



## Full wwPDB EM Validation Report ⓘ

Feb 13, 2024 – 12:57 PM EST

PDB ID : 3J5S  
EMDB ID : EMD-5784  
Title : EttA binds to ribosome exit site and regulates translation by restricting ribosome and tRNA dynamics  
Authors : Hashem, Y.  
Deposited on : 2013-11-15  
Resolution : 7.50 Å (reported)  
Based on initial models : 3R8T, 2WDG, 3R8O, 4FIN

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

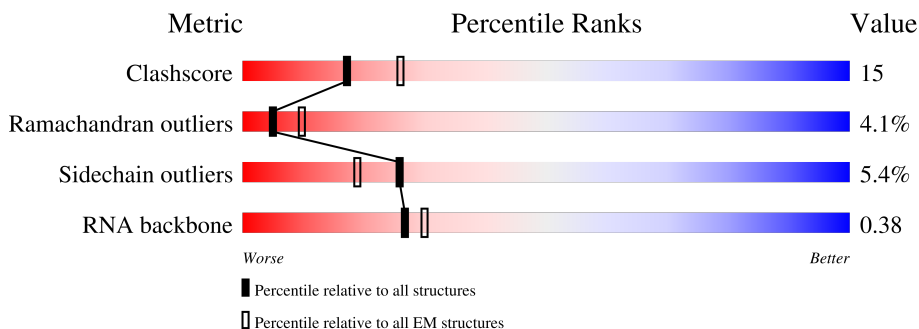
EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 7.50 Å.

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




| Metric                | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 158937                   | 4297                     |
| Ramachandran outliers | 154571                   | 4023                     |
| Sidechain outliers    | 154315                   | 3826                     |
| RNA backbone          | 4643                     | 859                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | B     | 101    |                  |
| 2   | A     | 360    |                  |
| 3   | E     | 77     |                  |
| 4   | D     | 561    |                  |
| 5   | F     | 234    |                  |
| 6   | G     | 178    |                  |
| 7   | H     | 50     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 8   | I     | 151    |  <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (23%), a green segment (61%), a yellow segment (30%), and a small orange segment (7%). The percentages are labeled above or below the segments.</p> |

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
|     |       |          | Total | C   | N   | O   | P  |         |       |
| 1   | B     | 32       | 687   | 306 | 126 | 223 | 32 | 0       | 0     |

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
|     |       |          | Total | C    | N   | O    | P   |         |       |
| 2   | A     | 174      | 3731  | 1663 | 674 | 1220 | 174 | 0       | 0     |

- Molecule 3 is a RNA chain called P-site tRNA FMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
|     |       |          | Total | C   | N   | O   | P  |         |       |
| 3   | E     | 77       | 1640  | 732 | 297 | 535 | 76 | 0       | 0     |

- Molecule 4 is a protein called Energy-dependent translational throttle A (EttA).

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 4   | D     | 554      | 4393  | 2764 | 781 | 837 | 11 | 0       | 0     |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -5      | HIS      | -      | expression tag | UNP P0A9W3 |
| D     | -4      | HIS      | -      | expression tag | UNP P0A9W3 |
| D     | -3      | HIS      | -      | expression tag | UNP P0A9W3 |
| D     | -2      | HIS      | -      | expression tag | UNP P0A9W3 |
| D     | -1      | HIS      | -      | expression tag | UNP P0A9W3 |
| D     | 0       | HIS      | -      | expression tag | UNP P0A9W3 |

- Molecule 5 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 5   | F     | 234      | 1733  | 1081 | 315 | 330 | 7 | 0       | 0     |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 6   | G     | 178      | 1420  | 905 | 251 | 258 | 6 | 0       | 0     |

- Molecule 7 is a protein called 50S ribosomal protein L33.

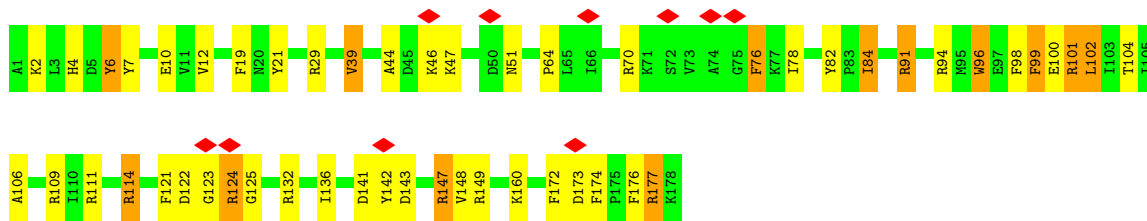
| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
|     |       |          | Total | C   | N  | O  |         |       |
| 7   | H     | 50       | 410   | 263 | 75 | 72 | 0       | 0     |

- Molecule 8 is a protein called 30S ribosomal protein S7.

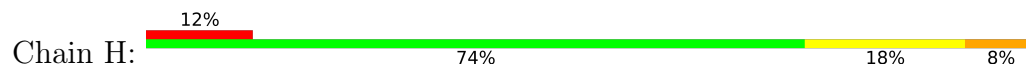
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 8   | I     | 151      | 1182  | 735 | 227 | 216 | 4 | 0       | 0     |



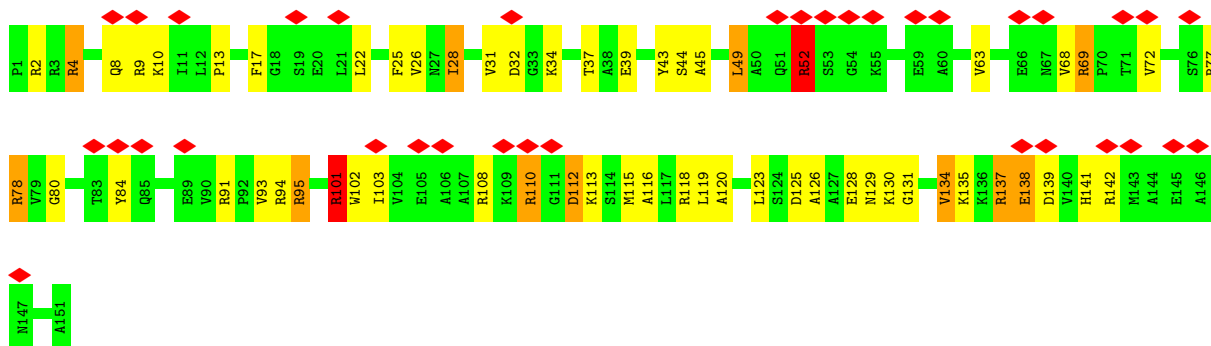




- Molecule 7: 50S ribosomal protein L33



- Molecule 8: 30S ribosomal protein S7





## 4 Experimental information

| Property                             | Value                          | Source    |
|--------------------------------------|--------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                | Depositor |
| Imposed symmetry                     | POINT, C1                      | Depositor |
| Number of particles used             | 39316                          | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF              | Depositor |
| CTF correction method                | Each micrograph                | Depositor |
| Microscope                           | FEI TECNAI F20                 | Depositor |
| Voltage (kV)                         | 200                            | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 17                             | Depositor |
| Minimum defocus (nm)                 | 1200                           | Depositor |
| Maximum defocus (nm)                 | 2500                           | Depositor |
| Magnification                        | 110637                         | Depositor |
| Image detector                       | GATAN ULTRASCAN 4000 (4k x 4k) | Depositor |
| Maximum map value                    | 338.729                        | Depositor |
| Minimum map value                    | -150.118                       | Depositor |
| Average map value                    | 3.621                          | Depositor |
| Map value standard deviation         | 39.948                         | Depositor |
| Recommended contour level            | 80.0                           | Depositor |
| Map size ( $\text{\AA}$ )            | 363.3544, 363.3544, 363.3544   | wwPDB     |
| Map dimensions                       | 134, 134, 134                  | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0               | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 2.7116, 2.7116, 2.7116         | Depositor |

## 5 Model quality i

### 5.1 Standard geometry i

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   | B     | 3.33         | 96/766 (12.5%)   | 3.35        | 147/1188 (12.4%)  |
| 2   | A     | 3.17         | 486/4174 (11.6%) | 3.15        | 702/6507 (10.8%)  |
| 3   | E     | 3.23         | 213/1832 (11.6%) | 3.28        | 351/2855 (12.3%)  |
| 4   | D     | 1.58         | 22/4474 (0.5%)   | 2.04        | 130/6034 (2.2%)   |
| 5   | F     | 1.52         | 5/1748 (0.3%)    | 1.97        | 49/2355 (2.1%)    |
| 6   | G     | 1.65         | 8/1444 (0.6%)    | 2.08        | 40/1937 (2.1%)    |
| 7   | H     | 1.63         | 2/417 (0.5%)     | 2.02        | 11/554 (2.0%)     |
| 8   | I     | 1.61         | 6/1196 (0.5%)    | 2.31        | 50/1602 (3.1%)    |
| All | All   | 2.41         | 838/16051 (5.2%) | 2.65        | 1480/23032 (6.4%) |

