 | a | 10 | ARG |
| 27 | a | 15 | ARG |
| 27 | a | 26 | CYS |
| 27 | a | 38 | LYS |
| 27 | a | 41 | ILE |
| 27 | a | 44 | ILE |
| 27 | a | 50 | VAL |
| 27 | a | 51 | ARG |
| 27 | a | 60 | ASP |
| 27 | a | 63 | VAL |
| 27 | a | 70 | LYS |
| 27 | a | 82 | LYS |
| 27 | a | 85 | ARG |
| 27 | a | 94 | ASP |
| 27 | a | 95 | ARG |
| 28 | b | 3 | LEU |
| 28 | b | 5 | LYS |
| 28 | b | 16 | LYS |
| 28 | b | 20 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | b | 23 | ARG |
| 28 | b | 26 | GLN |
| 28 | b | 41 | TYR |
| 28 | b | 42 | LYS |
| 28 | b | 49 | HIS |
| 28 | b | 51 | GLN |
| 28 | b | 53 | VAL |
| 28 | b | 83 | GLN |
| 28 | b | 84 | HIS |
| 29 | c | 5 | ARG |
| 29 | c | 7 | GLN |
| 29 | c | 13 | ARG |
| 29 | c | 35 | MET |
| 29 | c | 42 | ILE |
| 29 | c | 47 | LYS |
| 29 | c | 51 | ARG |
| 29 | c | 62 | GLU |
| 29 | c | 63 | ARG |
| 29 | c | 67 | ARG |
| 29 | c | 68 | LEU |
| 30 | d | 7 | TYR |
| 30 | d | 10 | HIS |
| 30 | d | 16 | GLN |
| 30 | d | 19 | ARG |
| 30 | d | 27 | ARG |
| 30 | d | 30 | LEU |
| 30 | d | 33 | LYS |
| 30 | d | 39 | CYS |
| 30 | d | 44 | ARG |
| 30 | d | 46 | TYR |
| 30 | d | 53 | ILE |
| 30 | d | 56 | ASP |
| 31 | e | 76 | VAL |
| 31 | e | 80 | LEU |
| 31 | e | 85 | LYS |
| 31 | e | 87 | ARG |
| 31 | e | 92 | LYS |
| 31 | e | 95 | LYS |
| 31 | e | 97 | GLU |
| 31 | e | 98 | LYS |
| 31 | e | 99 | LYS |
| 31 | e | 100 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | e | 103 | THR |
| 31 | e | 105 | ARG |
| 31 | e | 108 | ARG |
| 31 | e | 110 | MET |
| 31 | e | 114 | ARG |
| 31 | e | 115 | ARG |
| 31 | e | 118 | ASN |
| 31 | e | 120 | VAL |
| 31 | e | 122 | THR |
| 31 | e | 123 | PHE |
| 31 | e | 125 | LYS |
| 31 | e | 126 | LYS |
| 31 | e | 127 | LYS |
| 32 | f | 86 | THR |
| 32 | f | 88 | PRO |
| 32 | f | 89 | LYS |
| 32 | f | 90 | LYS |
| 32 | f | 94 | LYS |
| 32 | f | 95 | ARG |
| 32 | f | 96 | LYS |
| 32 | f | 97 | LYS |
| 32 | f | 104 | LYS |
| 32 | f | 109 | ASP |
| 32 | f | 110 | GLU |
| 32 | f | 111 | ASN |
| 32 | f | 113 | LYS |
| 32 | f | 116 | ARG |
| 32 | f | 118 | ARG |
| 32 | f | 121 | CYS |
| 32 | f | 130 | VAL |
| 32 | f | 135 | HIS |
| 32 | f | 136 | PHE |
| 32 | f | 139 | HIS |
| 32 | f | 150 | PHE |
| 33 | g | 8 | ARG |
| 33 | g | 24 | THR |
| 33 | g | 25 | PRO |
| 33 | g | 36 | ARG |
| 33 | g | 42 | MET |
| 33 | g | 44 | LYS |
| 33 | g | 47 | ARG |
| 33 | g | 50 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | g | 51 | ASN |
| 33 | g | 57 | ARG |
| 33 | g | 60 | ARG |
| 33 | g | 64 | HIS |
| 33 | g | 68 | ASP |
| 33 | g | 74 | ASP |
| 33 | g | 76 | GLN |
| 33 | g | 87 | LEU |
| 33 | g | 88 | ARG |
| 33 | g | 91 | ASP |
| 33 | g | 93 | THR |
| 33 | g | 100 | ARG |
| 33 | g | 118 | ARG |
| 33 | g | 119 | GLN |
| 33 | g | 131 | LEU |
| 33 | g | 139 | LYS |
| 33 | g | 140 | TYR |
| 33 | g | 143 | GLN |
| 33 | g | 145 | GLU |
| 33 | g | 146 | SER |
| 33 | g | 149 | GLU |
| 33 | g | 156 | PHE |
| 33 | g | 161 | SER |
| 33 | g | 175 | LYS |
| 33 | g | 183 | LYS |
| 33 | g | 185 | LYS |
| 33 | g | 192 | THR |
| 33 | g | 203 | ASP |
| 33 | g | 225 | LYS |
| 33 | g | 246 | TYR |
| 33 | g | 259 | TRP |
| 33 | g | 264 | LYS |
| 33 | g | 271 | LYS |
| 33 | g | 275 | ILE |
| 33 | g | 276 | SER |
| 33 | g | 277 | THR |
| 33 | g | 279 | SER |
| 33 | g | 280 | LYS |
| 33 | g | 289 | LEU |
| 33 | g | 294 | ASP |
| 37 | n | 34 | GLU |
| 37 | n | 35 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | n | 39 | ILE |
| 37 | n | 48 | GLU |
| 37 | n | 62 | ARG |
| 37 | n | 66 | ARG |
| 37 | n | 69 | VAL |
| 37 | n | 71 | ILE |
| 37 | n | 74 | SER |
| 37 | n | 78 | LEU |
| 37 | n | 81 | LEU |
| 37 | n | 83 | ASP |
| 37 | n | 85 | GLN |
| 37 | n | 95 | TYR |
| 37 | n | 101 | ARG |
| 37 | n | 102 | SER |
| 37 | n | 103 | LEU |
| 37 | n | 109 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 24 | HIS |
| 1 | A | 36 | GLN |
| 1 | A | 50 | ASN |
| 1 | A | 81 | ASN |
| 1 | A | 132 | GLN |
| 1 | A | 141 | ASN |
| 1 | A | 169 | HIS |
| 2 | B | 75 | GLN |
| 2 | B | 76 | ASN |
| 2 | B | 101 | HIS |
| 2 | B | 118 | GLN |
| 2 | B | 124 | HIS |
| 2 | B | 147 | ASN |
| 2 | B | 148 | ASN |
| 2 | B | 179 | ASN |
| 2 | B | 186 | ASN |
| 2 | B | 202 | GLN |
| 2 | B | 232 | HIS |
| 3 | C | 100 | GLN |
| 3 | C | 157 | ASN |
| 4 | D | 74 | GLN |
| 4 | D | 179 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 226 | GLN |
| 5 | E | 50 | ASN |
| 5 | E | 98 | ASN |
| 5 | E | 142 | HIS |
| 5 | E | 188 | ASN |
| 5 | E | 209 | HIS |
| 6 | F | 29 | GLN |
| 6 | F | 65 | GLN |
| 6 | F | 83 | ASN |
| 6 | F | 186 | ASN |
| 6 | F | 203 | ASN |
| 7 | G | 56 | ASN |
| 7 | G | 65 | GLN |
| 7 | G | 81 | HIS |
| 7 | G | 187 | HIS |
| 8 | H | 12 | ASN |
| 8 | H | 73 | GLN |
| 8 | H | 163 | GLN |
| 8 | H | 168 | HIS |
| 9 | I | 22 | HIS |
| 9 | I | 84 | ASN |
| 9 | I | 99 | ASN |
| 9 | I | 165 | GLN |
| 11 | K | 7 | ASN |
| 11 | K | 28 | HIS |
| 11 | K | 39 | ASN |
| 11 | K | 44 | HIS |
| 11 | K | 50 | GLN |
| 11 | K | 66 | HIS |
| 12 | L | 18 | GLN |
| 12 | L | 19 | ASN |
| 12 | L | 65 | ASN |
| 12 | L | 121 | GLN |
| 12 | L | 156 | GLN |
| 13 | M | 19 | GLN |
| 13 | M | 28 | HIS |
| 13 | M | 75 | ASN |
| 13 | M | 82 | ASN |
| 14 | N | 5 | HIS |
| 14 | N | 62 | GLN |
| 14 | N | 101 | HIS |
| 14 | N | 123 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | O | 20 | GLN |
| 16 | P | 41 | GLN |
| 16 | P | 53 | GLN |
| 16 | P | 79 | HIS |
| 16 | P | 103 | ASN |
| 16 | P | 114 | HIS |
| 16 | P | 128 | HIS |
| 17 | Q | 80 | GLN |
| 18 | R | 74 | GLN |
| 18 | R | 121 | GLN |
| 19 | S | 11 | HIS |
| 19 | S | 42 | HIS |
| 19 | S | 87 | GLN |
| 20 | T | 11 | GLN |
| 20 | T | 42 | HIS |
| 20 | T | 63 | HIS |
| 20 | T | 83 | GLN |
| 20 | T | 85 | ASN |
| 20 | T | 126 | GLN |
| 20 | T | 128 | GLN |
| 21 | U | 18 | HIS |
| 21 | U | 47 | ASN |
| 22 | V | 47 | ASN |
| 22 | V | 76 | HIS |
| 23 | W | 15 | ASN |
| 23 | W | 44 | HIS |
| 23 | W | 64 | ASN |
| 23 | W | 98 | GLN |
| 24 | X | 39 | ASN |
| 24 | X | 46 | HIS |
| 25 | Y | 29 | HIS |
| 25 | Y | 85 | ASN |
| 25 | Y | 89 | HIS |
| 25 | Y | 94 | HIS |
| 26 | Z | 103 | HIS |
| 27 | a | 80 | HIS |
| 28 | b | 49 | HIS |
| 28 | b | 83 | GLN |
| 28 | b | 84 | HIS |
| 29 | c | 26 | GLN |
| 30 | d | 26 | ASN |
| 30 | d | 28 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | e | 77 | HIS |
| 32 | f | 151 | ASN |
| 33 | g | 20 | GLN |
| 33 | g | 64 | HIS |
| 33 | g | 76 | GLN |
| 33 | g | 119 | GLN |
| 33 | g | 143 | GLN |
| 33 | g | 162 | ASN |
| 33 | g | 226 | HIS |
| 33 | g | 237 | ASN |
| 37 | n | 112 | HIS |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 34 | i | 1720/1863 (92%) | 496 (28%) | 0 |
| 35 | j | 74/75 (98%) | 17 (22%) | 0 |
| 36 | k | 12/24 (50%) | 3 (25%) | 0 |
| All | All | 1806/1962 (92%) | 516 (28%) | 0 |

All (516) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | i | 2 | A |
| 34 | i | 3 | C |
| 34 | i | 4 | C |
| 34 | i | 8 | U |
| 34 | i | 16 | G |
| 34 | i | 25 | A |
| 34 | i | 26 | U |
| 34 | i | 32 | U |
| 34 | i | 33 | G |
| 34 | i | 41 | G |
| 34 | i | 44 | U |
| 34 | i | 45 | A |
| 34 | i | 46 | A |
| 34 | i | 50 | A |
| 34 | i | 56 | G |
| 34 | i | 59 | U |
| 34 | i | 66 | G |
| 34 | i | 67 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | i | 68 | A |
| 34 | i | 70 | G |
| 34 | i | 72 | C |
| 34 | i | 73 | C |
| 34 | i | 74 | G |
| 34 | i | 75 | G |
| 34 | i | 76 | U |
| 34 | i | 77 | A |
| 34 | i | 78 | C |
| 34 | i | 79 | A |
| 34 | i | 80 | G |
| 34 | i | 99 | A |
| 34 | i | 103 | A |
| 34 | i | 113 | G |
| 34 | i | 126 | G |
| 34 | i | 139 | C |
| 34 | i | 140 | U |
| 34 | i | 141 | A |
| 34 | i | 142 | C |
| 34 | i | 143 | U |
| 34 | i | 147 | A |
| 34 | i | 148 | U |
| 34 | i | 155 | G |
| 34 | i | 160 | U |
| 34 | i | 161 | U |
| 34 | i | 162 | C |
| 34 | i | 170 | A |
| 34 | i | 176 | U |
| 34 | i | 182 | C |
| 34 | i | 183 | G |
| 34 | i | 187 | C |
| 34 | i | 188 | U |
| 34 | i | 189 | G |
| 34 | i | 190 | A |
| 34 | i | 191 | C |
| 34 | i | 197 | U |
| 34 | i | 198 | U |
| 34 | i | 199 | G |
| 34 | i | 203 | G |
| 34 | i | 205 | G |
| 34 | i | 206 | A |
| 34 | i | 212 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | i | 213 | C |
| 34 | i | 223 | A |
| 34 | i | 224 | U |
| 34 | i | 225 | C |
| 34 | i | 226 | A |
| 34 | i | 229 | A |
| 34 | i | 230 | C |
| 34 | i | 232 | A |
| 34 | i | 233 | A |
| 34 | i | 234 | C |
| 34 | i | 235 | C |
| 34 | i | 238 | G |
| 34 | i | 273 | G |
| 34 | i | 275 | C |
| 34 | i | 276 | U |
| 34 | i | 277 | U |
| 34 | i | 278 | U |
| 34 | i | 279 | G |
| 34 | i | 286 | C |
| 34 | i | 287 | U |
| 34 | i | 298 | G |
| 34 | i | 299 | G |
| 34 | i | 300 | G |
| 34 | i | 303 | G |
| 34 | i | 304 | A |
| 34 | i | 307 | G |
| 34 | i | 309 | A |
| 34 | i | 311 | C |
| 34 | i | 313 | C |
| 34 | i | 314 | U |
| 34 | i | 315 | C |
| 34 | i | 316 | C |
| 34 | i | 317 | G |
| 34 | i | 318 | U |
| 34 | i | 320 | G |
| 34 | i | 322 | G |
| 34 | i | 326 | A |
| 34 | i | 332 | C |
| 34 | i | 337 | G |
| 34 | i | 339 | A |
| 34 | i | 346 | C |
| 34 | i | 352 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | i | 354 | A |
| 34 | i | 357 | U |
| 34 | i | 359 | C |
| 34 | i | 375 | G |
| 34 | i | 376 | C |
| 34 | i | 379 | A |
| 34 | i | 382 | A |
| 34 | i | 390 | C |
| 34 | i | 397 | G |
| 34 | i | 398 | A |
| 34 | i | 399 | C |
| 34 | i | 416 | A |
| 34 | i | 438 | A |
| 34 | i | 440 | C |
| 34 | i | 442 | G |
| 34 | i | 449 | C |
| 34 | i | 454 | A |
| 34 | i | 456 | G |
| 34 | i | 460 | G |
| 34 | i | 461 | G |
| 34 | i | 462 | C |
| 34 | i | 463 | A |
| 34 | i | 464 | G |
| 34 | i | 466 | A |
| 34 | i | 472 | G |
| 34 | i | 477 | U |
| 34 | i | 482 | C |
| 34 | i | 484 | C |
| 34 | i | 486 | C |
| 34 | i | 515 | A |
| 34 | i | 521 | A |
| 34 | i | 522 | C |
| 34 | i | 523 | A |
| 34 | i | 525 | G |
| 34 | i | 537 | G |
| 34 | i | 539 | C |
| 34 | i | 541 | U |
| 34 | i | 542 | G |
| 34 | i | 543 | U |
| 34 | i | 546 | U |
| 34 | i | 547 | U |
| 34 | i | 549 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | i | 550 | A |
| 34 | i | 554 | A |
| 34 | i | 555 | G |
| 34 | i | 566 | A |
| 34 | i | 574 | A |
| 34 | i | 576 | G |
| 34 | i | 578 | G |
| 34 | i | 580 | A |
| 34 | i | 581 | U |
| 34 | i | 582 | C |
| 34 | i | 583 | C |
| 34 | i | 586 | U |
| 34 | i | 590 | G |
| 34 | i | 595 | A |
| 34 | i | 596 | G |
| 34 | i | 597 | U |
| 34 | i | 598 | C |
| 34 | i | 600 | G |
| 34 | i | 604 | G |
| 34 | i | 609 | A |
| 34 | i | 610 | G |
| 34 | i | 618 | A |
| 34 | i | 619 | A |
| 34 | i | 624 | A |
| 34 | i | 631 | A |
| 34 | i | 632 | U |
| 34 | i | 633 | A |
| 34 | i | 634 | G |
| 34 | i | 645 | A |
| 34 | i | 658 | A |