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   | B     | 0                   | 12                  |
| 2   | A     | 0                   | 84                  |
| 3   | E     | 0                   | 34                  |
| 4   | D     | 0                   | 23                  |
| 5   | F     | 0                   | 9                   |
| 6   | G     | 0                   | 6                   |
| 7   | H     | 0                   | 4                   |
| 8   | I     | 0                   | 6                   |
| All | All   | 0                   | 178                 |

All (838) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 3   | E     | 36   | A    | N9-C4 | -18.05 | 1.27        | 1.37     |
| 1   | B     | 1297 | G    | N9-C8 | 15.82  | 1.49        | 1.37     |
| 2   | A     | 1879 | C    | N1-C6 | 14.46  | 1.45        | 1.37     |
| 1   | B     | 1242 | G    | C8-N7 | -13.58 | 1.22        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | B     | 1236 | A    | C5-C4   | 13.00  | 1.47        | 1.38     |
| 3   | E     | 19   | G    | N7-C5   | 12.89  | 1.47        | 1.39     |
| 2   | A     | 2126 | A    | N3-C4   | -12.71 | 1.27        | 1.34     |
| 3   | E     | 74   | A    | N3-C4   | 12.13  | 1.42        | 1.34     |
| 2   | A     | 2140 | G    | N7-C5   | 11.96  | 1.46        | 1.39     |
| 3   | E     | 10   | G    | C8-N7   | 11.82  | 1.38        | 1.30     |
| 2   | A     | 1895 | C    | N1-C6   | 11.80  | 1.44        | 1.37     |
| 3   | E     | 9    | G    | N7-C5   | 11.66  | 1.46        | 1.39     |
| 2   | A     | 2179 | C    | C2-N3   | 11.44  | 1.45        | 1.35     |
| 3   | E     | 52   | C    | N1-C6   | 11.44  | 1.44        | 1.37     |
| 3   | E     | 2    | G    | N9-C8   | 11.41  | 1.45        | 1.37     |
| 2   | A     | 2186 | G    | N3-C4   | 11.28  | 1.43        | 1.35     |
| 1   | B     | 1305 | G    | N7-C5   | 11.16  | 1.46        | 1.39     |
| 1   | B     | 1334 | G    | C5-C4   | 11.09  | 1.46        | 1.38     |
| 2   | A     | 2097 | A    | N9-C4   | -11.05 | 1.31        | 1.37     |
| 2   | A     | 2114 | A    | C8-N7   | 10.97  | 1.39        | 1.31     |
| 1   | B     | 1290 | G    | N7-C5   | 10.84  | 1.45        | 1.39     |
| 2   | A     | 2095 | A    | N7-C5   | -10.82 | 1.32        | 1.39     |
| 3   | E     | 36   | A    | N7-C5   | -10.76 | 1.32        | 1.39     |
| 2   | A     | 2115 | G    | P-O5'   | -10.74 | 1.49        | 1.59     |
| 3   | E     | 58   | A    | C6-N1   | 10.73  | 1.43        | 1.35     |
| 2   | A     | 2096 | C    | N1-C6   | 10.71  | 1.43        | 1.37     |
| 3   | E     | 55   | U    | P-O5'   | -10.70 | 1.49        | 1.59     |
| 3   | E     | 46   | G    | N7-C5   | -10.64 | 1.32        | 1.39     |
| 3   | E     | 68   | C    | N1-C2   | -10.48 | 1.29        | 1.40     |
| 2   | A     | 1886 | U    | C5'-C4' | 10.42  | 1.63        | 1.51     |
| 2   | A     | 2100 | G    | N3-C4   | 10.32  | 1.42        | 1.35     |
| 3   | E     | 6    | G    | C6-N1   | 10.23  | 1.46        | 1.39     |
| 3   | E     | 10   | G    | N7-C5   | -10.20 | 1.33        | 1.39     |
| 3   | E     | 30   | G    | N1-C2   | -10.17 | 1.29        | 1.37     |
| 2   | A     | 2183 | A    | N9-C4   | -10.15 | 1.31        | 1.37     |
| 1   | B     | 1299 | A    | C6-N1   | -10.04 | 1.28        | 1.35     |
| 3   | E     | 57   | C    | N1-C6   | 10.02  | 1.43        | 1.37     |
| 3   | E     | 28   | U    | C4-C5   | -9.98  | 1.34        | 1.43     |
| 2   | A     | 2124 | G    | N9-C4   | -9.98  | 1.29        | 1.38     |
| 1   | B     | 1332 | A    | N9-C4   | 9.95   | 1.43        | 1.37     |
| 2   | A     | 1849 | G    | C5-C4   | 9.90   | 1.45        | 1.38     |
| 2   | A     | 2140 | G    | C5-C4   | 9.89   | 1.45        | 1.38     |
| 2   | A     | 1872 | A    | N9-C4   | -9.84  | 1.31        | 1.37     |
| 2   | A     | 2115 | G    | C5'-C4' | 9.84   | 1.63        | 1.51     |
| 2   | A     | 2094 | A    | C5-C4   | 9.83   | 1.45        | 1.38     |
| 2   | A     | 2110 | G    | C4'-C3' | 9.82   | 1.64        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1897 | G    | N9-C4   | -9.80 | 1.30        | 1.38     |
| 2   | A     | 2180 | U    | N1-C6   | 9.73  | 1.46        | 1.38     |
| 2   | A     | 2158 | A    | C5'-C4' | 9.70  | 1.62        | 1.51     |
| 1   | B     | 1298 | U    | C2'-C1' | -9.69 | 1.42        | 1.53     |
| 2   | A     | 2161 | C    | C5'-C4' | 9.64  | 1.62        | 1.51     |
| 2   | A     | 2161 | C    | P-O5'   | -9.62 | 1.50        | 1.59     |
| 2   | A     | 1869 | G    | C6-N1   | -9.61 | 1.32        | 1.39     |
| 2   | A     | 1852 | U    | N3-C4   | -9.58 | 1.29        | 1.38     |
| 2   | A     | 1893 | C    | N3-C4   | -9.57 | 1.27        | 1.33     |
| 2   | A     | 2153 | C    | C2-N3   | 9.53  | 1.43        | 1.35     |
| 1   | B     | 1305 | G    | C2'-C1' | -9.50 | 1.43        | 1.53     |
| 2   | A     | 2170 | A    | N3-C4   | -9.47 | 1.29        | 1.34     |
| 2   | A     | 2173 | A    | O3'-P   | -9.43 | 1.49        | 1.61     |
| 3   | E     | 22   | A    | N7-C5   | 9.43  | 1.45        | 1.39     |
| 2   | A     | 2144 | G    | N7-C5   | 9.38  | 1.44        | 1.39     |
| 2   | A     | 2122 | U    | O3'-P   | -9.35 | 1.50        | 1.61     |
| 2   | A     | 2166 | U    | C5'-C4' | 9.30  | 1.62        | 1.51     |
| 2   | A     | 2111 | U    | C5'-C4' | 9.30  | 1.62        | 1.51     |
| 1   | B     | 1239 | A    | O3'-P   | -9.28 | 1.50        | 1.61     |
| 3   | E     | 20   | G    | C4'-O4' | -9.28 | 1.33        | 1.45     |
| 2   | A     | 2123 | G    | C6-N1   | -9.25 | 1.33        | 1.39     |
| 3   | E     | 35   | C    | O3'-P   | -9.25 | 1.50        | 1.61     |
| 3   | E     | 5    | G    | C8-N7   | 9.23  | 1.36        | 1.30     |
| 1   | B     | 1290 | G    | N9-C4   | 9.19  | 1.45        | 1.38     |
| 2   | A     | 1885 | A    | N7-C5   | -9.18 | 1.33        | 1.39     |
| 3   | E     | 59   | A    | C8-N7   | 9.16  | 1.38        | 1.31     |
| 2   | A     | 1873 | G    | C6-N1   | 9.16  | 1.46        | 1.39     |
| 1   | B     | 1303 | C    | P-O5'   | -9.15 | 1.50        | 1.59     |
| 2   | A     | 1835 | G    | C8-N7   | 9.13  | 1.36        | 1.30     |
| 2   | A     | 1847 | A    | O3'-P   | -9.13 | 1.50        | 1.61     |
| 3   | E     | 12   | G    | C6-N1   | 9.12  | 1.46        | 1.39     |
| 2   | A     | 1838 | C    | C5'-C4' | 9.11  | 1.62        | 1.51     |
| 3   | E     | 66   | C    | N1-C6   | 9.09  | 1.42        | 1.37     |
| 2   | A     | 1857 | G    | N9-C4   | -9.07 | 1.30        | 1.38     |
| 2   | A     | 2112 | G    | C5'-C4' | 9.04  | 1.62        | 1.51     |
| 3   | E     | 2    | G    | N7-C5   | 9.04  | 1.44        | 1.39     |
| 1   | B     | 1333 | A    | N7-C5   | 9.04  | 1.44        | 1.39     |
| 3   | E     | 33   | C    | C2-N3   | -9.04 | 1.28        | 1.35     |
| 2   | A     | 1888 | G    | P-O5'   | -8.95 | 1.50        | 1.59     |
| 3   | E     | 48   | U    | O3'-P   | -8.95 | 1.50        | 1.61     |
| 1   | B     | 1290 | G    | C4'-C3' | 8.93  | 1.62        | 1.53     |
| 2   | A     | 2116 | G    | N9-C8   | -8.93 | 1.31        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | E     | 75   | C    | C4'-C3' | 8.91  | 1.62        | 1.53     |
| 3   | E     | 26   | C    | O3'-P   | 8.90  | 1.71        | 1.61     |
| 2   | A     | 1901 | A    | N9-C4   | 8.90  | 1.43        | 1.37     |
| 2   | A     | 2101 | A    | C5-C4   | 8.90  | 1.45        | 1.38     |
| 2   | A     | 2158 | A    | O3'-P   | -8.89 | 1.50        | 1.61     |
| 2   | A     | 1835 | G    | P-O5'   | -8.81 | 1.50        | 1.59     |
| 2   | A     | 2107 | G    | P-O5'   | -8.80 | 1.50        | 1.59     |
| 2   | A     | 1890 | A    | N7-C5   | -8.80 | 1.33        | 1.39     |
| 2   | A     | 2136 | G    | C2'-C1' | -8.80 | 1.43        | 1.53     |
| 2   | A     | 1845 | G    | N7-C5   | 8.79  | 1.44        | 1.39     |
| 3   | E     | 24   | C    | C5'-C4' | 8.77  | 1.61        | 1.51     |
| 2   | A     | 1849 | G    | N3-C4   | -8.71 | 1.29        | 1.35     |
| 2   | A     | 2119 | A    | C6-N6   | 8.69  | 1.41        | 1.33     |
| 3   | E     | 25   | U    | C2'-C1' | 8.69  | 1.62        | 1.53     |
| 3   | E     | 34   | U    | C2-N3   | 8.67  | 1.43        | 1.37     |
| 2   | A     | 2146 | C    | C5'-C4' | 8.67  | 1.61        | 1.51     |
| 3   | E     | 69   | C    | C5'-C4' | 8.66  | 1.61        | 1.51     |
| 2   | A     | 1849 | G    | N1-C2   | -8.62 | 1.30        | 1.37     |
| 1   | B     | 1245 | C    | N3-C4   | 8.61  | 1.40        | 1.33     |
| 1   | B     | 1304 | G    | N9-C8   | 8.61  | 1.43        | 1.37     |
| 1   | B     | 1299 | A    | N9-C4   | -8.60 | 1.32        | 1.37     |
| 1   | B     | 1294 | G    | C3'-C2' | -8.58 | 1.43        | 1.52     |
| 2   | A     | 1852 | U    | O3'-P   | -8.57 | 1.50        | 1.61     |
| 2   | A     | 2142 | A    | O3'-P   | -8.57 | 1.50        | 1.61     |
| 3   | E     | 74   | A    | P-O5'   | -8.57 | 1.51        | 1.59     |
| 3   | E     | 30   | G    | N7-C5   | 8.53  | 1.44        | 1.39     |
| 2   | A     | 1862 | G    | C6-N1   | -8.53 | 1.33        | 1.39     |
| 2   | A     | 2164 | C    | N1-C6   | 8.52  | 1.42        | 1.37     |
| 2   | A     | 1866 | A    | C2'-C1' | -8.48 | 1.44        | 1.53     |
| 2   | A     | 1835 | G    | N3-C4   | -8.47 | 1.29        | 1.35     |
| 2   | A     | 1867 | G    | O3'-P   | -8.47 | 1.50        | 1.61     |
| 2   | A     | 1839 | G    | O4'-C1' | 8.47  | 1.52        | 1.41     |
| 2   | A     | 1837 | C    | C1'-N1  | 8.45  | 1.61        | 1.48     |
| 2   | A     | 2171 | A    | N7-C5   | 8.44  | 1.44        | 1.39     |
| 2   | A     | 1840 | G    | N3-C4   | -8.39 | 1.29        | 1.35     |
| 2   | A     | 2124 | G    | P-O5'   | -8.36 | 1.51        | 1.59     |
| 2   | A     | 2167 | U    | C4'-O4' | 8.35  | 1.56        | 1.45     |
| 3   | E     | 23   | G    | N1-C2   | 8.33  | 1.44        | 1.37     |
| 2   | A     | 1874 | C    | C5'-C4' | 8.29  | 1.61        | 1.51     |
| 2   | A     | 2146 | C    | C4-N4   | -8.28 | 1.26        | 1.33     |
| 2   | A     | 2168 | G    | N7-C5   | -8.28 | 1.34        | 1.39     |
| 1   | B     | 1297 | G    | C2-N2   | -8.27 | 1.26        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | B     | 1334 | G    | N7-C5   | -8.24 | 1.34        | 1.39     |
| 3   | E     | 38   | A    | C5-C4   | 8.24  | 1.44        | 1.38     |
| 2   | A     | 2114 | A    | N9-C4   | 8.22  | 1.42        | 1.37     |
| 3   | E     | 26   | C    | N1-C6   | 8.22  | 1.42        | 1.37     |
| 2   | A     | 1878 | G    | C8-N7   | 8.22  | 1.35        | 1.30     |
| 2   | A     | 2171 | A    | O3'-P   | -8.22 | 1.51        | 1.61     |
| 2   | A     | 1902 | C    | C3'-C2' | -8.21 | 1.43        | 1.52     |
| 4   | D     | 244  | TYR  | CE2-CZ  | 8.18  | 1.49        | 1.38     |
| 1   | B     | 1301 | U    | P-O5'   | -8.18 | 1.51        | 1.59     |
| 3   | E     | 69   | C    | C2'-C1' | -8.17 | 1.44        | 1.53     |
| 1   | B     | 1289 | A    | C5'-C4' | 8.15  | 1.61        | 1.51     |
| 2   | A     | 1844 | C    | N1-C6   | 8.15  | 1.42        | 1.37     |
| 3   | E     | 47   | G    | C3'-O3' | 8.12  | 1.53        | 1.42     |
| 3   | E     | 63   | C    | N1-C6   | 8.09  | 1.42        | 1.37     |
| 2   | A     | 2097 | A    | N7-C5   | -8.09 | 1.34        | 1.39     |
| 1   | B     | 1239 | A    | N9-C4   | 8.06  | 1.42        | 1.37     |
| 3   | E     | 39   | A    | C3'-C2' | -8.05 | 1.43        | 1.52     |
| 3   | E     | 5    | G    | C2-N2   | -8.02 | 1.26        | 1.34     |
| 3   | E     | 44   | A    | C5-C4   | 8.01  | 1.44        | 1.38     |
| 1   | B     | 1295 | U    | C4'-C3' | -7.99 | 1.44        | 1.53     |
| 2   | A     | 2120 | G    | C8-N7   | -7.98 | 1.26        | 1.30     |
| 1   | B     | 1297 | G    | N7-C5   | 7.93  | 1.44        | 1.39     |
| 2   | A     | 2105 | U    | C4-C5   | 7.92  | 1.50        | 1.43     |
| 1   | B     | 1237 | C    | N3-C4   | -7.89 | 1.28        | 1.33     |
| 2   | A     | 1873 | G    | P-O5'   | -7.89 | 1.51        | 1.59     |
| 2   | A     | 1837 | C    | C4-C5   | 7.88  | 1.49        | 1.43     |
| 2   | A     | 1878 | G    | C4'-C3' | 7.88  | 1.61        | 1.53     |