| 34 | i | 659 | A |
| 34 | i | 660 | A |
| 34 | i | 661 | A |
| 34 | i | 662 | A |
| 34 | i | 669 | A |
| 34 | i | 678 | U |
| 34 | i | 679 | U |
| 34 | i | 683 | G |
| 34 | i | 684 | A |
| 34 | i | 685 | G |
| 34 | i | 686 | G |
| 34 | i | 687 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | i | 689 | G |
| 34 | i | 691 | G |
| 34 | i | 725 | C |
| 34 | i | 727 | G |
| 34 | i | 728 | U |
| 34 | i | 729 | C |
| 34 | i | 730 | C |
| 34 | i | 731 | C |
| 34 | i | 734 | C |
| 34 | i | 735 | C |
| 34 | i | 736 | C |
| 34 | i | 740 | G |
| 34 | i | 743 | U |
| 34 | i | 744 | C |
| 34 | i | 793 | C |
| 34 | i | 794 | G |
| 34 | i | 795 | U |
| 34 | i | 806 | A |
| 34 | i | 807 | A |
| 34 | i | 808 | A |
| 34 | i | 814 | A |
| 34 | i | 817 | G |
| 34 | i | 818 | U |
| 34 | i | 826 | A |
| 34 | i | 827 | G |
| 34 | i | 830 | C |
| 34 | i | 831 | C |
| 34 | i | 832 | G |
| 34 | i | 833 | A |
| 34 | i | 834 | G |
| 34 | i | 835 | C |
| 34 | i | 836 | C |
| 34 | i | 838 | C |
| 34 | i | 839 | C |
| 34 | i | 841 | G |
| 34 | i | 843 | A |
| 34 | i | 849 | C |
| 34 | i | 860 | A |
| 34 | i | 864 | G |
| 34 | i | 865 | A |
| 34 | i | 866 | A |
| 34 | i | 867 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | i | 869 | G |
| 34 | i | 870 | G |
| 34 | i | 871 | A |
| 34 | i | 872 | C |
| 34 | i | 873 | C |
| 34 | i | 874 | G |
| 34 | i | 877 | G |
| 34 | i | 882 | A |
| 34 | i | 883 | U |
| 34 | i | 884 | U |
| 34 | i | 886 | U |
| 34 | i | 890 | G |
| 34 | i | 891 | G |
| 34 | i | 893 | U |
| 34 | i | 899 | A |
| 34 | i | 900 | A |
| 34 | i | 907 | C |
| 34 | i | 909 | A |
| 34 | i | 910 | U |
| 34 | i | 916 | A |
| 34 | i | 917 | G |
| 34 | i | 929 | G |
| 34 | i | 947 | C |
| 34 | i | 951 | A |
| 34 | i | 962 | U |
| 34 | i | 965 | U |
| 34 | i | 966 | G |
| 34 | i | 967 | G |
| 34 | i | 972 | G |
| 34 | i | 974 | G |
| 34 | i | 986 | A |
| 34 | i | 988 | A |
| 34 | i | 995 | G |
| 34 | i | 997 | A |
| 34 | i | 1004 | A |
| 34 | i | 1013 | U |
| 34 | i | 1019 | A |
| 34 | i | 1021 | U |
| 34 | i | 1027 | A |
| 34 | i | 1035 | C |
| 34 | i | 1041 | U |
| 34 | i | 1045 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | i | 1046 | A |
| 34 | i | 1047 | G |
| 34 | i | 1048 | A |
| 34 | i | 1050 | G |
| 34 | i | 1056 | A |
| 34 | i | 1057 | U |
| 34 | i | 1058 | A |
| 34 | i | 1068 | U |
| 34 | i | 1069 | U |
| 34 | i | 1073 | A |
| 34 | i | 1074 | C |
| 34 | i | 1079 | A |
| 34 | i | 1092 | G |
| 34 | i | 1093 | G |
| 34 | i | 1105 | C |
| 34 | i | 1106 | G |
| 34 | i | 1107 | U |
| 34 | i | 1111 | U |
| 34 | i | 1112 | C |
| 34 | i | 1113 | C |
| 34 | i | 1114 | C |
| 34 | i | 1116 | U |
| 34 | i | 1119 | C |
| 34 | i | 1127 | G |
| 34 | i | 1132 | U |
| 34 | i | 1134 | C |
| 34 | i | 1136 | G |
| 34 | i | 1137 | G |
| 34 | i | 1139 | A |
| 34 | i | 1144 | A |
| 34 | i | 1145 | A |
| 34 | i | 1146 | A |
| 34 | i | 1149 | C |
| 34 | i | 1150 | U |
| 34 | i | 1151 | U |
| 34 | i | 1153 | G |
| 34 | i | 1154 | G |
| 34 | i | 1157 | U |
| 34 | i | 1162 | G |
| 34 | i | 1164 | G |
| 34 | i | 1199 | G |
| 34 | i | 1202 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | i | 1204 | A |
| 34 | i | 1205 | A |
| 34 | i | 1208 | G |
| 34 | i | 1210 | A |
| 34 | i | 1211 | C |
| 34 | i | 1212 | C |
| 34 | i | 1213 | A |
| 34 | i | 1217 | G |
| 34 | i | 1220 | G |
| 34 | i | 1232 | G |
| 34 | i | 1233 | C |
| 34 | i | 1238 | U |
| 34 | i | 1241 | G |
| 34 | i | 1247 | A |
| 34 | i | 1249 | A |
| 34 | i | 1250 | C |
| 34 | i | 1252 | G |
| 34 | i | 1253 | G |
| 34 | i | 1255 | A |
| 34 | i | 1256 | A |
| 34 | i | 1259 | U |
| 34 | i | 1260 | C |
| 34 | i | 1270 | G |
| 34 | i | 1271 | G |
| 34 | i | 1272 | A |
| 34 | i | 1274 | A |
| 34 | i | 1279 | C |
| 34 | i | 1280 | A |
| 34 | i | 1281 | G |
| 34 | i | 1296 | U |
| 34 | i | 1297 | A |
| 34 | i | 1299 | C |
| 34 | i | 1303 | U |
| 34 | i | 1304 | U |
| 34 | i | 1310 | U |
| 34 | i | 1311 | U |
| 34 | i | 1312 | C |
| 34 | i | 1313 | U |
| 34 | i | 1320 | G |
| 34 | i | 1325 | U |
| 34 | i | 1338 | U |
| 34 | i | 1339 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | i | 1344 | G |
| 34 | i | 1354 | U |
| 34 | i | 1367 | U |
| 34 | i | 1368 | U |
| 34 | i | 1369 | C |
| 34 | i | 1374 | A |
| 34 | i | 1390 | G |
| 34 | i | 1391 | C |
| 34 | i | 1392 | A |
| 34 | i | 1393 | U |
| 34 | i | 1394 | G |
| 34 | i | 1397 | A |
| 34 | i | 1398 | A |
| 34 | i | 1400 | U |
| 34 | i | 1402 | G |
| 34 | i | 1403 | U |
| 34 | i | 1405 | A |
| 34 | i | 1406 | C |
| 34 | i | 1408 | C |
| 34 | i | 1413 | C |
| 34 | i | 1414 | C |
| 34 | i | 1415 | C |
| 34 | i | 1422 | U |
| 34 | i | 1426 | C |
| 34 | i | 1431 | C |
| 34 | i | 1433 | C |
| 34 | i | 1445 | G |
| 34 | i | 1448 | A |
| 34 | i | 1450 | A |
| 34 | i | 1452 | G |
| 34 | i | 1455 | G |
| 34 | i | 1458 | U |
| 34 | i | 1461 | A |
| 34 | i | 1470 | A |
| 34 | i | 1471 | G |
| 34 | i | 1472 | A |
| 34 | i | 1473 | U |
| 34 | i | 1474 | U |
| 34 | i | 1485 | A |
| 34 | i | 1486 | G |
| 34 | i | 1489 | C |
| 34 | i | 1490 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | i | 1491 | G |
| 34 | i | 1504 | A |
| 34 | i | 1506 | G |
| 34 | i | 1507 | U |
| 34 | i | 1508 | C |
| 34 | i | 1511 | G |
| 34 | i | 1514 | U |
| 34 | i | 1515 | G |
| 34 | i | 1516 | C |
| 34 | i | 1519 | G |
| 34 | i | 1528 | A |
| 34 | i | 1530 | U |
| 34 | i | 1532 | A |
| 34 | i | 1535 | G |
| 34 | i | 1539 | C |
| 34 | i | 1540 | A |
| 34 | i | 1545 | G |
| 34 | i | 1546 | U |
| 34 | i | 1547 | G |
| 34 | i | 1548 | C |
| 34 | i | 1549 | C |
| 34 | i | 1551 | A |
| 34 | i | 1552 | C |
| 34 | i | 1553 | C |
| 34 | i | 1558 | G |
| 34 | i | 1559 | C |
| 34 | i | 1565 | G |
| 34 | i | 1573 | U |
| 34 | i | 1575 | A |
| 34 | i | 1577 | C |
| 34 | i | 1580 | U |
| 34 | i | 1582 | G |
| 34 | i | 1583 | A |
| 34 | i | 1593 | G |
| 34 | i | 1594 | U |
| 34 | i | 1595 | G |
| 34 | i | 1597 | U |
| 34 | i | 1599 | G |
| 34 | i | 1616 | U |
| 34 | i | 1617 | U |
| 34 | i | 1618 | A |
| 34 | i | 1627 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | i | 1628 | A |
| 34 | i | 1632 | A |
| 34 | i | 1633 | G |
| 34 | i | 1634 | G |
| 34 | i | 1643 | G |
| 34 | i | 1649 | G |
| 34 | i | 1652 | G |
| 34 | i | 1660 | G |
| 34 | i | 1675 | G |
| 34 | i | 1683 | C |
| 34 | i | 1690 | A |
| 34 | i | 1694 | A |
| 34 | i | 1696 | C |
| 34 | i | 1697 | G |
| 34 | i | 1716 | U |
| 34 | i | 1717 | G |
| 34 | i | 1722 | G |
| 34 | i | 1724 | U |
| 34 | i | 1741 | U |
| 34 | i | 1743 | G |
| 34 | i | 1745 | C |
| 34 | i | 1747 | C |
| 34 | i | 1748 | G |
| 34 | i | 1749 | C |
| 34 | i | 1750 | C |
| 34 | i | 1751 | G |
| 34 | i | 1755 | U |
| 34 | i | 1774 | G |
| 34 | i | 1775 | A |
| 34 | i | 1776 | G |
| 34 | i | 1777 | C |
| 34 | i | 1778 | G |
| 34 | i | 1779 | C |
| 34 | i | 1780 | U |
| 34 | i | 1790 | G |
| 34 | i | 1792 | C |
| 34 | i | 1799 | G |
| 34 | i | 1818 | A |
| 34 | i | 1819 | A |
| 34 | i | 1820 | G |
| 34 | i | 1822 | C |
| 34 | i | 1823 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | i | 1825 | A |
| 34 | i | 1826 | A |
| 34 | i | 1829 | A |
| 34 | i | 1832 | U |
| 34 | i | 1833 | U |
| 34 | i | 1843 | G |
| 34 | i | 1845 | A |
| 34 | i | 1846 | C |
| 34 | i | 1852 | G |
| 34 | i | 1855 | G |
| 34 | i | 1856 | G |
| 34 | i | 1857 | A |
| 34 | i | 1858 | U |
| 34 | i | 1859 | C |
| 34 | i | 1861 | U |
| 34 | i | 1863 | A |
| 35 | j | 4 | A |
| 35 | j | 5 | G |
| 35 | j | 8 | U |
| 35 | j | 16 | C |
| 35 | j | 17 | G |
| 35 | j | 18 | G |
| 35 | j | 19 | A |
| 35 | j | 20 | A |
| 35 | j | 46 | U |
| 35 | j | 47 | C |
| 35 | j | 48 | G |
| 35 | j | 52 | G |
| 35 | j | 66 | U |
| 35 | j | 70 | C |
| 35 | j | 72 | A |
| 35 | j | 74 | C |
| 35 | j | 75 | A |
| 36 | k | 14 | A |
| 36 | k | 15 | A |
| 36 | k | 22 | C |

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 34 | i | 11 |
| 10 | J | 3 |
| 19 | S | 2 |
| 7 | G | 1 |
| 4 | D | 1 |
| 31 | e | 1 |
| 9 | I | 1 |
| 3 | C | 1 |
| 21 | U | 1 |
| 18 | R | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | i | 326:A | O3' | 327:C | P | 9.94 |
| 1 | i | 309:A | O3' | 310:G | P | 7.21 |
| 1 | i | 209:C | O3' | 210:G | P | 6.66 |
| 1 | i | 1826:A | O3' | 1827:C | P | 5.44 |
| 1 | i | 304:A | O3' | 305:U | P | 4.93 |
| 1 | i | 1206:G | O3' | 1207:G | P | 4.13 |
| 1 | i | 1698:C | O3' | 1699:C | P | 3.74 |
| 1 | i | 183:G | O3' | 184:G | P | 3.17 |
| 1 | i | 550:A | O3' | 551:A | P | 2.80 |
| 1 | i | 515:A | O3' | 516:A | P | 2.53 |
| 1 | i | 1683:C | O3' | 1684:C | P | 2.23 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | D | 5:ILE | C | 6:SER | N | 1.82 |
| 1 | e | 95:LYS | C | 96:GLN | N | 1.76 |
| 1 | J | 118:GLY | C | 119:LEU | N | 1.73 |
| 1 | I | 43:ILE | C | 44:HIS | N | 1.67 |
| 1 | J | 146:SER | C | 147:PHE | N | 1.61 |
| 1 | U | 93:SER | C | 94:PRO | N | 1.61 |
| 1 | S | 141:ARG | C | 142:ARG | N | 1.60 |
| 1 | C | 93:LYS | C | 94:ILE | N | 1.18 |
| 1 | G | 130:PRO | C | 131:ARG | N | 1.16 |
| 1 | R | 1:MET | C | 2:GLY | N | 1.13 |
| 1 | S | 40:TYR | C | 41:ALA | N | 1.09 |
| 1 | J | 85:GLY | C | 86:VAL | N | 0.95 |

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1 | A | 208/295 (70%) | 0.77 | 40 (19%) 1 3 | 188, 273, 325, 347 | 0 |
| 2 | B | 215/264 (81%) | 1.44 | 75 (34%) 0 2 | 140, 249, 309, 321 | 0 |
| 3 | C | 226/278 (81%) | 2.76 | 109 (48%) 0 1 | 76, 163, 267, 285 | 0 |
| 4 | D | 227/243 (93%) | 4.76 | 165 (72%) 0 0 | 110, 175, 253, 280 | 0 |
| 5 | E | 263/263 (100%) | 2.66 | 135 (51%) 0 1 | 38, 138, 196, 225 | 0 |
| 6 | F | 191/204 (93%) | 5.07 | 154 (80%) 0 0 | 133, 175, 212, 224 | 0 |
| 7 | G | 237/249 (95%) | 1.41 | 73 (30%) 0 2 | 68, 198, 289, 311 | 0 |
| 8 | H | 190/194 (97%) | 0.10 | 22 (11%) 4 8 | 129, 278, 329, 340 | 0 |
| 9 | I | 206/208 (99%) | 3.73 | 119 (57%) 0 1 | 17, 164, 268, 289 | 0 |
| 10 | J | 182/194 (93%) | 0.70 | 34 (18%) 1 4 | 73, 158, 221, 259 | 0 |
| 11 | K | 98/165 (59%) | 1.83 | 29 (29%) 0 2 | 167, 238, 289, 308 | 0 |
| 12 | L | 158/158 (100%) | 1.68 | 62 (39%) 0 1 | 22, 90, 224, 255 | 0 |
| 13 | M | 124/132 (93%) | -0.16 | 5 (4%) 38 34 | 280, 347, 384, 417 | 0 |
| 14 | N | 150/151 (99%) | 0.74 | 23 (15%) 2 5 | 46, 118, 251, 261 | 0 |
| 15 | O | 136/151 (90%) | 2.04 | 52 (38%) 0 1 | 45, 205, 320, 353 | 0 |
| 16 | P | 127/145 (87%) | 3.24 | 71 (55%) 0 1 | 163, 254, 297, 310 | 0 |
| 17 | Q | 141/146 (96%) | 1.87 | 49 (34%) 0 2 | 108, 200, 225, 231 | 0 |
| 18 | R | 126/135 (93%) | 0.07 | 14 (11%) 5 9 | 130, 194, 302, 306 | 0 |
| 19 | S | 137/152 (90%) | 0.95 | 24 (17%) 1 4 | 151, 218, 239, 249 | 0 |
| 20 | T | 141/145 (97%) | 0.10 | 7 (4%) 28 28 | 161, 214, 230, 234 | 0 |
| 21 | U | 104/119 (87%) | 3.99 | 64 (61%) 0 0 | 116, 213, 258, 269 | 0 |
| 22 | V | 82/83 (98%) | 0.66 | 12 (14%) 2 6 | 175, 237, 316, 328 | 0 |
| 23 | W | 129/130 (99%) | 1.72 | 47 (36%) 0 1 | 75, 141, 196, 216 | 0 |
| 24 | X | 142/143 (99%) | 2.43 | 62 (43%) 0 1 | 22, 54, 84, 93 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25 | Y | 126/133 (94%) | 0.28 | 9 (7%) 16 16 | 85, 153, 198, 218 | 0 |
| 26 | Z | 75/125 (60%) | 0.84 | 13 (17%) 1 4 | 197, 207, 217, 225 | 0 |
| 27 | a | 107/115 (93%) | 1.57 | 27 (25%) 0 2 | 55, 111, 285, 317 | 0 |
| 28 | b | 84/84 (100%) | 0.05 | 6 (7%) 16 16 | 156, 236, 276, 286 | 0 |
| 29 | c | 64/69 (92%) | 2.52 | 36 (56%) 0 1 | 125, 173, 216, 221 | 0 |
| 30 | d | 53/56 (94%) | 1.75 | 21 (39%) 0 1 | 136, 159, 235, 256 | 0 |
| 31 | e | 59/133 (44%) | 0.73 | 12 (20%) 1 3 | 63, 136, 177, 192 | 0 |
| 32 | f | 71/156 (45%) | -0.55 | 0 100 100 | 145, 320, 392, 408 | 0 |
| 33 | g | 313/317 (98%) | 0.39 | 37 (11%) 4 8 | 190, 248, 277, 291 | 0 |
| 34 | i | 1797/1863 (96%) | 1.40 | 476 (26%) 0 2 | 13, 142, 348, 527 | 0 |
| 35 | j | 75/75 (100%) | 1.24 | 21 (28%) 0 2 | 308, 379, 421, 436 | 0 |
| 36 | k | 13/24 (54%) | 3.58 | 12 (92%) 0 0 | 186, 317, 324, 325 | 0 |
| 37 | n | 82/144 (56%) | 1.71 | 31 (37%) 0 1 | 212, 216, 222, 224 | 0 |
| All | All | 6859/7641 (89%) | 1.63 | 2148 (31%) 0 2 | 13, 190, 328, 527 | 0 |

All (2148) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 34 | i | 697 | G | 34.6 |
| 34 | i | 698 | G | 32.3 |
| 4 | D | 95 | GLY | 24.0 |
| 34 | i | 696 | G | 22.1 |
| 34 | i | 695 | C | 22.1 |
| 9 | I | 58 | LEU | 19.8 |
| 24 | X | 69 | CYS | 18.5 |
| 11 | K | 21 | MET | 16.0 |
| 11 | K | 20 | VAL | 15.9 |
| 34 | i | 694 | G | 15.8 |
| 4 | D | 88 | ALA | 15.5 |
| 6 | F | 189 | ALA | 15.5 |
| 4 | D | 186 | VAL | 15.3 |
| 9 | I | 173 | ALA | 15.3 |
| 3 | C | 87 | LEU | 15.2 |
| 5 | E | 73 | ASP | 14.8 |
| 9 | I | 104 | ILE | 14.7 |
| 9 | I | 95 | THR | 14.3 |
| 6 | F | 39 | ILE | 14.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9 | I | 36 | THR | 14.0 |
| 4 | D | 35 | SER | 14.0 |
| 4 | D | 101 | GLN | 13.8 |
| 5 | E | 74 | GLY | 13.7 |
| 4 | D | 50 | ILE | 13.6 |
| 3 | C | 84 | GLY | 13.4 |
| 4 | D | 96 | LEU | 13.4 |
| 6 | F | 66 | CYS | 13.3 |
| 21 | U | 25 | THR | 13.2 |
| 16 | P | 105 | VAL | 13.1 |
| 17 | Q | 53 | GLU | 13.1 |
| 4 | D | 98 | ALA | 13.1 |
| 21 | U | 26 | SER | 12.6 |
| 4 | D | 97 | CYS | 12.6 |
| 6 | F | 108 | PRO | 12.5 |
| 9 | I | 101 | ILE | 12.5 |
| 3 | C | 149 | PRO | 12.4 |
| 4 | D | 188 | ILE | 12.3 |
| 6 | F | 41 | VAL | 12.3 |
| 6 | F | 157 | GLY | 12.3 |
| 17 | Q | 54 | PRO | 12.2 |
| 24 | X | 83 | ALA | 12.2 |
| 6 | F | 40 | ALA | 12.2 |
| 4 | D | 19 | ALA | 12.2 |
| 4 | D | 36 | GLY | 12.2 |
| 4 | D | 52 | ALA | 12.1 |
| 6 | F | 64 | ALA | 12.1 |
| 15 | O | 129 | ILE | 12.1 |
| 16 | P | 87 | PRO | 12.0 |
| 21 | U | 110 | VAL | 12.0 |
| 9 | I | 100 | CYS | 12.0 |
| 9 | I | 57 | ALA | 11.9 |
| 4 | D | 70 | THR | 11.7 |
| 6 | F | 155 | CYS | 11.7 |
| 21 | U | 32 | LEU | 11.7 |
| 4 | D | 32 | ASP | 11.6 |
| 6 | F | 68 | ILE | 11.6 |
| 34 | i | 722 | C | 11.5 |
| 6 | F | 158 | ALA | 11.4 |
| 21 | U | 24 | LEU | 11.4 |
| 6 | F | 71 | ARG | 11.4 |
| 21 | U | 36 | CYS | 11.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | I | 81 | VAL | 11.3 |
| 6 | F | 106 | GLU | 11.3 |
| 6 | F | 109 | LEU | 11.3 |
| 16 | P | 94 | VAL | 11.2 |
| 5 | E | 88 | ASP | 11.2 |
| 11 | K | 22 | VAL | 11.2 |
| 4 | D | 33 | GLY | 11.2 |
| 6 | F | 107 | ASN | 11.1 |
| 5 | E | 91 | SER | 11.1 |
| 17 | Q | 50 | LYS | 11.0 |
| 4 | D | 91 | VAL | 11.0 |
| 9 | I | 105 | ASP | 11.0 |
| 9 | I | 63 | GLY | 10.9 |
| 6 | F | 111 | VAL | 10.9 |
| 4 | D | 136 | VAL | 10.9 |
| 6 | F | 183 | GLY | 10.9 |
| 9 | I | 102 | VAL | 10.9 |
| 3 | C | 121 | HIS | 10.8 |
| 5 | E | 69 | PHE | 10.8 |
| 6 | F | 154 | LEU | 10.7 |
| 11 | K | 68 | TYR | 10.7 |
| 3 | C | 147 | ILE | 10.7 |
| 4 | D | 102 | ALA | 10.7 |
| 9 | I | 174 | CYS | 10.6 |
| 7 | G | 36 | VAL | 10.6 |
| 2 | B | 100 | PHE | 10.6 |
| 6 | F | 113 | VAL | 10.5 |
| 9 | I | 186 | ASP | 10.5 |
| 6 | F | 73 | THR | 10.5 |
| 21 | U | 85 | HIS | 10.4 |
| 6 | F | 119 | SER | 10.4 |
| 3 | C | 150 | VAL | 10.4 |
| 4 | D | 94 | ARG | 10.4 |
| 6 | F | 70 | GLU | 10.3 |
| 11 | K | 63 | ALA | 10.3 |
| 16 | P | 95 | GLY | 10.3 |
| 9 | I | 76 | THR | 10.3 |
| 4 | D | 71 | ALA | 10.2 |
| 16 | P | 76 | VAL | 10.2 |
| 9 | I | 133 | GLU | 10.2 |
| 21 | U | 87 | ARG | 10.1 |
| 34 | i | 1419 | C | 10.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | I | 84 | ASN | 10.0 |
| 4 | D | 34 | TYR | 10.0 |
| 5 | E | 89 | VAL | 10.0 |
| 34 | i | 693 | A | 10.0 |
| 6 | F | 190 | ILE | 10.0 |
| 4 | D | 68 | GLU | 9.9 |
| 3 | C | 120 | GLY | 9.9 |
| 4 | D | 100 | ALA | 9.8 |
| 6 | F | 18 | LYS | 9.8 |
| 9 | I | 60 | LEU | 9.8 |
| 6 | F | 63 | LYS | 9.7 |
| 9 | I | 59 | ARG | 9.7 |
| 37 | n | 71 | ILE | 9.7 |
| 4 | D | 74 | GLN | 9.6 |
| 6 | F | 115 | ALA | 9.6 |
| 5 | E | 102 | ILE | 9.6 |
| 6 | F | 50 | PRO | 9.6 |
| 3 | C | 122 | VAL | 9.6 |
| 34 | i | 249 | C | 9.5 |
| 5 | E | 87 | MET | 9.5 |
| 3 | C | 116 | GLY | 9.5 |
| 16 | P | 88 | GLU | 9.5 |
| 5 | E | 86 | PHE | 9.4 |
| 4 | D | 51 | LEU | 9.4 |
| 24 | X | 82 | THR | 9.4 |
| 34 | i | 1762 | A | 9.4 |
| 3 | C | 148 | VAL | 9.4 |
| 6 | F | 29 | GLN | 9.4 |
| 6 | F | 110 | GLN | 9.3 |
| 6 | F | 67 | PRO | 9.3 |
| 21 | U | 112 | VAL | 9.3 |
| 34 | i | 1758 | G | 9.3 |
| 4 | D | 184 | ILE | 9.3 |
| 9 | I | 80 | ASP | 9.3 |
| 15 | O | 116 | LEU | 9.2 |
| 15 | O | 95 | ILE | 9.2 |
| 34 | i | 720 | A | 9.2 |
| 3 | C | 224 | ALA | 9.1 |
| 9 | I | 185 | ALA | 9.1 |
| 34 | i | 1580 | U | 9.1 |
| 4 | D | 20 | GLU | 9.1 |
| 34 | i | 1420 | G | 9.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 21 | U | 39 | LEU | 9.1 |
| 6 | F | 181 | ALA | 9.0 |
| 15 | O | 113 | GLN | 9.0 |
| 24 | X | 85 | VAL | 9.0 |
| 11 | K | 62 | PHE | 8.9 |
| 9 | I | 190 | LEU | 8.9 |
| 7 | G | 41 | LEU | 8.9 |
| 4 | D | 93 | THR | 8.8 |
| 9 | I | 83 | TYR | 8.8 |
| 6 | F | 75 | SER | 8.8 |
| 6 | F | 31 | ASN | 8.8 |
| 21 | U | 22 | ILE | 8.8 |
| 3 | C | 228 | ALA | 8.8 |
| 4 | D | 49 | ILE | 8.8 |
| 4 | D | 15 | GLY | 8.8 |
| 4 | D | 75 | LYS | 8.7 |
| 9 | I | 96 | LEU | 8.7 |
| 6 | F | 178 | ILE | 8.7 |
| 3 | C | 85 | ALA | 8.7 |
| 9 | I | 78 | ILE | 8.6 |
| 15 | O | 130 | GLU | 8.6 |
| 34 | i | 723 | G | 8.6 |
| 5 | E | 143 | ASP | 8.6 |
| 6 | F | 193 | LYS | 8.6 |
| 3 | C | 86 | ALA | 8.6 |
| 3 | C | 123 | GLY | 8.6 |
| 6 | F | 177 | LEU | 8.6 |
| 21 | U | 23 | THR | 8.6 |
| 4 | D | 66 | ILE | 8.6 |
| 27 | a | 45 | VAL | 8.5 |
| 6 | F | 112 | LEU | 8.5 |
| 3 | C | 220 | ASN | 8.5 |
| 4 | D | 175 | VAL | 8.5 |
| 4 | D | 53 | THR | 8.5 |
| 21 | U | 40 | ILE | 8.5 |
| 16 | P | 106 | GLU | 8.5 |
| 6 | F | 114 | ASN | 8.4 |
| 4 | D | 72 | VAL | 8.4 |
| 4 | D | 183 | GLY | 8.4 |
| 21 | U | 86 | LYS | 8.4 |
| 3 | C | 169 | VAL | 8.4 |
| 16 | P | 6 | GLN | 8.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 21 | U | 111 | GLU | 8.4 |
| 6 | F | 150 | ALA | 8.4 |
| 17 | Q | 57 | LEU | 8.3 |
| 15 | O | 131 | ASP | 8.3 |
| 9 | I | 129 | LEU | 8.3 |
| 34 | i | 1652 | G | 8.3 |
| 24 | X | 118 | VAL | 8.3 |
| 5 | E | 85 | GLY | 8.2 |
| 14 | N | 149 | LEU | 8.2 |
| 5 | E | 122 | LYS | 8.2 |
| 6 | F | 48 | TYR | 8.2 |
| 9 | I | 131 | PRO | 8.2 |
| 34 | i | 1653 | G | 8.2 |
| 34 | i | 1651 | G | 8.2 |
| 17 | Q | 112 | LEU | 8.2 |
| 5 | E | 71 | LYS | 8.1 |
| 24 | X | 115 | ILE | 8.1 |
| 3 | C | 198 | LEU | 8.1 |
| 4 | D | 30 | ALA | 8.1 |
| 11 | K | 70 | TYR | 8.1 |
| 3 | C | 89 | ASP | 8.1 |
| 6 | F | 151 | ILE | 8.1 |
| 16 | P | 89 | MET | 8.1 |
| 4 | D | 89 | GLU | 8.1 |
| 3 | C | 114 | ALA | 8.1 |
| 16 | P | 5 | GLU | 8.0 |
| 4 | D | 29 | LEU | 8.0 |
| 3 | C | 232 | THR | 8.0 |
| 34 | i | 1421 | G | 8.0 |
| 17 | Q | 115 | TYR | 8.0 |
| 9 | I | 38 | ILE | 8.0 |
| 21 | U | 89 | ILE | 8.0 |
| 6 | F | 116 | ILE | 8.0 |
| 4 | D | 22 | ASN | 7.9 |
| 9 | I | 189 | VAL | 7.9 |
| 24 | X | 67 | ARG | 7.9 |
| 4 | D | 119 | CYS | 7.9 |
| 21 | U | 114 | VAL | 7.9 |
| 7 | G | 18 | VAL | 7.9 |
| 34 | i | 125 | C | 7.9 |
| 16 | P | 86 | LEU | 7.9 |
| 6 | F | 184 | SER | 7.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | E | 65 | CYS | 7.9 |
| 9 | I | 85 | ALA | 7.8 |
| 9 | I | 43 | ILE | 7.8 |
| 5 | E | 237 | SER | 7.8 |
| 9 | I | 171 | LEU | 7.8 |
| 4 | D | 190 | LEU | 7.8 |
| 9 | I | 128 | LYS | 7.8 |
| 25 | Y | 17 | LEU | 7.8 |
| 24 | X | 70 | VAL | 7.7 |
| 5 | E | 60 | GLU | 7.7 |
| 3 | C | 202 | ALA | 7.7 |
| 4 | D | 103 | GLU | 7.7 |
| 6 | F | 118 | ASN | 7.7 |
| 4 | D | 73 | VAL | 7.7 |
| 21 | U | 21 | ARG | 7.7 |
| 4 | D | 86 | LEU | 7.7 |
| 14 | N | 146 | ALA | 7.7 |
| 6 | F | 180 | ALA | 7.6 |
| 5 | E | 72 | ILE | 7.6 |
| 9 | I | 39 | GLY | 7.6 |
| 19 | S | 67 | VAL | 7.6 |
| 3 | C | 226 | PHE | 7.6 |
| 3 | C | 225 | THR | 7.6 |
| 17 | Q | 58 | LEU | 7.6 |
| 3 | C | 201 | MET | 7.6 |
| 3 | C | 203 | GLY | 7.6 |
| 6 | F | 28 | VAL | 7.6 |
| 6 | F | 187 | SER | 7.6 |
| 3 | C | 117 | ASP | 7.6 |
| 21 | U | 35 | VAL | 7.6 |
| 3 | C | 230 | SER | 7.6 |
| 3 | C | 151 | ARG | 7.6 |
| 15 | O | 127 | GLY | 7.5 |
| 6 | F | 30 | ILE | 7.5 |
| 7 | G | 95 | LYS | 7.5 |
| 5 | E | 100 | ARG | 7.5 |
| 6 | F | 105 | GLY | 7.5 |
| 9 | I | 65 | PHE | 7.5 |
| 8 | H | 193 | GLN | 7.4 |
| 3 | C | 229 | ILE | 7.4 |
| 5 | E | 70 | ILE | 7.4 |
| 15 | O | 20 | GLN | 7.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | I | 61 | ASP | 7.4 |
| 23 | W | 103 | VAL | 7.4 |
| 9 | I | 121 | LEU | 7.4 |
| 34 | i | 1254 | A | 7.4 |
| 4 | D | 87 | TYR | 7.4 |
| 2 | B | 99 | ASN | 7.4 |
| 5 | E | 145 | ARG | 7.3 |
| 6 | F | 69 | VAL | 7.3 |
| 15 | O | 112 | ALA | 7.3 |
| 9 | I | 126 | GLY | 7.3 |
| 4 | D | 104 | SER | 7.3 |
| 24 | X | 117 | GLY | 7.3 |
| 5 | E | 238 | LEU | 7.3 |
| 5 | E | 43 | PRO | 7.3 |
| 16 | P | 113 | GLY | 7.3 |
| 4 | D | 180 | GLY | 7.3 |
| 6 | F | 117 | ILE | 7.3 |
| 9 | I | 103 | LEU | 7.2 |
| 5 | E | 90 | ILE | 7.2 |
| 6 | F | 176 | GLU | 7.2 |
| 24 | X | 130 | LEU | 7.2 |
| 4 | D | 137 | VAL | 7.2 |
| 4 | D | 38 | GLU | 7.2 |
| 19 | S | 117 | ILE | 7.2 |
| 4 | D | 24 | PHE | 7.2 |
| 6 | F | 46 | ALA | 7.2 |
| 7 | G | 50 | VAL | 7.2 |
| 34 | i | 1759 | C | 7.2 |
| 21 | U | 56 | MET | 7.1 |
| 16 | P | 10 | ARG | 7.1 |
| 34 | i | 1760 | C | 7.1 |
| 7 | G | 113 | ILE | 7.1 |
| 24 | X | 55 | VAL | 7.1 |
| 2 | B | 121 | ILE | 7.1 |
| 3 | C | 83 | LEU | 7.1 |
| 9 | I | 97 | VAL | 7.1 |
| 34 | i | 296 | U | 7.1 |
| 21 | U | 118 | ASP | 7.1 |
| 4 | D | 222 | PRO | 7.0 |
| 4 | D | 21 | LEU | 7.0 |
| 21 | U | 43 | ALA | 7.0 |