| 2   | A     | 1898 | U    | C4-C5   | 7.87  | 1.50        | 1.43     |
| 2   | A     | 2101 | A    | C6-N1   | 7.86  | 1.41        | 1.35     |
| 3   | E     | 39   | A    | C2-N3   | -7.86 | 1.26        | 1.33     |
| 2   | A     | 2161 | C    | C2-N3   | -7.85 | 1.29        | 1.35     |
| 3   | E     | 66   | C    | N3-C4   | 7.85  | 1.39        | 1.33     |
| 3   | E     | 18   | U    | C4'-C3' | -7.83 | 1.44        | 1.53     |
| 2   | A     | 2165 | C    | P-O5'   | -7.83 | 1.51        | 1.59     |
| 2   | A     | 1870 | C    | C5'-C4' | 7.82  | 1.60        | 1.51     |
| 2   | A     | 2170 | A    | N9-C4   | 7.82  | 1.42        | 1.37     |
| 2   | A     | 2119 | A    | N7-C5   | -7.81 | 1.34        | 1.39     |
| 2   | A     | 2152 | G    | N7-C5   | -7.80 | 1.34        | 1.39     |
| 2   | A     | 2175 | C    | N1-C6   | 7.80  | 1.41        | 1.37     |
| 2   | A     | 2176 | A    | P-O5'   | 7.80  | 1.67        | 1.59     |
| 2   | A     | 1876 | A    | C5'-C4' | 7.79  | 1.60        | 1.51     |
| 2   | A     | 1855 | U    | C2-N3   | -7.77 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 2151 | U    | N3-C4   | -7.77 | 1.31        | 1.38     |
| 3   | E     | 60   | A    | C2-N3   | 7.77  | 1.40        | 1.33     |
| 2   | A     | 2161 | C    | C4-C5   | 7.77  | 1.49        | 1.43     |
| 3   | E     | 77   | A    | C4'-O4' | -7.73 | 1.35        | 1.45     |
| 2   | A     | 2145 | C    | C3'-C2' | 7.73  | 1.61        | 1.52     |
| 3   | E     | 57   | C    | P-O5'   | -7.73 | 1.52        | 1.59     |
| 2   | A     | 2094 | A    | N3-C4   | -7.72 | 1.30        | 1.34     |
| 2   | A     | 2159 | G    | O3'-P   | -7.72 | 1.51        | 1.61     |
| 2   | A     | 2186 | G    | N9-C8   | -7.72 | 1.32        | 1.37     |
| 3   | E     | 4    | G    | N9-C4   | -7.71 | 1.31        | 1.38     |
| 2   | A     | 1844 | C    | C2'-C1' | -7.70 | 1.44        | 1.53     |
| 2   | A     | 1874 | C    | O3'-P   | -7.70 | 1.51        | 1.61     |
| 2   | A     | 2150 | C    | C2-N3   | -7.69 | 1.29        | 1.35     |
| 1   | B     | 1301 | U    | C2-N3   | 7.67  | 1.43        | 1.37     |
| 3   | E     | 46   | G    | C5-C4   | 7.65  | 1.43        | 1.38     |
| 2   | A     | 1890 | A    | C6-N6   | 7.63  | 1.40        | 1.33     |
| 3   | E     | 45   | A    | O3'-P   | -7.61 | 1.52        | 1.61     |
| 3   | E     | 42   | C    | P-O5'   | -7.59 | 1.52        | 1.59     |
| 2   | A     | 1874 | C    | N3-C4   | 7.58  | 1.39        | 1.33     |
| 3   | E     | 15   | G    | C5-C4   | 7.58  | 1.43        | 1.38     |
| 2   | A     | 2117 | A    | C5'-C4' | 7.58  | 1.60        | 1.51     |
| 1   | B     | 1335 | U    | C2-N3   | 7.57  | 1.43        | 1.37     |
| 3   | E     | 55   | U    | C5'-C4' | 7.57  | 1.60        | 1.51     |
| 2   | A     | 2130 | U    | C2'-C1' | -7.56 | 1.45        | 1.53     |
| 4   | D     | 334  | GLY  | CA-C    | -7.55 | 1.39        | 1.51     |
| 1   | B     | 1300 | G    | N9-C8   | -7.54 | 1.32        | 1.37     |
| 2   | A     | 1863 | G    | N9-C8   | 7.54  | 1.43        | 1.37     |
| 1   | B     | 1238 | A    | N7-C5   | 7.53  | 1.43        | 1.39     |
| 3   | E     | 13   | C    | N1-C6   | 7.53  | 1.41        | 1.37     |
| 2   | A     | 2144 | G    | C5'-C4' | 7.53  | 1.60        | 1.51     |
| 2   | A     | 1867 | G    | N3-C4   | 7.52  | 1.40        | 1.35     |
| 2   | A     | 2128 | G    | N9-C8   | -7.50 | 1.32        | 1.37     |
| 2   | A     | 2099 | U    | C3'-O3' | 7.50  | 1.52        | 1.42     |
| 2   | A     | 1847 | A    | N3-C4   | -7.49 | 1.30        | 1.34     |
| 2   | A     | 1850 | G    | P-O5'   | -7.49 | 1.52        | 1.59     |
| 3   | E     | 45   | A    | N9-C8   | 7.48  | 1.43        | 1.37     |
| 2   | A     | 2189 | U    | C3'-O3' | 7.47  | 1.52        | 1.42     |
| 2   | A     | 2180 | U    | O3'-P   | -7.47 | 1.52        | 1.61     |
| 2   | A     | 2135 | A    | N3-C4   | 7.46  | 1.39        | 1.34     |
| 2   | A     | 2165 | C    | C4-N4   | -7.45 | 1.27        | 1.33     |
| 2   | A     | 2181 | U    | P-O5'   | -7.43 | 1.52        | 1.59     |
| 2   | A     | 2187 | U    | C4'-C3' | 7.42  | 1.61        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 2107 | G    | C5-C4   | -7.40 | 1.33        | 1.38     |
| 2   | A     | 2128 | G    | C6-N1   | 7.39  | 1.44        | 1.39     |
| 2   | A     | 1858 | A    | C6-N1   | -7.39 | 1.30        | 1.35     |
| 4   | D     | 470  | GLU  | CD-OE1  | 7.39  | 1.33        | 1.25     |
| 3   | E     | 49   | C    | P-O5'   | -7.36 | 1.52        | 1.59     |
| 3   | E     | 30   | G    | P-O5'   | -7.36 | 1.52        | 1.59     |
| 3   | E     | 40   | C    | C2-N3   | -7.35 | 1.29        | 1.35     |
| 2   | A     | 2112 | G    | N9-C4   | 7.35  | 1.43        | 1.38     |
| 2   | A     | 2100 | G    | P-O5'   | -7.34 | 1.52        | 1.59     |
| 2   | A     | 2119 | A    | N9-C8   | 7.34  | 1.43        | 1.37     |
| 2   | A     | 1885 | A    | C5'-C4' | 7.33  | 1.60        | 1.51     |
| 3   | E     | 59   | A    | N9-C4   | -7.33 | 1.33        | 1.37     |
| 2   | A     | 2151 | U    | O3'-P   | -7.32 | 1.52        | 1.61     |
| 2   | A     | 2150 | C    | C2-O2   | 7.31  | 1.31        | 1.24     |
| 2   | A     | 2099 | U    | O3'-P   | -7.29 | 1.52        | 1.61     |
| 2   | A     | 2133 | G    | N7-C5   | -7.28 | 1.34        | 1.39     |
| 3   | E     | 43   | G    | C5-C6   | 7.25  | 1.49        | 1.42     |
| 3   | E     | 63   | C    | P-O5'   | -7.25 | 1.52        | 1.59     |
| 3   | E     | 27   | G    | C2-N2   | -7.23 | 1.27        | 1.34     |
| 3   | E     | 29   | C    | P-O5'   | -7.23 | 1.52        | 1.59     |
| 3   | E     | 36   | A    | N3-C4   | -7.22 | 1.30        | 1.34     |
| 2   | A     | 2178 | C    | C4-C5   | -7.21 | 1.37        | 1.43     |
| 2   | A     | 2099 | U    | C2'-C1' | -7.20 | 1.45        | 1.53     |
| 2   | A     | 1881 | C    | C3'-O3' | 7.18  | 1.52        | 1.42     |
| 1   | B     | 1302 | C    | C4-N4   | -7.17 | 1.27        | 1.33     |
| 2   | A     | 1906 | G    | C4'-C3' | -7.17 | 1.45        | 1.53     |
| 2   | A     | 2108 | A    | N9-C4   | -7.17 | 1.33        | 1.37     |