| 21 | U | 105 | SER | 7.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | a | 49 | ALA | 7.0 |
| 21 | U | 101 | ILE | 7.0 |
| 9 | I | 184 | ARG | 7.0 |
| 6 | F | 32 | ASP | 7.0 |
| 4 | D | 152 | PHE | 7.0 |
| 4 | D | 122 | VAL | 7.0 |
| 16 | P | 93 | MET | 7.0 |
| 24 | X | 10 | ALA | 7.0 |
| 2 | B | 156 | ALA | 6.9 |
| 4 | D | 135 | GLU | 6.9 |
| 4 | D | 37 | VAL | 6.9 |
| 6 | F | 123 | GLU | 6.9 |
| 9 | I | 64 | ASN | 6.9 |
| 29 | c | 65 | ALA | 6.9 |
| 34 | i | 248 | C | 6.9 |
| 10 | J | 74 | GLY | 6.9 |
| 21 | U | 115 | THR | 6.9 |
| 11 | K | 64 | TRP | 6.9 |
| 6 | F | 76 | MET | 6.8 |
| 3 | C | 119 | ASN | 6.8 |
| 24 | X | 84 | PHE | 6.8 |
| 34 | i | 1650 | C | 6.8 |
| 9 | I | 172 | LEU | 6.8 |
| 6 | F | 153 | LEU | 6.8 |
| 34 | i | 1493 | G | 6.8 |
| 7 | G | 37 | ALA | 6.8 |
| 11 | K | 67 | PHE | 6.8 |
| 16 | P | 27 | ASP | 6.8 |
| 15 | O | 21 | VAL | 6.8 |
| 3 | C | 168 | LYS | 6.7 |
| 5 | E | 64 | ILE | 6.7 |
| 29 | c | 64 | GLU | 6.7 |
| 34 | i | 3 | C | 6.7 |
| 7 | G | 96 | SER | 6.7 |
| 4 | D | 6 | SER | 6.7 |
| 34 | i | 1475 | G | 6.7 |
| 4 | D | 118 | ALA | 6.7 |
| 9 | I | 37 | LYS | 6.7 |
| 19 | S | 118 | ARG | 6.7 |
| 3 | C | 191 | SER | 6.7 |
| 33 | g | 32 | LEU | 6.7 |
| 17 | Q | 59 | GLY | 6.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 24 | X | 94 | ILE | 6.6 |
| 12 | L | 103 | GLU | 6.6 |
| 3 | C | 115 | ILE | 6.6 |
| 6 | F | 72 | LEU | 6.6 |
| 3 | C | 167 | CYS | 6.6 |
| 24 | X | 116 | PRO | 6.6 |
| 29 | c | 46 | VAL | 6.6 |
| 16 | P | 9 | LYS | 6.6 |
| 6 | F | 74 | ASN | 6.6 |
| 1 | A | 19 | LEU | 6.6 |
| 4 | D | 58 | VAL | 6.6 |
| 4 | D | 69 | LEU | 6.6 |
| 4 | D | 25 | LEU | 6.5 |
| 5 | E | 101 | LEU | 6.5 |
| 16 | P | 114 | HIS | 6.5 |
| 3 | C | 207 | CYS | 6.5 |
| 34 | i | 1662 | U | 6.5 |
| 34 | i | 1582 | G | 6.5 |
| 6 | F | 104 | THR | 6.5 |
| 11 | K | 61 | GLN | 6.5 |
| 21 | U | 117 | ALA | 6.5 |
| 4 | D | 221 | THR | 6.4 |
| 11 | K | 66 | HIS | 6.4 |
| 10 | J | 72 | PHE | 6.4 |
| 6 | F | 194 | ASP | 6.4 |
| 4 | D | 189 | MET | 6.4 |
| 23 | W | 129 | PHE | 6.4 |
| 35 | j | 31 | C | 6.4 |
| 27 | a | 36 | ILE | 6.4 |
| 5 | E | 61 | VAL | 6.4 |
| 16 | P | 26 | LEU | 6.4 |
| 5 | E | 84 | ALA | 6.4 |
| 4 | D | 28 | GLU | 6.4 |
| 7 | G | 97 | VAL | 6.4 |
| 4 | D | 67 | ARG | 6.3 |
| 6 | F | 124 | ASP | 6.3 |
| 6 | F | 100 | ILE | 6.3 |
| 4 | D | 65 | ARG | 6.3 |
| 6 | F | 38 | TYR | 6.3 |
| 5 | E | 182 | MET | 6.3 |
| 6 | F | 49 | LEU | 6.3 |
| 2 | B | 80 | ALA | 6.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 227 | LYS | 6.3 |
| 4 | D | 171 | ALA | 6.3 |
| 17 | Q | 51 | LEU | 6.3 |
| 34 | i | 1664 | G | 6.3 |
| 5 | E | 54 | TYR | 6.3 |
| 34 | i | 1761 | C | 6.3 |
| 6 | F | 174 | ALA | 6.3 |
| 2 | B | 43 | ASN | 6.3 |
| 21 | U | 102 | THR | 6.3 |
| 21 | U | 84 | ILE | 6.3 |
| 29 | c | 45 | ASN | 6.3 |
| 4 | D | 48 | ILE | 6.3 |
| 8 | H | 192 | PHE | 6.2 |
| 9 | I | 175 | ILE | 6.2 |
| 16 | P | 4 | VAL | 6.2 |
| 6 | F | 156 | THR | 6.2 |
| 17 | Q | 55 | VAL | 6.2 |
| 9 | I | 183 | GLY | 6.2 |
| 34 | i | 1579 | G | 6.2 |
| 5 | E | 236 | ILE | 6.2 |
| 16 | P | 53 | GLN | 6.2 |
| 3 | C | 204 | ILE | 6.2 |
| 9 | I | 99 | ASN | 6.2 |
| 7 | G | 35 | GLU | 6.2 |
| 5 | E | 92 | ILE | 6.2 |
| 6 | F | 185 | SER | 6.2 |
| 24 | X | 122 | VAL | 6.2 |
| 3 | C | 233 | TYR | 6.2 |
| 34 | i | 1661 | C | 6.2 |
| 34 | i | 1659 | A | 6.2 |
| 33 | g | 22 | ALA | 6.1 |
| 6 | F | 121 | PRO | 6.1 |
| 16 | P | 112 | ILE | 6.1 |
| 6 | F | 159 | ARG | 6.1 |
| 34 | i | 1252 | G | 6.1 |
| 17 | Q | 108 | ILE | 6.1 |
| 4 | D | 187 | LYS | 6.1 |
| 16 | P | 103 | ASN | 6.1 |
| 6 | F | 182 | LYS | 6.1 |
| 15 | O | 94 | HIS | 6.1 |
| 7 | G | 45 | TRP | 6.1 |
| 29 | c | 63 | ARG | 6.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | J | 94 | LEU | 6.1 |
| 16 | P | 24 | GLN | 6.1 |
| 16 | P | 104 | GLN | 6.1 |
| 34 | i | 250 | G | 6.1 |
| 5 | E | 124 | CYS | 6.1 |
| 34 | i | 1763 | C | 6.1 |
| 3 | C | 195 | PRO | 6.1 |
| 15 | O | 115 | ALA | 6.1 |
| 27 | a | 84 | VAL | 6.1 |
| 34 | i | 1649 | G | 6.0 |
| 21 | U | 90 | ASP | 6.0 |
| 4 | D | 220 | THR | 6.0 |
| 11 | K | 69 | TRP | 6.0 |
| 7 | G | 38 | ALA | 6.0 |
| 4 | D | 11 | PHE | 6.0 |
| 9 | I | 134 | GLU | 6.0 |
| 10 | J | 76 | ALA | 5.9 |
| 8 | H | 191 | GLU | 5.9 |
| 16 | P | 107 | ILE | 5.9 |
| 33 | g | 31 | ILE | 5.9 |
| 23 | W | 94 | LEU | 5.9 |
| 24 | X | 125 | VAL | 5.9 |
| 4 | D | 99 | ILE | 5.9 |
| 9 | I | 158 | ILE | 5.9 |
| 29 | c | 61 | SER | 5.9 |
| 5 | E | 141 | THR | 5.9 |
| 5 | E | 119 | ALA | 5.9 |
| 4 | D | 179 | GLN | 5.9 |
| 34 | i | 1057 | U | 5.9 |
| 7 | G | 17 | GLU | 5.9 |
| 4 | D | 12 | VAL | 5.9 |
| 9 | I | 86 | SER | 5.9 |
| 9 | I | 106 | SER | 5.8 |
| 18 | R | 111 | PHE | 5.8 |
| 24 | X | 100 | VAL | 5.8 |
| 36 | k | 18 | G | 5.8 |
| 16 | P | 111 | MET | 5.8 |
| 4 | D | 105 | LEU | 5.8 |
| 27 | a | 44 | ILE | 5.8 |
| 17 | Q | 111 | ILE | 5.8 |
| 2 | B | 46 | LYS | 5.8 |
| 4 | D | 16 | ILE | 5.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | F | 140 | ASP | 5.8 |
| 15 | O | 25 | GLU | 5.8 |
| 34 | i | 824 | G | 5.8 |
| 24 | X | 56 | GLY | 5.7 |
| 4 | D | 191 | PRO | 5.7 |
| 34 | i | 1693 | C | 5.7 |
| 5 | E | 123 | LEU | 5.7 |
| 7 | G | 44 | GLU | 5.7 |
| 34 | i | 251 | C | 5.7 |
| 4 | D | 7 | LYS | 5.7 |
| 6 | F | 173 | LEU | 5.7 |
| 15 | O | 119 | LEU | 5.7 |
| 12 | L | 142 | VAL | 5.7 |
| 24 | X | 114 | ASP | 5.7 |
| 7 | G | 153 | VAL | 5.7 |
| 11 | K | 19 | GLY | 5.7 |
| 14 | N | 147 | SER | 5.7 |
| 3 | C | 209 | THR | 5.7 |
| 17 | Q | 92 | LEU | 5.7 |
| 6 | F | 93 | VAL | 5.7 |
| 4 | D | 76 | ARG | 5.7 |
| 29 | c | 30 | VAL | 5.7 |
| 6 | F | 122 | ARG | 5.7 |
| 6 | F | 42 | LYS | 5.7 |
| 16 | P | 11 | THR | 5.7 |
| 27 | a | 46 | GLU | 5.7 |
| 5 | E | 97 | GLU | 5.7 |
| 9 | I | 90 | LEU | 5.7 |
| 12 | L | 143 | LEU | 5.7 |
| 23 | W | 72 | CYS | 5.7 |
| 34 | i | 1663 | U | 5.7 |
| 6 | F | 47 | LYS | 5.7 |
| 11 | K | 60 | GLU | 5.7 |
| 34 | i | 253 | G | 5.7 |
| 16 | P | 119 | PHE | 5.7 |
| 3 | C | 152 | ARG | 5.6 |
| 9 | I | 177 | SER | 5.6 |
| 21 | U | 88 | LEU | 5.6 |
| 16 | P | 92 | SER | 5.6 |
| 34 | i | 721 | C | 5.6 |
| 4 | D | 138 | VAL | 5.6 |
| 11 | K | 71 | LEU | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | C | 199 | LEU | 5.6 |
| 10 | J | 95 | ASP | 5.6 |
| 5 | E | 110 | ALA | 5.6 |
| 3 | C | 190 | ILE | 5.6 |
| 4 | D | 26 | THR | 5.6 |
| 9 | I | 130 | THR | 5.6 |
| 14 | N | 143 | SER | 5.6 |
| 4 | D | 131 | ALA | 5.6 |
| 5 | E | 42 | LEU | 5.6 |
| 21 | U | 82 | MET | 5.6 |
| 24 | X | 68 | LYS | 5.5 |
| 4 | D | 185 | LYS | 5.5 |
| 24 | X | 54 | LYS | 5.5 |
| 3 | C | 222 | ALA | 5.5 |
| 12 | L | 124 | ASP | 5.5 |
| 4 | D | 23 | GLU | 5.5 |
| 24 | X | 9 | THR | 5.5 |
| 12 | L | 109 | MET | 5.5 |
| 30 | d | 51 | GLY | 5.5 |
| 23 | W | 95 | PRO | 5.5 |
| 16 | P | 96 | VAL | 5.5 |
| 29 | c | 62 | GLU | 5.5 |
| 23 | W | 100 | GLY | 5.4 |
| 16 | P | 25 | LEU | 5.4 |
| 16 | P | 56 | LEU | 5.4 |
| 24 | X | 86 | PRO | 5.4 |
| 1 | A | 61 | ALA | 5.4 |
| 15 | O | 62 | VAL | 5.4 |
| 34 | i | 133 | C | 5.4 |
| 2 | B | 217 | MET | 5.4 |
| 29 | c | 50 | VAL | 5.4 |
| 15 | O | 26 | ASN | 5.4 |
| 6 | F | 197 | GLU | 5.4 |
| 23 | W | 102 | ILE | 5.4 |
| 9 | I | 187 | GLY | 5.4 |
| 6 | F | 27 | ASP | 5.4 |
| 16 | P | 85 | ILE | 5.4 |
| 5 | E | 44 | LEU | 5.4 |
| 34 | i | 1253 | G | 5.4 |
| 5 | E | 164 | LEU | 5.4 |
| 5 | E | 45 | ILE | 5.4 |
| 30 | d | 50 | ILE | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 739 | U | 5.3 |
| 5 | E | 82 | TYR | 5.3 |
| 4 | D | 18 | LYS | 5.3 |
| 5 | E | 109 | PHE | 5.3 |
| 34 | i | 1654 | U | 5.3 |
| 2 | B | 69 | VAL | 5.3 |
| 12 | L | 120 | VAL | 5.3 |
| 5 | E | 99 | PHE | 5.3 |
| 30 | d | 47 | ALA | 5.3 |
| 9 | I | 79 | ILE | 5.3 |
| 34 | i | 4 | C | 5.3 |
| 7 | G | 16 | ILE | 5.3 |
| 12 | L | 128 | VAL | 5.3 |
| 33 | g | 30 | MET | 5.3 |
| 5 | E | 160 | ILE | 5.3 |
| 6 | F | 97 | PHE | 5.3 |
| 14 | N | 150 | VAL | 5.3 |
| 3 | C | 180 | LEU | 5.3 |
| 34 | i | 299 | G | 5.3 |
| 5 | E | 239 | PRO | 5.3 |
| 3 | C | 192 | ALA | 5.3 |
| 34 | i | 397 | G | 5.2 |
| 4 | D | 17 | PHE | 5.2 |
| 4 | D | 129 | SER | 5.2 |
| 5 | E | 139 | LEU | 5.2 |
| 8 | H | 161 | ALA | 5.2 |
| 9 | I | 127 | ALA | 5.2 |
| 10 | J | 78 | LEU | 5.2 |
| 4 | D | 14 | ASP | 5.2 |
| 4 | D | 55 | THR | 5.2 |
| 34 | i | 679 | U | 5.2 |
| 34 | i | 126 | G | 5.2 |
| 9 | I | 162 | LEU | 5.2 |
| 21 | U | 33 | GLU | 5.2 |
| 16 | P | 90 | VAL | 5.2 |
| 23 | W | 101 | PHE | 5.2 |
| 7 | G | 49 | VAL | 5.2 |
| 24 | X | 57 | VAL | 5.2 |
| 22 | V | 10 | ASP | 5.2 |
| 4 | D | 163 | PRO | 5.2 |
| 4 | D | 134 | CYS | 5.2 |
| 27 | a | 47 | ALA | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | D | 10 | LYS | 5.1 |
| 3 | C | 219 | GLY | 5.1 |
| 16 | P | 108 | LYS | 5.1 |
| 34 | i | 1860 | A | 5.1 |
| 9 | I | 42 | ARG | 5.1 |
| 15 | O | 117 | ARG | 5.1 |
| 4 | D | 158 | ILE | 5.1 |
| 4 | D | 130 | GLY | 5.1 |
| 16 | P | 91 | GLY | 5.1 |
| 17 | Q | 85 | ARG | 5.1 |
| 4 | D | 13 | ALA | 5.1 |
| 3 | C | 223 | LYS | 5.1 |
| 7 | G | 83 | CYS | 5.1 |
| 18 | R | 110 | ASP | 5.1 |
| 34 | i | 1249 | A | 5.1 |
| 34 | i | 1474 | U | 5.1 |
| 11 | K | 65 | ARG | 5.1 |
| 27 | a | 37 | LYS | 5.1 |
| 21 | U | 113 | GLU | 5.1 |
| 15 | O | 96 | LYS | 5.1 |
| 7 | G | 19 | ASP | 5.1 |
| 7 | G | 191 | ARG | 5.1 |
| 5 | E | 35 | PRO | 5.1 |
| 2 | B | 101 | HIS | 5.1 |
| 2 | B | 226 | GLY | 5.0 |
| 9 | I | 120 | PRO | 5.0 |
| 9 | I | 139 | LYS | 5.0 |
| 34 | i | 823 | A | 5.0 |
| 24 | X | 81 | ILE | 5.0 |
| 12 | L | 145 | VAL | 5.0 |
| 24 | X | 111 | ALA | 5.0 |
| 34 | i | 1476 | A | 5.0 |
| 3 | C | 63 | LEU | 5.0 |
| 10 | J | 97 | ILE | 5.0 |
| 15 | O | 72 | TYR | 5.0 |
| 16 | P | 83 | MET | 5.0 |
| 34 | i | 298 | G | 5.0 |
| 4 | D | 9 | ARG | 5.0 |
| 6 | F | 25 | THR | 5.0 |
| 34 | i | 1581 | U | 5.0 |
| 3 | C | 178 | VAL | 5.0 |
| 15 | O | 128 | ARG | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 1092 | G | 5.0 |
| 23 | W | 127 | GLY | 5.0 |
| 24 | X | 90 | CYS | 5.0 |
| 12 | L | 80 | MET | 5.0 |
| 1 | A | 3 | GLY | 4.9 |
| 8 | H | 159 | ASP | 4.9 |
| 16 | P | 57 | LEU | 4.9 |
| 19 | S | 63 | GLU | 4.9 |
| 7 | G | 48 | TYR | 4.9 |
| 24 | X | 53 | GLU | 4.9 |
| 2 | B | 44 | ILE | 4.9 |
| 34 | i | 1655 | C | 4.9 |
| 5 | E | 129 | ILE | 4.9 |
| 6 | F | 20 | PHE | 4.9 |
| 17 | Q | 144 | SER | 4.9 |
| 34 | i | 1255 | A | 4.9 |
| 15 | O | 67 | ASP | 4.9 |
| 6 | F | 51 | HIS | 4.9 |
| 5 | E | 147 | ILE | 4.9 |
| 9 | I | 137 | LEU | 4.9 |
| 5 | E | 47 | PHE | 4.9 |
| 3 | C | 88 | LYS | 4.9 |
| 12 | L | 126 | VAL | 4.9 |
| 16 | P | 23 | ASP | 4.9 |
| 11 | K | 23 | ALA | 4.9 |
| 3 | C | 170 | THR | 4.8 |
| 6 | F | 169 | ILE | 4.8 |
| 34 | i | 130 | G | 4.8 |
| 6 | F | 17 | ILE | 4.8 |
| 19 | S | 64 | VAL | 4.8 |