| 2   | A     | 1862 | G    | C5-C6   | 7.16  | 1.49        | 1.42     |
| 2   | A     | 2173 | A    | C5-C6   | 7.16  | 1.47        | 1.41     |
| 2   | A     | 1846 | G    | C5'-C4' | 7.15  | 1.59        | 1.51     |
| 1   | B     | 1299 | A    | N3-C4   | 7.14  | 1.39        | 1.34     |
| 2   | A     | 2101 | A    | P-O5'   | -7.14 | 1.52        | 1.59     |
| 2   | A     | 2182 | U    | O3'-P   | -7.14 | 1.52        | 1.61     |
| 2   | A     | 2170 | A    | P-O5'   | -7.13 | 1.52        | 1.59     |
| 1   | B     | 1334 | G    | O3'-P   | -7.12 | 1.52        | 1.61     |
| 3   | E     | 55   | U    | C2'-C1' | -7.11 | 1.45        | 1.53     |
| 2   | A     | 1867 | G    | C6-O6   | 7.11  | 1.30        | 1.24     |
| 2   | A     | 2136 | G    | C5'-C4' | 7.11  | 1.59        | 1.51     |
| 3   | E     | 31   | G    | N3-C4   | 7.11  | 1.40        | 1.35     |
| 2   | A     | 2111 | U    | C3'-O3' | 7.10  | 1.52        | 1.42     |
| 2   | A     | 1894 | C    | N3-C4   | 7.09  | 1.39        | 1.33     |
| 1   | B     | 1297 | G    | N9-C4   | 7.08  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | B     | 1305 | G    | C6-N1   | -7.07 | 1.34        | 1.39     |
| 2   | A     | 2124 | G    | C6-O6   | -7.05 | 1.17        | 1.24     |
| 3   | E     | 43   | G    | N3-C4   | -7.04 | 1.30        | 1.35     |
| 2   | A     | 1906 | G    | N3-C4   | -7.03 | 1.30        | 1.35     |
| 2   | A     | 1893 | C    | P-O5'   | -7.03 | 1.52        | 1.59     |
| 1   | B     | 1334 | G    | N3-C4   | -7.02 | 1.30        | 1.35     |
| 3   | E     | 47   | G    | C8-N7   | 7.02  | 1.35        | 1.30     |
| 2   | A     | 2170 | A    | C5-C6   | -7.01 | 1.34        | 1.41     |
| 2   | A     | 2175 | C    | C5'-C4' | 6.99  | 1.59        | 1.51     |
| 3   | E     | 3    | C    | N1-C2   | 6.98  | 1.47        | 1.40     |
| 3   | E     | 11   | A    | N7-C5   | -6.98 | 1.35        | 1.39     |
| 3   | E     | 36   | A    | C5-C4   | 6.98  | 1.43        | 1.38     |
| 2   | A     | 1888 | G    | O3'-P   | -6.97 | 1.52        | 1.61     |
| 3   | E     | 10   | G    | C2-N2   | 6.96  | 1.41        | 1.34     |
| 2   | A     | 2158 | A    | N7-C5   | -6.96 | 1.35        | 1.39     |
| 2   | A     | 1863 | G    | O3'-P   | -6.94 | 1.52        | 1.61     |
| 2   | A     | 2160 | C    | C4'-O4' | 6.94  | 1.54        | 1.45     |
| 2   | A     | 1848 | A    | C6-N1   | 6.93  | 1.40        | 1.35     |
| 2   | A     | 2156 | G    | C2'-C1' | -6.93 | 1.45        | 1.53     |
| 2   | A     | 2175 | C    | O4'-C1' | -6.93 | 1.32        | 1.41     |
| 2   | A     | 2168 | G    | C6-N1   | 6.92  | 1.44        | 1.39     |
| 1   | B     | 1303 | C    | N1-C6   | 6.92  | 1.41        | 1.37     |
| 2   | A     | 1898 | U    | C5'-C4' | 6.92  | 1.59        | 1.51     |
| 2   | A     | 1892 | C    | N1-C6   | 6.92  | 1.41        | 1.37     |
| 2   | A     | 2112 | G    | C2-N3   | 6.91  | 1.38        | 1.32     |
| 2   | A     | 2173 | A    | C2'-C1' | 6.91  | 1.60        | 1.53     |
| 2   | A     | 1904 | G    | N7-C5   | 6.89  | 1.43        | 1.39     |
| 2   | A     | 2159 | G    | C5'-C4' | 6.89  | 1.59        | 1.51     |
| 3   | E     | 30   | G    | C3'-C2' | 6.88  | 1.60        | 1.52     |
| 3   | E     | 54   | G    | N9-C8   | -6.87 | 1.33        | 1.37     |
| 3   | E     | 23   | G    | C2-N2   | -6.87 | 1.27        | 1.34     |
| 3   | E     | 70   | C    | C5'-C4' | 6.86  | 1.59        | 1.51     |
| 2   | A     | 2158 | A    | C8-N7   | 6.84  | 1.36        | 1.31     |
| 2   | A     | 1866 | A    | C6-N1   | 6.84  | 1.40        | 1.35     |
| 3   | E     | 1    | C    | N3-C4   | 6.83  | 1.38        | 1.33     |
| 3   | E     | 42   | C    | C5'-C4' | 6.83  | 1.59        | 1.51     |
| 2   | A     | 2193 | G    | C6-N1   | 6.83  | 1.44        | 1.39     |
| 2   | A     | 1865 | U    | O3'-P   | -6.82 | 1.52        | 1.61     |
| 2   | A     | 2192 | U    | N1-C6   | -6.82 | 1.31        | 1.38     |
| 2   | A     | 2193 | G    | C8-N7   | 6.82  | 1.35        | 1.30     |
| 3   | E     | 23   | G    | C4'-C3' | 6.81  | 1.60        | 1.53     |
| 2   | A     | 2097 | A    | C8-N7   | -6.81 | 1.26        | 1.31     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | E     | 50   | G    | N7-C5   | -6.80 | 1.35        | 1.39     |
| 2   | A     | 2143 | C    | C3'-C2' | 6.79  | 1.60        | 1.52     |
| 3   | E     | 45   | A    | C5'-C4' | 6.78  | 1.59        | 1.51     |
| 2   | A     | 1838 | C    | P-O5'   | -6.77 | 1.52        | 1.59     |
| 3   | E     | 10   | G    | O4'-C1' | 6.77  | 1.50        | 1.41     |
| 2   | A     | 1847 | A    | C4'-C3' | 6.76  | 1.60        | 1.53     |
| 2   | A     | 1872 | A    | C5-C4   | 6.75  | 1.43        | 1.38     |
| 2   | A     | 2152 | G    | P-O5'   | -6.74 | 1.53        | 1.59     |
| 1   | B     | 1237 | C    | O3'-P   | -6.74 | 1.53        | 1.61     |
| 2   | A     | 2192 | U    | C5'-C4' | 6.72  | 1.59        | 1.51     |
| 1   | B     | 1243 | C    | N3-C4   | 6.71  | 1.38        | 1.33     |
| 3   | E     | 52   | C    | O4'-C1' | -6.71 | 1.32        | 1.41     |
| 1   | B     | 1292 | G    | O3'-P   | -6.70 | 1.53        | 1.61     |
| 1   | B     | 1245 | C    | C4'-C3' | 6.67  | 1.60        | 1.53     |
| 2   | A     | 1838 | C    | N3-C4   | 6.67  | 1.38        | 1.33     |
| 2   | A     | 2133 | G    | C5'-C4' | 6.67  | 1.59        | 1.51     |
| 2   | A     | 2177 | C    | N3-C4   | 6.66  | 1.38        | 1.33     |
| 3   | E     | 45   | A    | N1-C2   | 6.66  | 1.40        | 1.34     |
| 2   | A     | 1834 | U    | O3'-P   | -6.65 | 1.53        | 1.61     |
| 2   | A     | 1866 | A    | N3-C4   | 6.64  | 1.38        | 1.34     |
| 1   | B     | 1238 | A    | C6-N6   | 6.63  | 1.39        | 1.33     |
| 2   | A     | 2186 | G    | C3'-O3' | 6.62  | 1.51        | 1.42     |
| 2   | A     | 2184 | A    | C6-N1   | -6.60 | 1.30        | 1.35     |
| 3   | E     | 39   | A    | N3-C4   | -6.60 | 1.30        | 1.34     |
| 3   | E     | 28   | U    | C4'-C3' | 6.59  | 1.60        | 1.53     |
| 1   | B     | 1297 | G    | C8-N7   | 6.58  | 1.34        | 1.30     |