| 12 | L | 9 | ALA | 4.8 |
| 27 | a | 79 | ILE | 4.8 |
| 9 | I | 44 | HIS | 4.8 |
| 7 | G | 121 | ILE | 4.8 |
| 6 | F | 148 | ASN | 4.8 |
| 14 | N | 148 | ALA | 4.8 |
| 34 | i | 9 | U | 4.8 |
| 11 | K | 15 | LEU | 4.8 |
| 4 | D | 90 | LYS | 4.8 |
| 2 | B | 45 | GLY | 4.8 |
| 4 | D | 63 | GLY | 4.8 |
| 6 | F | 139 | VAL | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | F | 89 | THR | 4.8 |
| 4 | D | 182 | LEU | 4.8 |
| 5 | E | 95 | THR | 4.8 |
| 2 | B | 223 | PHE | 4.8 |
| 22 | V | 11 | LEU | 4.8 |
| 34 | i | 1736 | U | 4.8 |
| 4 | D | 181 | VAL | 4.8 |
| 30 | d | 9 | SER | 4.8 |
| 6 | F | 120 | GLY | 4.8 |
| 4 | D | 77 | PHE | 4.7 |
| 9 | I | 109 | TYR | 4.7 |
| 5 | E | 118 | GLU | 4.7 |
| 7 | G | 73 | VAL | 4.7 |
| 4 | D | 126 | ILE | 4.7 |
| 7 | G | 27 | PHE | 4.7 |
| 34 | i | 94 | G | 4.7 |
| 34 | i | 687 | G | 4.7 |
| 34 | i | 1530 | U | 4.7 |
| 1 | A | 65 | ILE | 4.7 |
| 24 | X | 126 | ALA | 4.7 |
| 16 | P | 84 | ILE | 4.7 |
| 6 | F | 204 | ARG | 4.7 |
| 7 | G | 84 | TYR | 4.7 |
| 33 | g | 33 | SER | 4.7 |
| 34 | i | 462 | C | 4.7 |
| 5 | E | 36 | HIS | 4.7 |
| 17 | Q | 117 | ARG | 4.7 |
| 34 | i | 441 | G | 4.7 |
| 5 | E | 55 | ALA | 4.7 |
| 4 | D | 173 | ARG | 4.7 |
| 17 | Q | 89 | SER | 4.7 |
| 34 | i | 1541 | G | 4.7 |
| 3 | C | 171 | GLY | 4.7 |
| 4 | D | 121 | GLY | 4.7 |
| 21 | U | 27 | ARG | 4.7 |
| 5 | E | 83 | PRO | 4.7 |
| 34 | i | 1251 | G | 4.6 |
| 9 | I | 94 | LYS | 4.6 |
| 9 | I | 124 | LYS | 4.6 |
| 34 | i | 736 | C | 4.6 |
| 6 | F | 191 | LYS | 4.6 |
| 7 | G | 120 | ASP | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | E | 98 | ASN | 4.6 |
| 34 | i | 1665 | C | 4.6 |
| 3 | C | 113 | VAL | 4.6 |
| 15 | O | 31 | CYS | 4.6 |
| 21 | U | 116 | ILE | 4.6 |
| 18 | R | 89 | SER | 4.6 |
| 9 | I | 166 | PHE | 4.6 |
| 34 | i | 22 | A | 4.6 |
| 17 | Q | 6 | PRO | 4.6 |
| 21 | U | 50 | VAL | 4.6 |
| 33 | g | 58 | ALA | 4.6 |
| 16 | P | 28 | MET | 4.6 |
| 34 | i | 1544 | U | 4.6 |
| 34 | i | 1093 | G | 4.6 |
| 34 | i | 1390 | G | 4.6 |
| 34 | i | 295 | C | 4.6 |
| 5 | E | 157 | ASN | 4.6 |
| 9 | I | 62 | VAL | 4.6 |
| 5 | E | 121 | TYR | 4.6 |
| 36 | k | 20 | U | 4.6 |
| 5 | E | 77 | ARG | 4.6 |
| 7 | G | 114 | VAL | 4.6 |
| 37 | n | 92 | ILE | 4.6 |
| 16 | P | 110 | GLU | 4.6 |
| 12 | L | 7 | GLU | 4.6 |
| 34 | i | 2 | A | 4.6 |
| 4 | D | 167 | TYR | 4.6 |
| 7 | G | 42 | GLY | 4.5 |
| 14 | N | 144 | SER | 4.5 |
| 34 | i | 294 | C | 4.5 |
| 21 | U | 42 | GLY | 4.5 |
| 9 | I | 179 | PRO | 4.5 |
| 1 | A | 60 | LEU | 4.5 |
| 12 | L | 73 | LEU | 4.5 |
| 37 | n | 91 | VAL | 4.5 |
| 27 | a | 48 | ALA | 4.5 |
| 3 | C | 221 | PHE | 4.5 |
| 9 | I | 122 | GLY | 4.5 |
| 29 | c | 60 | GLU | 4.5 |
| 4 | D | 108 | LYS | 4.5 |
| 3 | C | 173 | CYS | 4.5 |
| 24 | X | 124 | LYS | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 23 | G | 4.5 |
| 12 | L | 8 | ARG | 4.5 |
| 23 | W | 9 | ASP | 4.5 |
| 1 | A | 63 | ARG | 4.5 |
| 34 | i | 434 | G | 4.4 |
| 5 | E | 48 | LEU | 4.4 |
| 16 | P | 78 | THR | 4.4 |
| 36 | k | 13 | C | 4.4 |
| 36 | k | 11 | A | 4.4 |
| 6 | F | 15 | PRO | 4.4 |
| 15 | O | 97 | LEU | 4.4 |
| 3 | C | 235 | TYR | 4.4 |
| 34 | i | 1250 | C | 4.4 |
| 5 | E | 226 | PHE | 4.4 |
| 34 | i | 659 | A | 4.4 |
| 9 | I | 82 | VAL | 4.4 |
| 35 | j | 73 | C | 4.4 |
| 26 | Z | 87 | ALA | 4.4 |
| 6 | F | 52 | SER | 4.4 |
| 20 | T | 35 | ASP | 4.4 |
| 6 | F | 90 | VAL | 4.4 |
| 34 | i | 375 | G | 4.4 |
| 21 | U | 38 | ASP | 4.4 |
| 23 | W | 61 | ILE | 4.4 |
| 34 | i | 1083 | A | 4.4 |
| 6 | F | 170 | ALA | 4.4 |
| 34 | i | 93 | U | 4.4 |
| 6 | F | 24 | SER | 4.4 |
| 34 | i | 1666 | G | 4.4 |
| 9 | I | 87 | ASN | 4.4 |
| 34 | i | 1485 | A | 4.4 |
| 16 | P | 109 | PRO | 4.4 |
| 34 | i | 1543 | G | 4.4 |
| 7 | G | 82 | SER | 4.4 |
| 15 | O | 22 | ALA | 4.4 |
| 34 | i | 302 | C | 4.4 |
| 17 | Q | 48 | GLN | 4.4 |
| 8 | H | 163 | GLN | 4.3 |
| 14 | N | 84 | LEU | 4.3 |
| 14 | N | 145 | THR | 4.3 |
| 16 | P | 116 | LEU | 4.3 |
| 14 | N | 141 | TYR | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 21 | U | 108 | PRO | 4.3 |
| 17 | Q | 52 | LEU | 4.3 |
| 27 | a | 78 | ALA | 4.3 |
| 34 | i | 1153 | G | 4.3 |
| 4 | D | 169 | ASP | 4.3 |
| 6 | F | 186 | ASN | 4.3 |
| 5 | E | 117 | GLU | 4.3 |
| 7 | G | 34 | THR | 4.3 |
| 10 | J | 73 | GLU | 4.3 |
| 34 | i | 303 | G | 4.3 |
| 34 | i | 1855 | G | 4.3 |
| 3 | C | 175 | SER | 4.3 |
| 12 | L | 110 | SER | 4.3 |
| 3 | C | 208 | TYR | 4.3 |
| 2 | B | 135 | LEU | 4.3 |
| 9 | I | 136 | ILE | 4.3 |
| 10 | J | 57 | ALA | 4.3 |
| 29 | c | 56 | LEU | 4.3 |
| 34 | i | 206 | A | 4.3 |
| 5 | E | 63 | LYS | 4.3 |
| 6 | F | 96 | ALA | 4.3 |
| 29 | c | 44 | ARG | 4.3 |
| 2 | B | 215 | VAL | 4.3 |
| 12 | L | 141 | ASN | 4.3 |
| 16 | P | 60 | LEU | 4.3 |
| 34 | i | 129 | C | 4.3 |
| 34 | i | 509 | A | 4.3 |
| 2 | B | 81 | PHE | 4.3 |
| 27 | a | 72 | HIS | 4.3 |
| 7 | G | 152 | ASP | 4.2 |
| 34 | i | 1548 | C | 4.2 |
| 4 | D | 64 | ARG | 4.2 |
| 34 | i | 293 | A | 4.2 |
| 10 | J | 75 | ASN | 4.2 |
| 34 | i | 37 | C | 4.2 |
| 34 | i | 1089 | A | 4.2 |
| 34 | i | 1496 | G | 4.2 |
| 6 | F | 92 | ILE | 4.2 |
| 19 | S | 71 | MET | 4.2 |
| 6 | F | 172 | CYS | 4.2 |
| 6 | F | 147 | VAL | 4.2 |
| 34 | i | 1746 | C | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 57 | LYS | 4.2 |
| 6 | F | 149 | GLN | 4.2 |
| 31 | e | 76 | VAL | 4.2 |
| 34 | i | 1757 | G | 4.2 |
| 23 | W | 112 | ASP | 4.2 |
| 3 | C | 156 | GLY | 4.2 |
| 34 | i | 177 | G | 4.2 |
| 34 | i | 733 | G | 4.2 |
| 21 | U | 53 | PRO | 4.2 |
| 6 | F | 179 | ASN | 4.2 |
| 31 | e | 87 | ARG | 4.2 |
| 34 | i | 132 | U | 4.2 |
| 37 | n | 94 | LYS | 4.2 |
| 34 | i | 1540 | A | 4.2 |
| 34 | i | 378 | U | 4.2 |
| 3 | C | 200 | LEU | 4.2 |
| 15 | O | 70 | SER | 4.2 |
| 4 | D | 8 | LYS | 4.2 |
| 4 | D | 107 | TYR | 4.2 |
| 9 | I | 34 | ALA | 4.2 |
| 7 | G | 3 | LEU | 4.2 |
| 34 | i | 618 | A | 4.2 |
| 2 | B | 230 | GLU | 4.2 |
| 34 | i | 1647 | G | 4.2 |
| 37 | n | 47 | LEU | 4.2 |
| 5 | E | 67 | GLN | 4.1 |
| 4 | D | 54 | ARG | 4.1 |
| 6 | F | 21 | GLY | 4.1 |
| 34 | i | 366 | A | 4.1 |
| 34 | i | 657 | U | 4.1 |
| 5 | E | 155 | LYS | 4.1 |
| 8 | H | 189 | PHE | 4.1 |
| 3 | C | 182 | PRO | 4.1 |
| 7 | G | 75 | LEU | 4.1 |
| 12 | L | 75 | GLY | 4.1 |
| 34 | i | 301 | C | 4.1 |
| 36 | k | 10 | C | 4.1 |
| 4 | D | 174 | HIS | 4.1 |
| 28 | b | 24 | LEU | 4.1 |
| 37 | n | 69 | VAL | 4.1 |
| 34 | i | 1573 | U | 4.1 |
| 5 | E | 140 | VAL | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | F | 141 | VAL | 4.1 |
| 16 | P | 75 | VAL | 4.1 |
| 6 | F | 33 | ILE | 4.1 |
| 6 | F | 138 | ALA | 4.1 |
| 9 | I | 145 | ILE | 4.1 |
| 19 | S | 116 | LYS | 4.1 |
| 3 | C | 176 | VAL | 4.1 |
| 5 | E | 248 | ILE | 4.1 |
| 5 | E | 259 | LYS | 4.1 |
| 5 | E | 46 | ILE | 4.1 |
| 7 | G | 77 | LEU | 4.1 |
| 23 | W | 10 | ALA | 4.1 |
| 8 | H | 190 | PRO | 4.1 |
| 15 | O | 126 | ILE | 4.1 |
| 34 | i | 212 | G | 4.1 |
| 34 | i | 50 | A | 4.1 |
| 34 | i | 1486 | G | 4.1 |
| 6 | F | 14 | THR | 4.1 |
| 12 | L | 140 | PHE | 4.1 |
| 4 | D | 92 | ALA | 4.1 |
| 21 | U | 109 | GLY | 4.1 |
| 34 | i | 688 | U | 4.1 |
| 24 | X | 113 | GLY | 4.0 |
| 34 | i | 1088 | G | 4.1 |
| 7 | G | 180 | VAL | 4.0 |
| 4 | D | 84 | VAL | 4.0 |
| 2 | B | 151 | ARG | 4.0 |
| 12 | L | 101 | ARG | 4.0 |
| 5 | E | 144 | ALA | 4.0 |
| 9 | I | 165 | GLN | 4.0 |
| 19 | S | 48 | ALA | 4.0 |
| 6 | F | 37 | ASP | 4.0 |
| 34 | i | 440 | C | 4.0 |
| 5 | E | 249 | ALA | 4.0 |
| 4 | D | 177 | LEU | 4.0 |
| 6 | F | 23 | TRP | 4.0 |
| 21 | U | 37 | ALA | 4.0 |
| 5 | E | 252 | ARG | 4.0 |
| 5 | E | 162 | ILE | 4.0 |
| 22 | V | 82 | ASN | 4.0 |
| 23 | W | 128 | PHE | 4.0 |
| 34 | i | 367 | G | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | E | 159 | THR | 4.0 |
| 24 | X | 71 | ARG | 4.0 |
| 24 | X | 66 | ILE | 4.0 |
| 1 | A | 62 | ALA | 4.0 |
| 34 | i | 405 | A | 4.0 |
| 24 | X | 58 | GLU | 4.0 |
| 6 | F | 61 | PHE | 4.0 |
| 36 | k | 19 | U | 4.0 |
| 34 | i | 609 | A | 4.0 |
| 4 | D | 168 | VAL | 4.0 |
| 23 | W | 37 | PHE | 4.0 |
| 34 | i | 810 | U | 4.0 |
| 6 | F | 161 | ALA | 4.0 |
| 17 | Q | 135 | PRO | 4.0 |
| 28 | b | 23 | ARG | 4.0 |
| 37 | n | 70 | TRP | 4.0 |
| 1 | A | 2 | SER | 4.0 |
| 6 | F | 171 | GLU | 4.0 |
| 5 | E | 169 | ILE | 3.9 |
| 34 | i | 1539 | C | 3.9 |
| 1 | A | 94 | THR | 3.9 |
| 9 | I | 93 | THR | 3.9 |
| 34 | i | 734 | C | 3.9 |
| 23 | W | 53 | ILE | 3.9 |
| 5 | E | 154 | ILE | 3.9 |
| 8 | H | 162 | GLN | 3.9 |
| 1 | A | 66 | VAL | 3.9 |
| 24 | X | 93 | PHE | 3.9 |
| 34 | i | 692 | U | 3.9 |
| 4 | D | 57 | ASN | 3.9 |
| 27 | a | 12 | LYS | 3.9 |
| 5 | E | 76 | VAL | 3.9 |
| 3 | C | 111 | ALA | 3.9 |
| 17 | Q | 88 | ILE | 3.9 |
| 37 | n | 93 | LEU | 3.9 |
| 18 | R | 87 | GLU | 3.9 |
| 34 | i | 365 | U | 3.9 |
| 30 | d | 23 | VAL | 3.9 |
| 15 | O | 28 | PHE | 3.9 |
| 17 | Q | 56 | LEU | 3.9 |
| 23 | W | 126 | LEU | 3.9 |
| 37 | n | 59 | CYS | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 12 | L | 111 | VAL | 3.9 |
| 34 | i | 1542 | C | 3.9 |
| 34 | i | 339 | A | 3.9 |
| 33 | g | 92 | LEU | 3.9 |
| 34 | i | 252 | C | 3.9 |
| 35 | j | 32 | C | 3.9 |
| 12 | L | 94 | HIS | 3.9 |
| 34 | i | 610 | G | 3.9 |
| 34 | i | 1400 | U | 3.9 |
| 8 | H | 142 | LYS | 3.8 |
| 34 | i | 438 | A | 3.8 |
| 17 | Q | 119 | LEU | 3.8 |
| 21 | U | 20 | ILE | 3.8 |
| 23 | W | 104 | LEU | 3.8 |
| 34 | i | 497 | G | 3.8 |
| 4 | D | 79 | PHE | 3.8 |
| 9 | I | 156 | ALA | 3.8 |
| 34 | i | 330 | C | 3.8 |
| 34 | i | 825 | C | 3.8 |
| 34 | i | 411 | G | 3.8 |
| 9 | I | 108 | PRO | 3.8 |
| 33 | g | 257 | LYS | 3.8 |
| 29 | c | 43 | ILE | 3.8 |
| 24 | X | 134 | TYR | 3.8 |
| 2 | B | 39 | PHE | 3.8 |
| 34 | i | 1648 | U | 3.8 |
| 3 | C | 112 | PHE | 3.8 |
| 4 | D | 151 | LYS | 3.8 |
| 6 | F | 152 | TRP | 3.8 |
| 15 | O | 27 | VAL | 3.8 |
| 28 | b | 25 | VAL | 3.8 |
| 12 | L | 108 | ASN | 3.8 |
| 6 | F | 35 | LEU | 3.8 |
| 16 | P | 7 | LYS | 3.8 |
| 4 | D | 139 | SER | 3.8 |
| 15 | O | 114 | SER | 3.8 |
| 5 | E | 52 | LEU | 3.8 |
| 2 | B | 102 | GLY | 3.8 |
| 35 | j | 75 | A | 3.8 |
| 8 | H | 137 | SER | 3.8 |
| 16 | P | 45 | LEU | 3.8 |
| 4 | D | 4 | GLN | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 84 | PHE | 3.8 |
| 9 | I | 163 | GLU | 3.7 |
| 9 | I | 159 | SER | 3.7 |
| 12 | L | 74 | SER | 3.7 |
| 16 | P | 71 | GLU | 3.7 |
| 34 | i | 439 | A | 3.7 |
| 12 | L | 129 | GLY | 3.7 |
| 37 | n | 65 | LEU | 3.7 |
| 3 | C | 79 | ILE | 3.7 |
| 7 | G | 52 | ILE | 3.7 |
| 12 | L | 21 | LYS | 3.7 |
| 34 | i | 404 | A | 3.7 |
| 34 | i | 729 | C | 3.7 |
| 12 | L | 86 | ILE | 3.7 |
| 16 | P | 21 | ASP | 3.7 |
| 34 | i | 1538 | U | 3.7 |
| 34 | i | 1861 | U | 3.7 |
| 16 | P | 77 | LYS | 3.7 |
| 34 | i | 1082 | G | 3.7 |
| 3 | C | 73 | ILE | 3.7 |