| 2   | A     | 2108 | A    | C6-N1   | 6.58  | 1.40        | 1.35     |
| 2   | A     | 2143 | C    | P-O5'   | -6.57 | 1.53        | 1.59     |
| 2   | A     | 2186 | G    | C2-N2   | -6.56 | 1.27        | 1.34     |
| 2   | A     | 2125 | G    | C2-N2   | -6.55 | 1.28        | 1.34     |
| 2   | A     | 2140 | G    | C2'-C1' | -6.55 | 1.46        | 1.53     |
| 3   | E     | 49   | C    | C2-N3   | 6.55  | 1.41        | 1.35     |
| 2   | A     | 2127 | G    | O4'-C1' | 6.54  | 1.50        | 1.41     |
| 2   | A     | 2129 | C    | C4-N4   | -6.54 | 1.28        | 1.33     |
| 3   | E     | 47   | G    | N7-C5   | 6.54  | 1.43        | 1.39     |
| 4   | D     | 441  | ARG  | CD-NE   | 6.54  | 1.57        | 1.46     |
| 2   | A     | 2119 | A    | N3-C4   | -6.53 | 1.30        | 1.34     |
| 2   | A     | 2174 | C    | C5'-C4' | 6.53  | 1.59        | 1.51     |
| 3   | E     | 30   | G    | C5-C4   | -6.50 | 1.33        | 1.38     |
| 2   | A     | 2124 | G    | C2-N3   | -6.50 | 1.27        | 1.32     |
| 3   | E     | 52   | C    | C2-N3   | -6.50 | 1.30        | 1.35     |
| 2   | A     | 2142 | A    | N1-C2   | -6.50 | 1.28        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1903 | G    | C6-N1   | -6.49 | 1.35        | 1.39     |
| 2   | A     | 1843 | C    | C3'-C2' | -6.47 | 1.45        | 1.52     |
| 2   | A     | 2133 | G    | N3-C4   | -6.46 | 1.30        | 1.35     |
| 2   | A     | 2153 | C    | C5'-C4' | 6.45  | 1.59        | 1.51     |
| 2   | A     | 1839 | G    | O3'-P   | -6.45 | 1.53        | 1.61     |
| 1   | B     | 1299 | A    | P-O5'   | -6.45 | 1.53        | 1.59     |
| 2   | A     | 1866 | A    | N9-C4   | -6.45 | 1.33        | 1.37     |
| 2   | A     | 2191 | A    | P-O5'   | -6.45 | 1.53        | 1.59     |
| 2   | A     | 2179 | C    | N1-C2   | -6.44 | 1.33        | 1.40     |
| 3   | E     | 64   | G    | N9-C8   | 6.44  | 1.42        | 1.37     |
| 3   | E     | 43   | G    | O3'-P   | -6.44 | 1.53        | 1.61     |
| 3   | E     | 73   | A    | C5-C4   | 6.44  | 1.43        | 1.38     |
| 4   | D     | 220  | TYR  | CG-CD2  | 6.42  | 1.47        | 1.39     |
| 2   | A     | 1872 | A    | N3-C4   | -6.42 | 1.30        | 1.34     |
| 2   | A     | 2104 | C    | C2'-C1' | -6.42 | 1.46        | 1.53     |
| 2   | A     | 2129 | C    | C5-C6   | -6.42 | 1.29        | 1.34     |
| 2   | A     | 2142 | A    | C6-N1   | 6.42  | 1.40        | 1.35     |
| 2   | A     | 2170 | A    | C6-N6   | 6.42  | 1.39        | 1.33     |
| 1   | B     | 1335 | U    | C4-C5   | 6.41  | 1.49        | 1.43     |
| 2   | A     | 2170 | A    | N9-C8   | 6.41  | 1.42        | 1.37     |
| 3   | E     | 38   | A    | C2'-C1' | 6.40  | 1.60        | 1.53     |
| 2   | A     | 1859 | U    | N1-C6   | -6.40 | 1.32        | 1.38     |
| 2   | A     | 2164 | C    | C5-C6   | -6.40 | 1.29        | 1.34     |
| 3   | E     | 58   | A    | C2-N3   | 6.39  | 1.39        | 1.33     |
| 2   | A     | 1879 | C    | C5'-C4' | 6.39  | 1.59        | 1.51     |
| 2   | A     | 2151 | U    | C4'-C3' | 6.38  | 1.60        | 1.53     |
| 3   | E     | 4    | G    | C5-C4   | -6.38 | 1.33        | 1.38     |
| 2   | A     | 1869 | G    | C2-N3   | -6.37 | 1.27        | 1.32     |
| 2   | A     | 2169 | A    | N9-C4   | -6.37 | 1.34        | 1.37     |
| 3   | E     | 50   | G    | C2'-C1' | -6.36 | 1.46        | 1.53     |
| 2   | A     | 1834 | U    | C2-N3   | 6.36  | 1.42        | 1.37     |
| 2   | A     | 2095 | A    | C3'-O3' | 6.36  | 1.51        | 1.42     |
| 2   | A     | 2105 | U    | C2'-C1' | -6.36 | 1.46        | 1.53     |
| 2   | A     | 2136 | G    | C6-N1   | 6.33  | 1.44        | 1.39     |
| 2   | A     | 1862 | G    | C2-N2   | -6.33 | 1.28        | 1.34     |
| 3   | E     | 6    | G    | C5'-C4' | 6.32  | 1.58        | 1.51     |
| 2   | A     | 1835 | G    | N9-C8   | 6.31  | 1.42        | 1.37     |
| 2   | A     | 2147 | A    | N3-C4   | -6.31 | 1.31        | 1.34     |
| 3   | E     | 25   | U    | C4-C5   | -6.30 | 1.37        | 1.43     |
| 2   | A     | 2149 | U    | C5'-C4' | 6.30  | 1.58        | 1.51     |
| 2   | A     | 2174 | C    | N3-C4   | 6.30  | 1.38        | 1.33     |
| 2   | A     | 2138 | G    | N1-C2   | 6.29  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 2172 | U    | O3'-P   | -6.29 | 1.53        | 1.61     |
| 2   | A     | 2178 | C    | O3'-P   | -6.28 | 1.53        | 1.61     |
| 2   | A     | 1853 | A    | C6-N6   | -6.28 | 1.28        | 1.33     |
| 2   | A     | 2188 | U    | O3'-P   | -6.27 | 1.53        | 1.61     |
| 3   | E     | 7    | G    | N9-C4   | 6.24  | 1.43        | 1.38     |
| 3   | E     | 26   | C    | C2-N3   | -6.24 | 1.30        | 1.35     |
| 1   | B     | 1304 | G    | C4'-O4' | 6.24  | 1.53        | 1.45     |
| 2   | A     | 1877 | A    | C6-N1   | 6.23  | 1.40        | 1.35     |
| 1   | B     | 1292 | G    | N9-C8   | 6.23  | 1.42        | 1.37     |
| 2   | A     | 2175 | C    | O5'-C5' | 6.22  | 1.54        | 1.44     |
| 2   | A     | 2112 | G    | C6-O6   | 6.22  | 1.29        | 1.24     |
| 2   | A     | 2174 | C    | C5-C6   | 6.21  | 1.39        | 1.34     |
| 2   | A     | 1856 | U    | C4-C5   | -6.21 | 1.38        | 1.43     |
| 2   | A     | 2152 | G    | C5-C4   | -6.21 | 1.34        | 1.38     |
| 2   | A     | 2119 | A    | O3'-P   | -6.20 | 1.53        | 1.61     |
| 4   | D     | 124  | GLU  | CB-CG   | 6.20  | 1.64        | 1.52     |
| 2   | A     | 1901 | A    | O3'-P   | -6.19 | 1.53        | 1.61     |
| 1   | B     | 1336 | C    | C4'-C3' | 6.19  | 1.59        | 1.53     |
| 3   | E     | 42   | C    | N1-C6   | 6.19  | 1.40        | 1.37     |
| 3   | E     | 29   | C    | C4-C5   | -6.19 | 1.38        | 1.43     |
| 2   | A     | 1840 | G    | C6-N1   | -6.19 | 1.35        | 1.39     |
| 2   | A     | 2184 | A    | N9-C4   | -6.18 | 1.34        | 1.37     |
| 2   | A     | 1851 | U    | C5'-C4' | 6.18  | 1.58        | 1.51     |
| 2   | A     | 1860 | G    | N3-C4   | -6.18 | 1.31        | 1.35     |
| 2   | A     | 1902 | C    | C4'-C3' | 6.18  | 1.59        | 1.53     |
| 2   | A     | 2127 | G    | N9-C8   | 6.18  | 1.42        | 1.37     |
| 3   | E     | 13   | C    | C4-C5   | 6.17  | 1.47        | 1.43     |
| 2   | A     | 2128 | G    | C2-N2   | -6.17 | 1.28        | 1.34     |
| 3   | E     | 30   | G    | C6-O6   | -6.16 | 1.18        | 1.24     |
| 3   | E     | 9    | G    | C6-N1   | 6.16  | 1.43        | 1.39     |
| 2   | A     | 2133 | G    | C6-N1   | 6.16  | 1.43        | 1.39     |
| 2   | A     | 2127 | G    | N7-C5   | -6.15 | 1.35        | 1.39     |
| 2   | A     | 1884 | G    | C6-N1   | 6.15  | 1.43        | 1.39     |
| 2   | A     | 2112 | G    | C2-N2   | -6.15 | 1.28        | 1.34     |
| 1   | B     | 1241 | G    | N3-C4   | -6.14 | 1.31        | 1.35     |
| 2   | A     | 1879 | C    | C2-N3   | 6.14  | 1.40        | 1.35     |
| 2   | A     | 2147 | A    | C2'-C1' | -6.14 | 1.46        | 1.53     |
| 3   | E     | 64   | G    | C5'-C4' | 6.14  | 1.58        | 1.51     |
| 2   | A     | 2157 | G    | P-O5'   | -6.13 | 1.53        | 1.59     |
| 2   | A     | 2116 | G    | C8-N7   | 6.13  | 1.34        | 1.30     |
| 1   | B     | 1239 | A    | C1'-N9  | -6.13 | 1.38        | 1.46     |
| 2   | A     | 2176 | A    | N7-C5   | 6.12  | 1.43        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | E     | 29   | C    | N1-C6   | 6.12  | 1.40        | 1.37     |
| 2   | A     | 2175 | C    | C3'-C2' | -6.12 | 1.46        | 1.52     |
| 3   | E     | 13   | C    | C2-N3   | -6.12 | 1.30        | 1.35     |
| 3   | E     | 19   | G    | N3-C4   | 6.12  | 1.39        | 1.35     |
| 2   | A     | 1834 | U    | P-O5'   | -6.12 | 1.53        | 1.59     |
| 3   | E     | 33   | C    | C4'-C3' | -6.11 | 1.46        | 1.53     |
| 1   | B     | 1305 | G    | C4'-O4' | -6.11 | 1.37        | 1.45     |
| 2   | A     | 2133 | G    | O3'-P   | -6.11 | 1.53        | 1.61     |
| 2   | A     | 2149 | U    | N3-C4   | 6.10  | 1.44        | 1.38     |
| 2   | A     | 2158 | A    | C4'-C3' | 6.10  | 1.59        | 1.53     |
| 3   | E     | 48   | U    | N1-C6   | -6.10 | 1.32        | 1.38     |
| 2   | A     | 1895 | C    | C2-O2   | -6.10 | 1.19        | 1.24     |
| 6   | G     | 174  | PHE  | CE2-CZ  | 6.10  | 1.49        | 1.37     |
| 2   | A     | 1896 | G    | C2'-C1' | -6.10 | 1.46        | 1.53     |
| 3   | E     | 21   | U    | C2'-O2' | 6.10  | 1.49        | 1.41     |
| 2   | A     | 2149 | U    | C4'-O4' | -6.09 | 1.37        | 1.45     |
| 2   | A     | 2154 | A    | C5'-C4' | -6.09 | 1.44        | 1.51     |
| 1   | B     | 1298 | U    | N3-C4   | -6.09 | 1.32        | 1.38     |
| 2   | A     | 2101 | A    | C5'-C4' | 6.08  | 1.58        | 1.51     |
| 3   | E     | 49   | C    | N1-C6   | -6.08 | 1.33        | 1.37     |
| 3   | E     | 14   | A    | N3-C4   | -6.08 | 1.31        | 1.34     |
| 1   | B     | 1294 | G    | N9-C8   | 6.07  | 1.42        | 1.37     |
| 2   | A     | 2192 | U    | C2-N3   | -6.07 | 1.33        | 1.37     |
| 1   | B     | 1295 | U    | C2-N3   | 6.07  | 1.42        | 1.37     |
| 2   | A     | 1848 | A    | P-O5'   | -6.07 | 1.53        | 1.59     |
| 2   | A     | 1875 | G    | O3'-P   | -6.07 | 1.53        | 1.61     |
| 2   | A     | 2186 | G    | C6-N1   | -6.07 | 1.35        | 1.39     |
| 1   | B     | 1243 | C    | C5'-C4' | 6.06  | 1.58        | 1.51     |
| 2   | A     | 2155 | U    | C3'-O3' | 6.06  | 1.50        | 1.42     |
| 2   | A     | 1907 | G    | C6-N1   | 6.05  | 1.43        | 1.39     |
| 1   | B     | 1294 | G    | P-O5'   | -6.05 | 1.53        | 1.59     |
| 1   | B     | 1304 | G    | O3'-P   | -6.05 | 1.53        | 1.61     |
| 3   | E     | 42   | C    | C1'-N1  | 6.05  | 1.57        | 1.48     |
| 3   | E     | 61   | U    | P-O5'   | -6.05 | 1.53        | 1.59     |
| 1   | B     | 1291 | U    | C2'-C1' | -6.04 | 1.46        | 1.53     |
| 2   | A     | 1846 | G    | C2-N3   | 6.03  | 1.37        | 1.32     |
| 3   | E     | 69   | C    | N1-C6   | -6.03 | 1.33        | 1.37     |
| 2   | A     | 2104 | C    | C4'-C3' | 6.03  | 1.59        | 1.53     |
| 3   | E     | 19   | G    | P-O5'   | -6.03 | 1.53        | 1.59     |
| 2   | A     | 1877 | A    | C4'-C3' | -6.02 | 1.46        | 1.53     |
| 3   | E     | 64   | G    | C2'-C1' | -6.02 | 1.46        | 1.53     |
| 3   | E     | 69   | C    | C3'-C2' | -6.02 | 1.46        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | B     | 1241 | G    | N7-C5   | -6.01 | 1.35        | 1.39     |
| 2   | A     | 1896 | G    | P-O5'   | -6.01 | 1.53        | 1.59     |
| 1   | B     | 1238 | A    | C6-N1   | 6.00  | 1.39        | 1.35     |
| 3   | E     | 49   | C    | O3'-P   | -6.00 | 1.53        | 1.61     |
| 1   | B     | 1244 | G    | O3'-P   | -6.00 | 1.53        | 1.61     |
| 3   | E     | 2    | G    | C2-N2   | -6.00 | 1.28        | 1.34     |
| 2   | A     | 1901 | A    | N1-C2   | -6.00 | 1.28        | 1.34     |
| 2   | A     | 2119 | A    | N9-C4   | -6.00 | 1.34        | 1.37     |
| 3   | E     | 77   | A    | C8-N7   | -6.00 | 1.27        | 1.31     |
| 2   | A     | 2114 | A    | C4'-C3' | 6.00  | 1.59        | 1.53     |
| 3   | E     | 42   | C    | C2-N3   | -5.99 | 1.30        | 1.35     |
| 2   | A     | 1871 | A    | C2'-C1' | -5.99 | 1.46        | 1.53     |
| 2   | A     | 1869 | G    | N9-C4   | -5.98 | 1.33        | 1.38     |
| 2   | A     | 2171 | A    | N3-C4   | -5.98 | 1.31        | 1.34     |
| 2   | A     | 1884 | G    | C2'-C1' | 5.98  | 1.59        | 1.53     |
| 2   | A     | 1907 | G    | C2-N3   | 5.98  | 1.37        | 1.32     |
| 3   | E     | 44   | A    | N3-C4   | 5.97  | 1.38        | 1.34     |
| 2   | A     | 1875 | G    | N1-C2   | 5.97  | 1.42        | 1.37     |
| 2   | A     | 1893 | C    | N1-C2   | 5.97  | 1.46        | 1.40     |
| 3   | E     | 34   | U    | C3'-C2' | -5.97 | 1.46        | 1.52     |
| 2   | A     | 1856 | U    | N3-C4   | 5.96  | 1.43        | 1.38     |
| 3   | E     | 43   | G    | C4'-C3' | 5.96  | 1.59        | 1.53     |
| 2   | A     | 2170 | A    | N7-C5   | 5.95  | 1.42        | 1.39     |
| 3   | E     | 72   | C    | C4'-C3' | 5.95  | 1.59        | 1.53     |
| 2   | A     | 2099 | U    | C4-O4   | -5.94 | 1.18        | 1.23     |