| 19 | S | 50 | ILE | 3.7 |
| 37 | n | 72 | ASN | 3.7 |
| 34 | i | 1859 | C | 3.7 |
| 29 | c | 58 | LEU | 3.7 |
| 2 | B | 32 | ASP | 3.7 |
| 5 | E | 112 | HIS | 3.7 |
| 34 | i | 338 | A | 3.7 |
| 6 | F | 56 | TYR | 3.7 |
| 6 | F | 78 | MET | 3.7 |
| 34 | i | 403 | G | 3.7 |
| 5 | E | 18 | TRP | 3.7 |
| 9 | I | 188 | TYR | 3.7 |
| 22 | V | 27 | LYS | 3.7 |
| 34 | i | 1583 | A | 3.7 |
| 5 | E | 251 | GLU | 3.7 |
| 7 | G | 192 | ILE | 3.7 |
| 29 | c | 42 | ILE | 3.7 |
| 34 | i | 987 | G | 3.7 |
| 33 | g | 55 | PRO | 3.7 |
| 9 | I | 35 | ASN | 3.7 |
| 17 | Q | 134 | GLY | 3.7 |
| 4 | D | 31 | GLU | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 21 | U | 91 | LEU | 3.7 |
| 7 | G | 74 | ARG | 3.7 |
| 21 | U | 70 | CYS | 3.7 |
| 12 | L | 105 | ARG | 3.7 |
| 9 | I | 67 | TRP | 3.7 |
| 34 | i | 329 | A | 3.7 |
| 34 | i | 1482 | A | 3.7 |
| 34 | i | 1818 | A | 3.7 |
| 34 | i | 1523 | G | 3.7 |
| 12 | L | 68 | ILE | 3.7 |
| 7 | G | 179 | LEU | 3.6 |
| 34 | i | 660 | A | 3.6 |
| 14 | N | 82 | PRO | 3.6 |
| 29 | c | 57 | THR | 3.6 |
| 17 | Q | 93 | VAL | 3.6 |
| 23 | W | 124 | LYS | 3.6 |
| 16 | P | 41 | GLN | 3.6 |
| 4 | D | 157 | MET | 3.6 |
| 30 | d | 38 | MET | 3.6 |
| 21 | U | 107 | GLU | 3.6 |
| 7 | G | 5 | ILE | 3.6 |
| 34 | i | 243 | C | 3.6 |
| 1 | A | 59 | LEU | 3.6 |
| 34 | i | 1355 | U | 3.6 |
| 1 | A | 67 | ALA | 3.6 |
| 7 | G | 1 | MET | 3.6 |
| 34 | i | 1491 | G | 3.6 |
| 7 | G | 51 | ARG | 3.6 |
| 2 | B | 153 | THR | 3.6 |
| 5 | E | 120 | LYS | 3.6 |
| 28 | b | 16 | LYS | 3.6 |
| 10 | J | 61 | LEU | 3.6 |
| 9 | I | 138 | ASN | 3.6 |
| 1 | A | 15 | VAL | 3.6 |
| 6 | F | 192 | LYS | 3.6 |
| 17 | Q | 46 | THR | 3.6 |
| 34 | i | 1578 | C | 3.6 |
| 9 | I | 148 | LYS | 3.6 |
| 33 | g | 21 | ILE | 3.6 |
| 4 | D | 208 | VAL | 3.6 |
| 30 | d | 37 | ASN | 3.6 |
| 34 | i | 1090 | C | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | E | 146 | THR | 3.6 |
| 34 | i | 813 | G | 3.6 |
| 34 | i | 1389 | G | 3.6 |
| 34 | i | 1586 | C | 3.6 |
| 2 | B | 86 | LEU | 3.6 |
| 2 | B | 141 | GLY | 3.6 |
| 34 | i | 658 | A | 3.5 |
| 16 | P | 20 | VAL | 3.5 |
| 24 | X | 87 | ASN | 3.5 |
| 9 | I | 132 | GLU | 3.5 |
| 33 | g | 42 | MET | 3.5 |
| 34 | i | 814 | A | 3.5 |
| 23 | W | 60 | LYS | 3.5 |
| 34 | i | 1487 | G | 3.5 |
| 4 | D | 223 | ILE | 3.5 |
| 8 | H | 160 | LYS | 3.5 |
| 23 | W | 13 | SER | 3.5 |
| 4 | D | 46 | THR | 3.5 |
| 34 | i | 176 | U | 3.5 |
| 9 | I | 75 | LYS | 3.5 |
| 24 | X | 6 | GLY | 3.5 |
| 34 | i | 1205 | A | 3.5 |
| 34 | i | 268 | G | 3.5 |
| 23 | W | 27 | ILE | 3.5 |
| 12 | L | 119 | ASP | 3.5 |
| 12 | L | 88 | ILE | 3.5 |
| 34 | i | 682 | G | 3.5 |
| 34 | i | 1138 | G | 3.5 |
| 34 | i | 207 | U | 3.5 |
| 30 | d | 52 | PHE | 3.5 |
| 1 | A | 58 | LEU | 3.5 |
| 2 | B | 133 | TYR | 3.5 |
| 34 | i | 208 | G | 3.5 |
| 36 | k | 12 | A | 3.5 |
| 2 | B | 140 | VAL | 3.5 |
| 5 | E | 81 | THR | 3.5 |
| 15 | O | 19 | PRO | 3.5 |
| 34 | i | 1549 | C | 3.5 |
| 35 | j | 70 | C | 3.5 |
| 29 | c | 8 | PRO | 3.5 |
| 9 | I | 155 | ASN | 3.5 |
| 30 | d | 22 | ARG | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 1445 | G | 3.5 |
| 3 | C | 189 | ILE | 3.5 |
| 19 | S | 68 | ILE | 3.5 |
| 29 | c | 47 | LYS | 3.5 |
| 4 | D | 39 | VAL | 3.5 |
| 23 | W | 125 | ILE | 3.5 |
| 15 | O | 73 | ALA | 3.5 |
| 21 | U | 97 | ILE | 3.5 |
| 34 | i | 258 | G | 3.5 |
| 3 | C | 179 | ARG | 3.4 |
| 9 | I | 91 | VAL | 3.5 |
| 5 | E | 225 | ILE | 3.4 |
| 21 | U | 31 | SER | 3.4 |
| 27 | a | 16 | GLY | 3.4 |
| 23 | W | 40 | VAL | 3.4 |
| 15 | O | 93 | LEU | 3.4 |
| 10 | J | 66 | LYS | 3.4 |
| 31 | e | 88 | GLY | 3.4 |
| 33 | g | 231 | ASP | 3.4 |
| 34 | i | 254 | G | 3.4 |
| 34 | i | 364 | G | 3.4 |
| 34 | i | 1352 | G | 3.4 |
| 34 | i | 1134 | C | 3.4 |
| 2 | B | 224 | GLU | 3.4 |
| 37 | n | 90 | ASP | 3.4 |
| 4 | D | 125 | PHE | 3.4 |
| 23 | W | 130 | PHE | 3.4 |
| 9 | I | 140 | LYS | 3.4 |
| 34 | i | 735 | C | 3.4 |
| 5 | E | 161 | GLN | 3.4 |
| 14 | N | 142 | GLU | 3.4 |
| 13 | M | 95 | ASP | 3.4 |
| 33 | g | 23 | THR | 3.4 |
| 37 | n | 40 | LYS | 3.4 |
| 2 | B | 92 | GLN | 3.4 |
| 34 | i | 1658 | A | 3.4 |
| 3 | C | 174 | GLY | 3.4 |
| 10 | J | 87 | LEU | 3.4 |
| 10 | J | 93 | LYS | 3.4 |
| 34 | i | 21 | U | 3.4 |
| 34 | i | 1745 | C | 3.4 |
| 24 | X | 91 | LEU | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 24 | X | 133 | LEU | 3.4 |
| 34 | i | 644 | A | 3.4 |
| 16 | P | 70 | MET | 3.4 |
| 30 | d | 46 | TYR | 3.4 |
| 2 | B | 73 | ASP | 3.4 |
| 6 | F | 44 | LYS | 3.4 |
| 9 | I | 40 | PRO | 3.4 |
| 34 | i | 549 | G | 3.4 |
| 34 | i | 209 | C | 3.4 |
| 34 | i | 1081 | C | 3.4 |
| 1 | A | 18 | PHE | 3.4 |
| 8 | H | 165 | ASN | 3.3 |
| 34 | i | 1418 | G | 3.3 |
| 4 | D | 141 | LYS | 3.3 |
| 6 | F | 175 | ASP | 3.3 |
| 34 | i | 13 | C | 3.3 |
| 34 | i | 435 | A | 3.3 |
| 5 | E | 142 | HIS | 3.3 |
| 6 | F | 95 | HIS | 3.3 |
| 29 | c | 14 | VAL | 3.3 |
| 34 | i | 244 | C | 3.3 |
| 17 | Q | 114 | GLN | 3.3 |
| 4 | D | 40 | ARG | 3.3 |
| 15 | O | 120 | ALA | 3.3 |
| 10 | J | 16 | PRO | 3.3 |
| 37 | n | 111 | GLU | 3.3 |
| 23 | W | 76 | SER | 3.3 |
| 34 | i | 328 | G | 3.3 |
| 34 | i | 1392 | A | 3.3 |
| 2 | B | 78 | GLU | 3.3 |
| 5 | E | 228 | ILE | 3.3 |
| 2 | B | 181 | LEU | 3.3 |
| 29 | c | 31 | ARG | 3.3 |
| 34 | i | 997 | A | 3.3 |
| 16 | P | 33 | LEU | 3.3 |
| 1 | A | 4 | ALA | 3.3 |
| 33 | g | 41 | ILE | 3.3 |
| 3 | C | 217 | THR | 3.3 |
| 9 | I | 169 | GLY | 3.3 |
| 34 | i | 730 | C | 3.3 |
| 36 | k | 22 | C | 3.3 |
| 2 | B | 207 | LEU | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 15 | O | 40 | THR | 3.3 |
| 7 | G | 112 | VAL | 3.3 |
| 34 | i | 724 | C | 3.3 |
| 34 | i | 1058 | A | 3.3 |
| 2 | B | 225 | LEU | 3.3 |
| 2 | B | 212 | VAL | 3.3 |
| 12 | L | 134 | LEU | 3.3 |
| 34 | i | 297 | C | 3.3 |
| 20 | T | 36 | THR | 3.3 |
| 4 | D | 81 | GLU | 3.3 |
| 6 | F | 45 | TYR | 3.3 |
| 34 | i | 385 | G | 3.3 |
| 34 | i | 436 | G | 3.3 |
| 31 | e | 124 | GLY | 3.3 |
| 34 | i | 14 | C | 3.3 |
| 34 | i | 1735 | C | 3.3 |
| 29 | c | 41 | SER | 3.3 |
| 34 | i | 1852 | G | 3.3 |
| 34 | i | 996 | C | 3.3 |
| 34 | i | 53 | C | 3.3 |
| 24 | X | 112 | VAL | 3.2 |
| 34 | i | 175 | A | 3.2 |
| 34 | i | 1817 | A | 3.2 |
| 8 | H | 143 | ARG | 3.2 |
| 9 | I | 170 | LYS | 3.2 |
| 29 | c | 59 | LEU | 3.2 |
| 10 | J | 96 | TYR | 3.2 |
| 16 | P | 69 | PRO | 3.2 |
| 34 | i | 1094 | C | 3.2 |
| 6 | F | 43 | GLU | 3.2 |
| 1 | A | 178 | LEU | 3.2 |
| 2 | B | 209 | ASP | 3.2 |
| 33 | g | 272 | GLN | 3.2 |
| 34 | i | 636 | G | 3.2 |
| 24 | X | 102 | VAL | 3.2 |
| 34 | i | 1228 | U | 3.2 |
| 18 | R | 91 | LEU | 3.2 |
| 33 | g | 56 | GLN | 3.2 |
| 24 | X | 129 | SER | 3.2 |
| 29 | c | 66 | ARG | 3.2 |
| 3 | C | 124 | LEU | 3.2 |
| 7 | G | 76 | LEU | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | F | 130 | ARG | 3.2 |
| 24 | X | 141 | PRO | 3.2 |
| 34 | i | 309 | A | 3.2 |
| 2 | B | 211 | PHE | 3.2 |
| 5 | E | 41 | CYS | 3.2 |
| 34 | i | 1484 | C | 3.2 |
| 37 | n | 77 | ILE | 3.2 |
| 1 | A | 161 | ILE | 3.2 |
| 34 | i | 1191 | A | 3.2 |
| 34 | i | 1483 | A | 3.2 |
| 29 | c | 7 | GLN | 3.2 |
| 3 | C | 181 | ILE | 3.2 |
| 17 | Q | 49 | TYR | 3.2 |
| 34 | i | 467 | G | 3.2 |
| 17 | Q | 102 | GLU | 3.2 |
| 31 | e | 123 | PHE | 3.2 |
| 1 | A | 51 | LEU | 3.2 |
| 4 | D | 123 | LEU | 3.2 |
| 12 | L | 87 | VAL | 3.2 |
| 18 | R | 90 | ALA | 3.2 |
| 12 | L | 106 | HIS | 3.2 |
| 19 | S | 123 | LEU | 3.2 |
| 29 | c | 54 | ASP | 3.2 |
| 1 | A | 186 | ARG | 3.2 |
| 2 | B | 82 | ARG | 3.2 |
| 5 | E | 258 | ALA | 3.2 |
| 34 | i | 1853 | A | 3.2 |
| 34 | i | 468 | G | 3.2 |
| 21 | U | 57 | PRO | 3.2 |
| 23 | W | 34 | ILE | 3.2 |
| 17 | Q | 110 | ASP | 3.2 |
| 2 | B | 70 | SER | 3.2 |
| 2 | B | 154 | SER | 3.2 |
| 3 | C | 165 | VAL | 3.2 |
| 34 | i | 396 | U | 3.2 |
| 34 | i | 1151 | U | 3.2 |
| 34 | i | 822 | A | 3.2 |
| 34 | i | 1190 | A | 3.2 |
| 6 | F | 103 | LEU | 3.2 |
| 5 | E | 257 | ALA | 3.2 |
| 18 | R | 112 | GLY | 3.2 |
| 21 | U | 106 | ILE | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | I | 198 | TYR | 3.1 |
| 3 | C | 126 | MET | 3.1 |
| 10 | J | 98 | LEU | 3.1 |
| 5 | E | 165 | GLU | 3.1 |
| 5 | E | 21 | ASP | 3.1 |
| 8 | H | 187 | PHE | 3.1 |
| 34 | i | 49 | C | 3.1 |
| 10 | J | 92 | MET | 3.1 |
| 33 | g | 57 | ARG | 3.1 |
| 7 | G | 109 | LEU | 3.1 |
| 34 | i | 307 | G | 3.1 |
| 3 | C | 197 | LYS | 3.1 |
| 24 | X | 119 | ARG | 3.1 |
| 31 | e | 122 | THR | 3.1 |
| 34 | i | 637 | U | 3.1 |
| 34 | i | 32 | U | 3.1 |
| 34 | i | 1495 | U | 3.1 |
| 23 | W | 110 | ILE | 3.1 |
| 34 | i | 876 | G | 3.1 |
| 27 | a | 62 | TYR | 3.1 |
| 34 | i | 662 | A | 3.1 |
| 12 | L | 112 | HIS | 3.1 |
| 7 | G | 115 | LYS | 3.1 |
| 7 | G | 116 | LYS | 3.1 |
| 34 | i | 202 | U | 3.1 |
| 34 | i | 1858 | U | 3.1 |
| 31 | e | 90 | THR | 3.1 |
| 33 | g | 250 | ALA | 3.1 |
| 7 | G | 93 | LYS | 3.1 |
| 9 | I | 56 | ARG | 3.1 |
| 15 | O | 23 | GLU | 3.1 |
| 34 | i | 1470 | A | 3.1 |
| 1 | A | 145 | ILE | 3.1 |
| 15 | O | 58 | GLY | 3.1 |
| 4 | D | 106 | ARG | 3.1 |
| 34 | i | 247 | C | 3.1 |
| 34 | i | 10 | G | 3.1 |
| 9 | I | 135 | GLU | 3.1 |
| 24 | X | 123 | VAL | 3.1 |
| 27 | a | 20 | PRO | 3.1 |
| 34 | i | 1327 | C | 3.1 |
| 34 | i | 1737 | C | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | E | 253 | ASP | 3.1 |
| 34 | i | 1584 | A | 3.1 |
| 35 | j | 72 | A | 3.1 |
| 4 | D | 27 | ARG | 3.1 |
| 9 | I | 110 | ARG | 3.1 |
| 12 | L | 59 | LYS | 3.1 |
| 2 | B | 122 | GLU | 3.1 |
| 10 | J | 71 | LEU | 3.1 |
| 35 | j | 37 | A | 3.1 |
| 33 | g | 249 | CYS | 3.1 |
| 27 | a | 65 | PRO | 3.0 |
| 34 | i | 811 | U | 3.0 |
| 34 | i | 1139 | A | 3.0 |
| 1 | A | 64 | ALA | 3.0 |
| 3 | C | 227 | ASP | 3.0 |
| 6 | F | 26 | ASP | 3.0 |
| 8 | H | 158 | LEU | 3.0 |
| 3 | C | 91 | VAL | 3.0 |
| 31 | e | 75 | LYS | 3.0 |
| 14 | N | 20 | ARG | 3.0 |
| 34 | i | 1350 | G | 3.0 |
| 7 | G | 24 | LEU | 3.0 |
| 9 | I | 114 | GLU | 3.0 |
| 10 | J | 91 | LYS | 3.0 |
| 11 | K | 25 | LYS | 3.0 |
| 12 | L | 77 | VAL | 3.0 |
| 6 | F | 36 | GLN | 3.0 |
| 2 | B | 143 | THR | 3.0 |
| 9 | I | 182 | CYS | 3.0 |
| 19 | S | 6 | PRO | 3.0 |
| 24 | X | 11 | ARG | 3.0 |
| 27 | a | 86 | ASN | 3.0 |
| 30 | d | 6 | LEU | 3.0 |
| 30 | d | 36 | LEU | 3.0 |
| 3 | C | 164 | THR | 3.0 |
| 5 | E | 138 | HIS | 3.0 |
| 34 | i | 1324 | G | 3.0 |
| 34 | i | 1497 | C | 3.0 |
| 6 | F | 188 | TYR | 3.0 |
| 23 | W | 38 | LEU | 3.0 |
| 26 | Z | 108 | ILE | 3.0 |
| 34 | i | 1642 | A | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 331 | C | 3.0 |
| 34 | i | 1524 | C | 3.0 |
| 12 | L | 79 | LYS | 3.0 |
| 30 | d | 49 | ASP | 3.0 |
| 37 | n | 60 | HIS | 3.0 |
| 5 | E | 175 | PHE | 3.0 |
| 34 | i | 1494 | A | 3.0 |
| 7 | G | 117 | GLY | 3.0 |
| 12 | L | 130 | GLU | 3.0 |
| 34 | i | 1150 | U | 3.0 |
| 5 | E | 126 | VAL | 3.0 |
| 17 | Q | 63 | PHE | 3.0 |
| 24 | X | 127 | ASN | 3.0 |
| 34 | i | 548 | G | 3.0 |
| 2 | B | 229 | MET | 3.0 |
| 34 | i | 379 | A | 3.0 |
| 10 | J | 90 | GLY | 3.0 |
| 1 | A | 24 | HIS | 3.0 |
| 6 | F | 146 | ARG | 3.0 |
| 34 | i | 1764 | G | 3.0 |
| 34 | i | 1843 | G | 3.0 |
| 25 | Y | 50 | THR | 3.0 |
| 34 | i | 1587 | C | 3.0 |
| 3 | C | 205 | ASP | 3.0 |
| 34 | i | 1477 | G | 3.0 |
| 34 | i | 1585 | C | 3.0 |
| 2 | B | 36 | PRO | 3.0 |
| 3 | C | 125 | GLY | 3.0 |
| 26 | Z | 50 | PHE | 3.0 |
| 29 | c | 32 | VAL | 3.0 |
| 37 | n | 67 | LYS | 3.0 |
| 14 | N | 81 | ALA | 3.0 |
| 15 | O | 111 | GLY | 3.0 |
| 20 | T | 118 | ASP | 3.0 |
| 25 | Y | 18 | LEU | 3.0 |
| 33 | g | 78 | ALA | 3.0 |
| 9 | I | 41 | ARG | 3.0 |
| 36 | k | 17 | U | 3.0 |
| 34 | i | 1353 | A | 2.9 |
| 35 | j | 71 | U | 2.9 |
| 6 | F | 57 | ALA | 2.9 |
| 34 | i | 944 | C | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 995 | G | 2.9 |
| 34 | i | 1575 | A | 2.9 |
| 34 | i | 1660 | G | 2.9 |
| 12 | L | 113 | LEU | 2.9 |
| 34 | i | 656 | U | 2.9 |
| 34 | i | 1657 | U | 2.9 |
| 6 | F | 201 | LYS | 2.9 |
| 4 | D | 5 | ILE | 2.9 |
| 34 | i | 410 | G | 2.9 |
| 34 | i | 645 | A | 2.9 |
| 5 | E | 227 | VAL | 2.9 |
| 10 | J | 70 | ARG | 2.9 |
| 11 | K | 42 | ASN | 2.9 |
| 5 | E | 103 | TYR | 2.9 |
| 27 | a | 19 | GLN | 2.9 |
| 34 | i | 5 | U | 2.9 |
| 34 | i | 128 | U | 2.9 |
| 17 | Q | 39 | LEU | 2.9 |
| 19 | S | 49 | ASP | 2.9 |
| 37 | n | 78 | LEU | 2.9 |
| 34 | i | 1133 | U | 2.9 |
| 34 | i | 459 | A | 2.9 |
| 5 | E | 75 | LYS | 2.9 |
| 34 | i | 1447 | G | 2.9 |
| 34 | i | 1354 | U | 2.9 |
| 23 | W | 96 | SER | 2.9 |
| 34 | i | 1212 | C | 2.9 |
| 2 | B | 221 | PRO | 2.9 |
| 12 | L | 22 | ARG | 2.9 |
| 17 | Q | 47 | LEU | 2.9 |
| 23 | W | 6 | VAL | 2.9 |
| 1 | A | 159 | ILE | 2.9 |
| 24 | X | 120 | PHE | 2.9 |
| 4 | D | 61 | GLU | 2.9 |
| 34 | i | 643 | A | 2.9 |
| 27 | a | 95 | ARG | 2.9 |
| 31 | e | 79 | SER | 2.9 |
| 11 | K | 59 | LYS | 2.9 |
| 15 | O | 61 | LYS | 2.9 |
| 17 | Q | 103 | ALA | 2.9 |
| 34 | i | 43 | U | 2.9 |
| 34 | i | 833 | A | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 23 | W | 77 | PRO | 2.9 |
| 21 | U | 51 | LYS | 2.9 |
| 26 | Z | 69 | THR | 2.9 |
| 33 | g | 43 | TRP | 2.9 |
| 9 | I | 77 | ARG | 2.8 |
| 17 | Q | 104 | SER | 2.8 |
| 21 | U | 29 | VAL | 2.8 |
| 19 | S | 42 | HIS | 2.8 |
| 19 | S | 127 | TRP | 2.8 |
| 16 | P | 17 | TYR | 2.8 |
| 15 | O | 132 | VAL | 2.8 |
| 21 | U | 54 | VAL | 2.8 |
| 34 | i | 1547 | G | 2.8 |
| 3 | C | 196 | LYS | 2.8 |
| 4 | D | 59 | LEU | 2.8 |
| 4 | D | 62 | LYS | 2.8 |
| 37 | n | 79 | VAL | 2.8 |
| 3 | C | 80 | ASP | 2.8 |
| 34 | i | 100 | U | 2.8 |
| 34 | i | 982 | G | 2.8 |
| 27 | a | 53 | ILE | 2.8 |
| 4 | D | 109 | LEU | 2.8 |
| 4 | D | 164 | VAL | 2.8 |
| 33 | g | 290 | ALA | 2.8 |
| 21 | U | 100 | GLN | 2.8 |
| 24 | X | 41 | PHE | 2.8 |
| 14 | N | 83 | ASP | 2.8 |
| 37 | n | 80 | GLY | 2.8 |
| 6 | F | 99 | ILE | 2.8 |
| 23 | W | 111 | MET | 2.8 |
| 24 | X | 128 | VAL | 2.8 |
| 37 | n | 48 | GLU | 2.8 |
| 10 | J | 19 | PRO | 2.8 |
| 14 | N | 139 | TRP | 2.8 |
| 34 | i | 300 | G | 2.8 |
| 34 | i | 506 | A | 2.8 |
| 34 | i | 832 | G | 2.8 |
| 34 | i | 1856 | G | 2.8 |
| 1 | A | 56 | GLU | 2.8 |
| 5 | E | 66 | MET | 2.8 |
| 24 | X | 99 | GLU | 2.8 |
| 26 | Z | 101 | SER | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 35 | j | 55 | C | 2.8 |
| 6 | F | 34 | SER | 2.8 |
| 29 | c | 52 | GLU | 2.8 |
| 10 | J | 77 | LEU | 2.8 |
| 23 | W | 11 | LEU | 2.8 |
| 4 | D | 85 | GLU | 2.8 |
| 12 | L | 127 | THR | 2.8 |
| 36 | k | 16 | A | 2.8 |
| 7 | G | 150 | GLU | 2.8 |
| 37 | n | 73 | THR | 2.8 |
| 3 | C | 160 | GLY | 2.8 |
| 34 | i | 1422 | U | 2.8 |
| 15 | O | 71 | PRO | 2.8 |
| 11 | K | 37 | ASP | 2.8 |
| 20 | T | 90 | SER | 2.8 |
| 9 | I | 66 | SER | 2.8 |
| 17 | Q | 130 | LYS | 2.8 |
| 1 | A | 16 | LEU | 2.8 |
| 5 | E | 80 | ILE | 2.8 |
| 34 | i | 203 | G | 2.8 |
| 34 | i | 415 | G | 2.8 |
| 2 | B | 228 | LEU | 2.8 |
| 4 | D | 170 | THR | 2.8 |
| 21 | U | 44 | LYS | 2.8 |
| 34 | i | 424 | G | 2.8 |
| 34 | i | 877 | G | 2.8 |
| 34 | i | 1446 | G | 2.8 |
| 15 | O | 24 | GLY | 2.8 |
| 7 | G | 78 | SER | 2.8 |
| 2 | B | 95 | ASN | 2.7 |
| 5 | E | 167 | GLY | 2.7 |
| 5 | E | 158 | ASP | 2.7 |
| 12 | L | 117 | PHE | 2.7 |
| 34 | i | 24 | C | 2.7 |
| 34 | i | 1135 | C | 2.7 |
| 34 | i | 1161 | G | 2.7 |
| 29 | c | 15 | THR | 2.7 |
| 34 | i | 389 | C | 2.7 |
| 9 | I | 23 | LYS | 2.7 |
| 22 | V | 80 | SER | 2.7 |
| 33 | g | 93 | THR | 2.7 |
| 4 | D | 132 | LYS | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | Z | 43 | LYS | 2.7 |
| 23 | W | 73 | GLY | 2.7 |
| 34 | i | 36 | U | 2.7 |
| 3 | C | 194 | VAL | 2.7 |
| 12 | L | 147 | LYS | 2.7 |
| 19 | S | 119 | ALA | 2.7 |
| 36 | k | 14 | A | 2.7 |
| 34 | i | 269 | C | 2.7 |
| 34 | i | 578 | G | 2.7 |
| 34 | i | 699 | C | 2.7 |
| 34 | i | 855 | G | 2.7 |
| 4 | D | 153 | VAL | 2.7 |
| 29 | c | 16 | LYS | 2.7 |
| 24 | X | 139 | GLU | 2.7 |
| 9 | I | 176 | ALA | 2.7 |
| 20 | T | 37 | VAL | 2.7 |
| 34 | i | 306 | C | 2.7 |
| 34 | i | 340 | C | 2.7 |
| 34 | i | 1522 | C | 2.7 |
| 34 | i | 62 | G | 2.7 |
| 34 | i | 204 | G | 2.7 |
| 7 | G | 43 | GLU | 2.7 |
| 7 | G | 125 | THR | 2.7 |
| 7 | G | 188 | LYS | 2.7 |
| 34 | i | 117 | C | 2.7 |
| 5 | E | 255 | ARG | 2.7 |
| 24 | X | 142 | ARG | 2.7 |
| 34 | i | 613 | G | 2.7 |
| 34 | i | 808 | A | 2.7 |
| 34 | i | 1154 | G | 2.7 |
| 34 | i | 1744 | G | 2.7 |
| 23 | W | 14 | ILE | 2.7 |
| 35 | j | 34 | A | 2.7 |
| 4 | D | 219 | PRO | 2.7 |
| 4 | D | 117 | ARG | 2.7 |
| 10 | J | 157 | ILE | 2.7 |
| 34 | i | 1698 | C | 2.7 |
| 3 | C | 183 | ALA | 2.7 |
| 31 | e | 77 | HIS | 2.7 |
| 27 | a | 64 | LEU | 2.7 |
| 1 | A | 55 | TRP | 2.7 |
| 34 | i | 118 | C | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 21 | U | 83 | ARG | 2.7 |
| 22 | V | 81 | GLN | 2.7 |
| 18 | R | 88 | VAL | 2.7 |
| 7 | G | 195 | LYS | 2.6 |
| 34 | i | 11 | A | 2.6 |
| 33 | g | 255 | SER | 2.6 |
| 34 | i | 1344 | G | 2.6 |
| 5 | E | 262 | SER | 2.6 |
| 2 | B | 103 | MET | 2.6 |
| 7 | G | 176 | ILE | 2.6 |
| 21 | U | 61 | LEU | 2.6 |
| 33 | g | 71 | ILE | 2.6 |
| 17 | Q | 136 | GLY | 2.6 |
| 5 | E | 183 | VAL | 2.6 |
| 6 | F | 86 | LYS | 2.6 |
| 6 | F | 142 | SER | 2.6 |
| 15 | O | 33 | ILE | 2.6 |
| 34 | i | 505 | G | 2.6 |
| 12 | L | 146 | THR | 2.6 |
| 5 | E | 125 | LYS | 2.6 |
| 16 | P | 125 | PRO | 2.6 |
| 19 | S | 78 | LYS | 2.6 |
| 35 | j | 38 | C | 2.6 |
| 4 | D | 128 | GLU | 2.6 |
| 34 | i | 1229 | G | 2.6 |
| 34 | i | 1443 | G | 2.6 |
| 2 | B | 74 | LEU | 2.6 |
| 30 | d | 34 | TYR | 2.6 |
| 34 | i | 292 | A | 2.6 |
| 34 | i | 1091 | U | 2.6 |
| 34 | i | 1198 | U | 2.6 |
| 34 | i | 1537 | C | 2.6 |
| 13 | M | 129 | LYS | 2.6 |
| 14 | N | 151 | ALA | 2.6 |
| 24 | X | 98 | ASP | 2.6 |
| 14 | N | 88 | LEU | 2.6 |
| 33 | g | 13 | GLY | 2.6 |
| 4 | D | 120 | TYR | 2.6 |
| 27 | a | 71 | LEU | 2.6 |
| 34 | i | 377 | C | 2.6 |
| 5 | E | 57 | THR | 2.6 |
| 30 | d | 11 | PRO | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 257 | G | 2.6 |
| 14 | N | 92 | ILE | 2.6 |
| 6 | F | 94 | LYS | 2.6 |
| 2 | B | 79 | VAL | 2.6 |
| 2 | B | 119 | THR | 2.6 |
| 34 | i | 1554 | C | 2.6 |
| 34 | i | 1708 | C | 2.6 |
| 6 | F | 19 | LEU | 2.6 |
| 34 | i | 77 | A | 2.6 |
| 12 | L | 11 | GLN | 2.6 |
| 3 | C | 215 | THR | 2.6 |
| 5 | E | 163 | ASP | 2.6 |
| 16 | P | 30 | TYR | 2.6 |
| 7 | G | 154 | ARG | 2.6 |
| 26 | Z | 49 | LEU | 2.6 |
| 35 | j | 15 | G | 2.6 |
| 2 | B | 98 | THR | 2.6 |
| 12 | L | 85 | THR | 2.6 |
| 25 | Y | 44 | LEU | 2.6 |
| 34 | i | 92 | A | 2.5 |
| 34 | i | 260 | G | 2.5 |
| 34 | i | 903 | G | 2.5 |
| 34 | i | 1454 | G | 2.5 |
| 12 | L | 4 | ILE | 2.5 |
| 3 | C | 82 | PHE | 2.5 |
| 25 | Y | 52 | PRO | 2.5 |
| 34 | i | 725 | C | 2.5 |
| 2 | B | 47 | THR | 2.5 |
| 16 | P | 80 | LEU | 2.5 |
| 25 | Y | 47 | MET | 2.5 |
| 34 | i | 1351 | C | 2.5 |
| 19 | S | 44 | VAL | 2.5 |
| 22 | V | 79 | VAL | 2.5 |
| 34 | i | 1854 | A | 2.5 |
| 7 | G | 122 | PRO | 2.5 |
| 1 | A | 52 | LYS | 2.5 |
| 3 | C | 188 | GLY | 2.5 |
| 12 | L | 78 | THR | 2.5 |
| 6 | F | 143 | PRO | 2.5 |
| 34 | i | 1160 | G | 2.5 |
| 7 | G | 39 | ASP | 2.5 |
| 7 | G | 187 | HIS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 1679 | C | 2.5 |
| 34 | i | 510 | A | 2.5 |
| 5 | E | 261 | SER | 2.5 |
| 34 | i | 945 | G | 2.5 |
| 15 | O | 121 | ARG | 2.5 |
| 25 | Y | 51 | THR | 2.5 |
| 8 | H | 139 | ILE | 2.5 |
| 33 | g | 232 | GLY | 2.5 |
| 7 | G | 138 | ALA | 2.5 |
| 7 | G | 151 | ASP | 2.5 |
| 34 | i | 131 | C | 2.5 |
| 34 | i | 608 | C | 2.5 |
| 34 | i | 1060 | C | 2.5 |
| 34 | i | 1846 | C | 2.5 |
| 8 | H | 156 | VAL | 2.5 |
| 2 | B | 139 | CYS | 2.5 |
| 10 | J | 137 | VAL | 2.5 |
| 34 | i | 220 | C | 2.5 |
| 3 | C | 72 | PRO | 2.5 |
| 1 | A | 53 | ARG | 2.5 |
| 6 | F | 135 | ARG | 2.5 |
| 29 | c | 29 | GLN | 2.5 |
| 3 | C | 166 | ARG | 2.5 |
| 14 | N | 41 | ALA | 2.5 |
| 34 | i | 221 | A | 2.5 |
| 34 | i | 580 | A | 2.5 |
| 5 | E | 24 | THR | 2.5 |
| 34 | i | 425 | A | 2.5 |
| 34 | i | 310 | G | 2.5 |
| 34 | i | 341 | G | 2.5 |
| 3 | C | 210 | SER | 2.5 |
| 4 | D | 114 | ALA | 2.5 |
| 16 | P | 44 | ARG | 2.5 |
| 13 | M | 9 | GLY | 2.5 |
| 23 | W | 123 | GLY | 2.5 |
| 26 | Z | 67 | LEU | 2.5 |
| 37 | n | 74 | SER | 2.5 |
| 34 | i | 494 | G | 2.5 |
| 34 | i | 929 | G | 2.5 |
| 35 | j | 30 | G | 2.5 |
| 17 | Q | 91 | ALA | 2.5 |
| 34 | i | 1056 | A | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 231 | LEU | 2.5 |
| 16 | P | 118 | GLU | 2.4 |
| 18 | R | 86 | PRO | 2.4 |
| 37 | n | 89 | ALA | 2.4 |
| 5 | E | 150 | PRO | 2.4 |
| 7 | G | 102 | VAL | 2.4 |
| 12 | L | 144 | LYS | 2.4 |
| 19 | S | 115 | LYS | 2.4 |
| 26 | Z | 100 | VAL | 2.4 |
| 29 | c | 17 | VAL | 2.4 |
| 18 | R | 92 | ASP | 2.4 |
| 17 | Q | 107 | GLU | 2.4 |
| 23 | W | 29 | PRO | 2.4 |
| 30 | d | 35 | GLY | 2.4 |
| 34 | i | 54 | A | 2.4 |
| 3 | C | 118 | TYR | 2.4 |
| 34 | i | 174 | C | 2.4 |
| 34 | i | 376 | C | 2.4 |
| 35 | j | 16 | C | 2.4 |
| 34 | i | 33 | G | 2.4 |
| 34 | i | 428 | G | 2.4 |
| 34 | i | 1039 | G | 2.4 |
| 10 | J | 79 | ARG | 2.4 |
| 1 | A | 174 | MET | 2.4 |
| 3 | C | 62 | SER | 2.4 |
| 2 | B | 19 | LYS | 2.4 |
| 27 | a | 35 | ALA | 2.4 |
| 34 | i | 508 | G | 2.4 |
| 3 | C | 144 | LYS | 2.4 |
| 6 | F | 203 | ASN | 2.4 |
| 34 | i | 487 | C | 2.4 |
| 6 | F | 134 | VAL | 2.4 |
| 33 | g | 256 | ILE | 2.4 |
| 5 | E | 111 | VAL | 2.4 |
| 22 | V | 70 | LEU | 2.4 |
| 34 | i | 95 | G | 2.4 |
| 34 | i | 1105 | C | 2.4 |
| 34 | i | 1468 | C | 2.4 |
| 34 | i | 1577 | C | 2.4 |
| 2 | B | 105 | LEU | 2.4 |
| 4 | D | 200 | PRO | 2.4 |
| 7 | G | 111 | LEU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 1667 | U | 2.4 |
| 5 | E | 192 | ILE | 2.4 |
| 17 | Q | 96 | TYR | 2.4 |
| 17 | Q | 131 | LYS | 2.4 |
| 22 | V | 12 | TYR | 2.4 |
| 34 | i | 395 | G | 2.4 |
| 11 | K | 49 | MET | 2.4 |
| 23 | W | 113 | HIS | 2.4 |
| 34 | i | 1336 | U | 2.4 |
| 12 | L | 96 | ILE | 2.4 |
| 27 | a | 75 | VAL | 2.4 |
| 9 | I | 180 | GLY | 2.4 |
| 25 | Y | 53 | ASP | 2.4 |
| 34 | i | 305 | U | 2.4 |
| 37 | n | 95 | TYR | 2.4 |
| 21 | U | 58 | THR | 2.4 |
| 18 | R | 93 | GLN | 2.4 |
| 34 | i | 99 | A | 2.4 |
| 34 | i | 194 | C | 2.4 |
| 34 | i | 612 | C | 2.4 |
| 34 | i | 1646 | A | 2.4 |
| 5 | E | 115 | THR | 2.4 |
| 16 | P | 36 | LEU | 2.4 |
| 31 | e | 81 | ALA | 2.4 |
| 24 | X | 51 | VAL | 2.4 |
| 34 | i | 363 | G | 2.4 |
| 34 | i | 917 | G | 2.4 |
| 4 | D | 116 | ARG | 2.4 |
| 4 | D | 47 | GLU | 2.4 |
| 2 | B | 77 | ASP | 2.4 |
| 33 | g | 299 | PHE | 2.4 |
| 34 | i | 1747 | C | 2.4 |
| 33 | g | 271 | LYS | 2.4 |
| 36 | k | 21 | U | 2.4 |
| 37 | n | 61 | ILE | 2.4 |
| 12 | L | 137 | THR | 2.4 |
| 5 | E | 34 | GLY | 2.4 |
| 17 | Q | 105 | LYS | 2.3 |
| 34 | i | 674 | G | 2.4 |
| 34 | i | 1330 | G | 2.4 |
| 34 | i | 1743 | G | 2.4 |
| 27 | a | 11 | ALA | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 107 | A | 2.3 |
| 34 | i | 1391 | C | 2.3 |
| 37 | n | 66 | ARG | 2.3 |
| 2 | B | 93 | GLY | 2.3 |
| 6 | F | 196 | LEU | 2.3 |
| 21 | U | 59 | LYS | 2.3 |
| 13 | M | 130 | CYS | 2.3 |
| 17 | Q | 116 | ASP | 2.3 |
| 19 | S | 65 | GLU | 2.3 |
| 34 | i | 834 | G | 2.3 |
| 34 | i | 863 | G | 2.3 |
| 5 | E | 31 | PRO | 2.3 |
| 6 | F | 101 | HIS | 2.3 |
| 37 | n | 62 | ARG | 2.3 |
| 8 | H | 112 | ASN | 2.3 |
| 5 | E | 78 | ALA | 2.3 |
| 3 | C | 214 | CYS | 2.3 |
| 33 | g | 40 | ILE | 2.3 |
| 34 | i | 943 | G | 2.3 |
| 34 | i | 1325 | U | 2.3 |
| 34 | i | 1243 | C | 2.3 |
| 34 | i | 1643 | G | 2.3 |
| 1 | A | 175 | TRP | 2.3 |
| 17 | Q | 81 | ILE | 2.3 |
| 29 | c | 28 | THR | 2.3 |
| 34 | i | 719 | C | 2.3 |
| 34 | i | 1395 | C | 2.3 |
| 34 | i | 1536 | G | 2.3 |
| 35 | j | 12 | G | 2.3 |
| 3 | C | 211 | ALA | 2.3 |
| 7 | G | 62 | PRO | 2.3 |
| 7 | G | 40 | ALA | 2.3 |
| 34 | i | 486 | C | 2.3 |
| 12 | L | 5 | GLN | 2.3 |
| 4 | D | 2 | ALA | 2.3 |
| 34 | i | 458 | A | 2.3 |
| 34 | i | 826 | A | 2.3 |
| 34 | i | 386 | U | 2.3 |
| 34 | i | 879 | U | 2.3 |
| 30 | d | 43 | PHE | 2.3 |
| 21 | U | 96 | GLU | 2.3 |
| 34 | i | 90 | G | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 545 | A | 2.3 |
| 34 | i | 1167 | G | 2.3 |
| 6 | F | 133 | THR | 2.3 |
| 34 | i | 1084 | U | 2.3 |
| 11 | K | 72 | THR | 2.3 |
| 5 | E | 93 | ASP | 2.3 |
| 21 | U | 103 | SER | 2.3 |
| 34 | i | 8 | U | 2.3 |
| 34 | i | 812 | A | 2.3 |
| 34 | i | 1079 | A | 2.3 |
| 34 | i | 1469 | G | 2.3 |
| 11 | K | 11 | ILE | 2.3 |
| 18 | R | 41 | ILE | 2.3 |
| 3 | C | 92 | LEU | 2.3 |
| 16 | P | 22 | LEU | 2.3 |
| 22 | V | 37 | ALA | 2.3 |
| 31 | e | 82 | ARG | 2.3 |
| 34 | i | 1707 | A | 2.3 |
| 34 | i | 1722 | G | 2.3 |
| 6 | F | 54 | GLY | 2.3 |
| 3 | C | 90 | LYS | 2.3 |
| 3 | C | 193 | PRO | 2.3 |
| 33 | g | 289 | LEU | 2.3 |
| 5 | E | 184 | THR | 2.3 |
| 10 | J | 141 | VAL | 2.3 |
| 15 | O | 148 | GLY | 2.3 |
| 34 | i | 809 | A | 2.3 |
| 15 | O | 35 | ALA | 2.3 |
| 30 | d | 33 | LYS | 2.3 |
| 34 | i | 579 | G | 2.3 |
| 34 | i | 587 | G | 2.3 |
| 37 | n | 56 | LYS | 2.3 |
| 23 | W | 105 | THR | 2.3 |
| 16 | P | 59 | ARG | 2.3 |
| 24 | X | 59 | ALA | 2.3 |
| 34 | i | 1481 | U | 2.3 |
| 3 | C | 130 | LYS | 2.3 |
| 7 | G | 23 | LYS | 2.3 |
| 16 | P | 115 | TYR | 2.3 |
| 24 | X | 101 | LEU | 2.3 |
| 34 | i | 861 | A | 2.3 |
| 4 | D | 124 | ARG | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 360 | G | 2.3 |
| 34 | i | 1337 | C | 2.3 |
| 34 | i | 1836 | C | 2.3 |
| 35 | j | 13 | C | 2.3 |
| 8 | H | 141 | GLY | 2.3 |
| 15 | O | 92 | ALA | 2.3 |
| 2 | B | 210 | VAL | 2.3 |
| 4 | D | 41 | VAL | 2.3 |
| 30 | d | 31 | ILE | 2.2 |
| 1 | A | 93 | ALA | 2.2 |
| 20 | T | 32 | GLU | 2.2 |
| 23 | W | 41 | MET | 2.2 |
| 24 | X | 140 | ARG | 2.2 |
| 34 | i | 891 | G | 2.2 |
| 34 | i | 991 | G | 2.2 |
| 34 | i | 1137 | G | 2.2 |
| 34 | i | 1842 | U | 2.2 |
| 27 | a | 67 | LEU | 2.2 |
| 7 | G | 85 | ARG | 2.2 |
| 10 | J | 153 | SER | 2.2 |
| 1 | A | 5 | LEU | 2.2 |
| 34 | i | 966 | G | 2.2 |
| 4 | D | 60 | GLY | 2.2 |
| 15 | O | 29 | GLY | 2.2 |
| 29 | c | 55 | VAL | 2.2 |
| 18 | R | 109 | LEU | 2.2 |
| 12 | L | 83 | GLN | 2.2 |
| 33 | g | 254 | PRO | 2.2 |
| 10 | J | 60 | LEU | 2.2 |
| 34 | i | 492 | C | 2.2 |
| 34 | i | 1142 | C | 2.2 |
| 15 | O | 89 | GLY | 2.2 |
| 5 | E | 29 | PRO | 2.2 |
| 6 | F | 137 | GLN | 2.2 |
| 34 | i | 406 | U | 2.2 |
| 9 | I | 88 | ASN | 2.2 |
| 34 | i | 1140 | A | 2.2 |
| 5 | E | 168 | LYS | 2.2 |
| 6 | F | 65 | GLN | 2.2 |
| 14 | N | 103 | GLU | 2.2 |
| 15 | O | 91 | THR | 2.2 |
| 4 | D | 172 | VAL | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 15 | O | 108 | PRO | 2.2 |
| 16 | P | 8 | LYS | 2.2 |
| 34 | i | 1678 | C | 2.2 |
| 34 | i | 124 | U | 2.2 |
| 10 | J | 86 | VAL | 2.2 |
| 14 | N | 19 | ARG | 2.2 |
| 34 | i | 817 | G | 2.2 |
| 34 | i | 1162 | G | 2.2 |
| 35 | j | 33 | C | 2.2 |
| 34 | i | 1507 | U | 2.2 |
| 21 | U | 99 | LYS | 2.2 |
| 34 | i | 1040 | G | 2.2 |
| 9 | I | 146 | GLN | 2.2 |
| 12 | L | 26 | GLY | 2.2 |
| 34 | i | 38 | A | 2.2 |
| 3 | C | 231 | LYS | 2.2 |
| 34 | i | 383 | U | 2.2 |
| 4 | D | 133 | GLY | 2.2 |
| 9 | I | 107 | THR | 2.2 |
| 26 | Z | 88 | LEU | 2.2 |
| 24 | X | 65 | ALA | 2.2 |
| 29 | c | 51 | ARG | 2.2 |
| 34 | i | 267 | G | 2.2 |
| 4 | D | 176 | LEU | 2.2 |
| 34 | i | 1826 | A | 2.2 |
| 23 | W | 75 | ILE | 2.2 |
| 34 | i | 12 | U | 2.2 |
| 34 | i | 859 | U | 2.2 |
| 9 | I | 141 | ARG | 2.2 |
| 5 | E | 50 | ASN | 2.2 |
| 33 | g | 69 | VAL | 2.2 |
| 4 | D | 218 | LEU | 2.2 |
| 5 | E | 49 | ARG | 2.2 |
| 6 | F | 144 | LEU | 2.2 |
| 26 | Z | 58 | LEU | 2.2 |
| 34 | i | 282 | G | 2.2 |
| 34 | i | 946 | C | 2.2 |
| 26 | Z | 70 | PRO | 2.2 |
| 2 | B | 113 | MET | 2.2 |
| 15 | O | 145 | GLY | 2.2 |
| 30 | d | 45 | GLN | 2.2 |
| 34 | i | 314 | U | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 607 | G | 2.2 |
| 34 | i | 1455 | G | 2.2 |
| 34 | i | 1478 | C | 2.2 |
| 34 | i | 1492 | U | 2.2 |
| 8 | H | 188 | GLU | 2.2 |
| 9 | I | 74 | ARG | 2.2 |
| 22 | V | 78 | ILE | 2.2 |
| 5 | E | 156 | MET | 2.2 |
| 14 | N | 36 | GLN | 2.2 |
| 16 | P | 120 | SER | 2.2 |
| 5 | E | 68 | ARG | 2.2 |
| 19 | S | 21 | ASP | 2.2 |
| 34 | i | 1835 | C | 2.2 |
| 5 | E | 250 | GLU | 2.1 |
| 12 | L | 61 | PRO | 2.1 |
| 3 | C | 107 | THR | 2.1 |
| 23 | W | 54 | ASP | 2.1 |
| 7 | G | 190 | ARG | 2.1 |
| 12 | L | 138 | VAL | 2.1 |
| 13 | M | 100 | PRO | 2.1 |
| 34 | i | 106 | C | 2.1 |
| 34 | i | 1087 | C | 2.1 |
| 2 | B | 109 | LYS | 2.1 |
| 16 | P | 14 | LYS | 2.1 |
| 19 | S | 62 | ASP | 2.1 |
| 2 | B | 213 | ARG | 2.1 |
| 4 | D | 78 | GLY | 2.1 |
| 33 | g | 70 | VAL | 2.1 |
| 7 | G | 156 | TYR | 2.1 |
| 18 | R | 94 | GLU | 2.1 |
| 3 | C | 159 | ILE | 2.1 |
| 28 | b | 4 | ALA | 2.1 |
| 29 | c | 10 | LYS | 2.1 |
| 29 | c | 12 | ALA | 2.1 |
| 12 | L | 70 | GLY | 2.1 |
| 5 | E | 232 | ASN | 2.1 |
| 9 | I | 113 | TYR | 2.1 |
| 1 | A | 68 | ILE | 2.1 |
| 21 | U | 46 | LYS | 2.1 |
| 22 | V | 69 | ILE | 2.1 |
| 3 | C | 146 | SER | 2.1 |
| 19 | S | 46 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | i | 433 | U | 2.1 |
| 34 | i | 902 | U | 2.1 |
| 9 | I | 117 | TYR | 2.1 |
| 9 | I | 149 | TYR | 2.1 |
| 23 | W | 30 | CYS | 2.1 |
| 34 | i | 1444 | A | 2.1 |
| 2 | B | 164 | ILE | 2.1 |
| 12 | L | 6 | THR | 2.1 |
| 17 | Q | 34 | VAL | 2.1 |
| 34 | i | 201 | G | 2.1 |
| 34 | i | 1396 | U | 2.1 |
| 30 | d | 42 | CYS | 2.1 |
| 5 | E | 116 | PRO | 2.1 |
| 25 | Y | 40 | ILE | 2.1 |
| 10 | J | 65 | GLU | 2.1 |
| 34 | i | 1399 | C | 2.1 |
| 34 | i | 1656 | A | 2.1 |
| 35 | j | 49 | A | 2.1 |
| 34 | i | 172 | U | 2.1 |
| 34 | i | 818 | U | 2.1 |
| 2 | B | 83 | LYS | 2.1 |
| 34 | i | 400 | G | 2.1 |
| 34 | i | 1721 | G | 2.1 |
| 1 | A | 36 | GLN | 2.1 |
| 17 | Q | 70 | VAL | 2.1 |
| 28 | b | 12 | PRO | 2.1 |
| 3 | C | 110 | LYS | 2.1 |
| 34 | i | 1242 | A | 2.1 |
| 34 | i | 1479 | A | 2.1 |
| 34 | i | 1551 | A | 2.1 |
| 35 | j | 14 | A | 2.1 |
| 9 | I | 152 | ARG | 2.1 |
| 23 | W | 8 | ALA | 2.1 |
| 17 | Q | 42 | ILE | 2.1 |
| 37 | n | 63 | GLY | 2.1 |
| 17 | Q | 146 | ARG | 2.1 |
| 10 | J | 100 | LEU | 2.1 |
| 11 | K | 46 | MET | 2.1 |
| 11 | K | 45 | VAL | 2.1 |
| 4 | D | 150 | MET | 2.1 |
| 34 | i | 242 | G | 2.1 |
| 34 | i | 261 | G | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 15 | O | 42 | VAL | 2.1 |
| 34 | i | 1328 | A | 2.1 |
| 1 | A | 23 | THR | 2.1 |
| 11 | K | 58 | VAL | 2.1 |
| 26 | Z | 59 | CYS | 2.1 |
| 34 | i | 1393 | U | 2.1 |
| 6 | F | 91 | ARG | 2.1 |
| 33 | g | 288 | SER | 2.1 |
| 10 | J | 188 | GLY | 2.1 |
| 8 | H | 154 | ILE | 2.1 |
| 2 | B | 68 | GLU | 2.1 |
| 12 | L | 66 | VAL | 2.1 |
| 3 | C | 218 | LEU | 2.1 |
| 6 | F | 53 | ALA | 2.1 |
| 34 | i | 1394 | G | 2.1 |
| 34 | i | 1571 | G | 2.1 |
| 12 | L | 102 | PHE | 2.1 |
| 11 | K | 79 | LEU | 2.1 |
| 2 | B | 38 | MET | 2.1 |
| 19 | S | 45 | LEU | 2.1 |
| 34 | i | 1334 | G | 2.1 |
| 7 | G | 141 | ILE | 2.1 |
| 34 | i | 382 | A | 2.1 |
| 34 | i | 1857 | A | 2.1 |
| 12 | L | 81 | LYS | 2.1 |
| 24 | X | 40 | PRO | 2.1 |
| 34 | i | 216 | U | 2.1 |
| 1 | A | 20 | ALA | 2.1 |
| 34 | i | 1163 | G | 2.0 |
| 34 | i | 160 | U | 2.0 |
| 1 | A | 182 | VAL | 2.0 |
| 5 | E | 128 | LYS | 2.0 |
| 35 | j | 67 | C | 2.0 |
| 37 | n | 75 | ASP | 2.0 |
| 6 | F | 16 | ASP | 2.0 |
| 34 | i | 634 | G | 2.0 |
| 2 | B | 71 | LEU | 2.0 |
| 23 | W | 7 | LEU | 2.0 |
| 2 | B | 233 | GLY | 2.0 |
| 9 | I | 15 | GLY | 2.0 |
| 21 | U | 71 | GLY | 2.0 |
| 2 | B | 205 | TYR | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | F | 125 | SER | 2.0 |
| 5 | E | 62 | LYS | 2.0 |
| 2 | B | 120 | MET | 2.0 |
| 3 | C | 206 | ASP | 2.0 |
| 12 | L | 135 | SER | 2.0 |
| 34 | i | 337 | G | 2.0 |
| 20 | T | 99 | VAL | 2.0 |
| 34 | i | 1553 | C | 2.0 |
| 5 | E | 2 | ALA | 2.0 |
| 1 | A | 12 | GLU | 2.0 |
| 6 | F | 195 | GLU | 2.0 |
| 2 | B | 188 | LEU | 2.0 |
| 4 | D | 112 | GLY | 2.0 |
| 6 | F | 162 | ALA | 2.0 |
| 23 | W | 28 | ARG | 2.0 |
| 33 | g | 75 | GLY | 2.0 |
| 35 | j | 36 | A | 2.0 |
| 34 | i | 635 | C | 2.0 |
| 34 | i | 1639 | C | 2.0 |
| 5 | E | 256 | LEU | 2.0 |
| 9 | I | 55 | TYR | 2.0 |
| 34 | i | 91 | A | 2.0 |
| 34 | i | 1038 | A | 2.0 |
| 9 | I | 125 | LYS | 2.0 |
| 34 | i | 139 | C | 2.0 |
| 7 | G | 181 | THR | 2.0 |
| 16 | P | 101 | THR | 2.0 |
| 2 | B | 37 | ALA | 2.0 |
| 9 | I | 13 | LYS | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.