| 1   | B     | 1292 | G    | C5'-C4' | 5.94  | 1.58        | 1.51     |
| 2   | A     | 2137 | U    | C4'-O4' | 5.94  | 1.53        | 1.45     |
| 2   | A     | 2111 | U    | N3-C4   | -5.93 | 1.33        | 1.38     |
| 3   | E     | 12   | G    | C5'-C4' | 5.93  | 1.58        | 1.51     |
| 2   | A     | 1857 | G    | C6-N1   | -5.92 | 1.35        | 1.39     |
| 3   | E     | 73   | A    | N9-C8   | 5.92  | 1.42        | 1.37     |
| 5   | F     | 32   | GLU  | CA-CB   | 5.92  | 1.67        | 1.53     |
| 4   | D     | 189  | PRO  | N-CD    | -5.90 | 1.39        | 1.47     |
| 2   | A     | 1888 | G    | C6-N1   | 5.90  | 1.43        | 1.39     |
| 2   | A     | 2172 | U    | C2'-C1' | 5.90  | 1.59        | 1.53     |
| 2   | A     | 2176 | A    | C5-C4   | -5.90 | 1.34        | 1.38     |
| 2   | A     | 2182 | U    | O4'-C1' | 5.90  | 1.49        | 1.41     |
| 2   | A     | 1885 | A    | C5-C4   | 5.90  | 1.42        | 1.38     |
| 8   | I     | 2    | ARG  | CD-NE   | 5.90  | 1.56        | 1.46     |
| 6   | G     | 132  | ARG  | CZ-NH1  | 5.89  | 1.40        | 1.33     |
| 2   | A     | 2142 | A    | N9-C4   | 5.89  | 1.41        | 1.37     |
| 3   | E     | 20   | G    | N9-C8   | -5.89 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | B     | 1245 | C    | C2'-C1' | -5.88 | 1.46        | 1.53     |
| 2   | A     | 2119 | A    | C8-N7   | -5.88 | 1.27        | 1.31     |
| 2   | A     | 1835 | G    | N1-C2   | -5.88 | 1.33        | 1.37     |
| 2   | A     | 1891 | G    | N9-C8   | -5.88 | 1.33        | 1.37     |
| 2   | A     | 2181 | U    | N3-C4   | 5.88  | 1.43        | 1.38     |
| 2   | A     | 1848 | A    | C5'-C4' | 5.87  | 1.58        | 1.51     |
| 2   | A     | 2134 | A    | C8-N7   | -5.87 | 1.27        | 1.31     |
| 3   | E     | 13   | C    | C2'-C1' | -5.87 | 1.46        | 1.53     |
| 1   | B     | 1299 | A    | N7-C5   | 5.87  | 1.42        | 1.39     |
| 2   | A     | 1846 | G    | C4'-C3' | 5.87  | 1.59        | 1.53     |
| 2   | A     | 1904 | G    | P-O5'   | -5.87 | 1.53        | 1.59     |
| 2   | A     | 1848 | A    | C3'-C2' | -5.87 | 1.46        | 1.52     |
| 2   | A     | 2122 | U    | N1-C2   | -5.86 | 1.33        | 1.38     |
| 2   | A     | 2154 | A    | N9-C4   | -5.86 | 1.34        | 1.37     |
| 3   | E     | 26   | C    | N3-C4   | 5.86  | 1.38        | 1.33     |
| 1   | B     | 1332 | A    | P-O5'   | -5.85 | 1.53        | 1.59     |
| 2   | A     | 2111 | U    | O3'-P   | -5.85 | 1.54        | 1.61     |
| 2   | A     | 2117 | A    | N1-C2   | -5.84 | 1.29        | 1.34     |
| 2   | A     | 2095 | A    | C5-C6   | 5.84  | 1.46        | 1.41     |
| 2   | A     | 1868 | C    | C2-N3   | -5.83 | 1.31        | 1.35     |
| 2   | A     | 1838 | C    | C2-N3   | 5.83  | 1.40        | 1.35     |
| 2   | A     | 2155 | U    | P-O5'   | -5.83 | 1.53        | 1.59     |
| 2   | A     | 2119 | A    | C4'-O4' | 5.82  | 1.53        | 1.45     |
| 2   | A     | 2191 | A    | C2-N3   | -5.82 | 1.28        | 1.33     |
| 2   | A     | 1893 | C    | C3'-C2' | 5.82  | 1.59        | 1.52     |
| 2   | A     | 2144 | G    | C2-N2   | -5.81 | 1.28        | 1.34     |
| 8   | I     | 138  | GLU  | CD-OE1  | -5.81 | 1.19        | 1.25     |
| 2   | A     | 2171 | A    | P-O5'   | -5.81 | 1.53        | 1.59     |
| 8   | I     | 4    | ARG  | CD-NE   | 5.80  | 1.56        | 1.46     |
| 2   | A     | 2181 | U    | C2-N3   | -5.79 | 1.33        | 1.37     |
| 1   | B     | 1293 | C    | C4-N4   | -5.78 | 1.28        | 1.33     |
| 2   | A     | 1850 | G    | C8-N7   | 5.78  | 1.34        | 1.30     |
| 2   | A     | 2127 | G    | C2-N3   | 5.78  | 1.37        | 1.32     |
| 2   | A     | 1850 | G    | C5-C4   | -5.76 | 1.34        | 1.38     |
| 2   | A     | 2190 | G    | N9-C8   | 5.75  | 1.41        | 1.37     |
| 2   | A     | 1835 | G    | C2-N3   | 5.75  | 1.37        | 1.32     |
| 2   | A     | 1895 | C    | O3'-P   | -5.75 | 1.54        | 1.61     |
| 3   | E     | 11   | A    | C5-C6   | -5.75 | 1.35        | 1.41     |
| 2   | A     | 2134 | A    | C5-C6   | 5.75  | 1.46        | 1.41     |
| 2   | A     | 2136 | G    | C5-C4   | -5.75 | 1.34        | 1.38     |
| 3   | E     | 48   | U    | P-O5'   | 5.74  | 1.65        | 1.59     |
| 3   | E     | 4    | G    | N1-C2   | -5.74 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1845 | G    | C5'-C4' | 5.74  | 1.58        | 1.51     |
| 2   | A     | 2115 | G    | O4'-C1' | 5.73  | 1.49        | 1.41     |
| 2   | A     | 2098 | U    | C2'-C1' | -5.72 | 1.47        | 1.53     |
| 2   | A     | 2181 | U    | N1-C6   | -5.72 | 1.32        | 1.38     |
| 2   | A     | 2131 | U    | C4-C5   | 5.71  | 1.48        | 1.43     |
| 2   | A     | 1835 | G    | C5-C4   | 5.71  | 1.42        | 1.38     |
| 2   | A     | 1884 | G    | P-O5'   | -5.71 | 1.54        | 1.59     |
| 3   | E     | 9    | G    | C4'-O4' | -5.71 | 1.38        | 1.45     |
| 1   | B     | 1242 | G    | N7-C5   | -5.70 | 1.35        | 1.39     |
| 2   | A     | 1857 | G    | C2'-C1' | -5.70 | 1.47        | 1.53     |
| 2   | A     | 2117 | A    | C4'-C3' | 5.70  | 1.59        | 1.53     |
| 2   | A     | 1881 | C    | C4-N4   | -5.70 | 1.28        | 1.33     |
| 7   | H     | 27   | ARG  | CD-NE   | 5.69  | 1.56        | 1.46     |
| 2   | A     | 1895 | C    | C4'-C3' | -5.68 | 1.46        | 1.52     |
| 1   | B     | 1294 | G    | C5-C6   | 5.68  | 1.48        | 1.42     |
| 1   | B     | 1243 | C    | O3'-P   | -5.68 | 1.54        | 1.61     |
| 2   | A     | 2117 | A    | C2-N3   | -5.68 | 1.28        | 1.33     |
| 2   | A     | 2139 | U    | P-O5'   | -5.68 | 1.54        | 1.59     |
| 2   | A     | 2103 | C    | C4-C5   | -5.68 | 1.38        | 1.43     |
| 3   | E     | 13   | C    | N3-C4   | 5.67  | 1.38        | 1.33     |
| 1   | B     | 1298 | U    | O3'-P   | -5.66 | 1.54        | 1.61     |
| 3   | E     | 23   | G    | C3'-C2' | -5.66 | 1.46        | 1.52     |
| 2   | A     | 1847 | A    | C6-N1   | -5.65 | 1.31        | 1.35     |
| 2   | A     | 2112 | G    | C5-C4   | -5.65 | 1.34        | 1.38     |
| 2   | A     | 2144 | G    | C3'-O3' | 5.65  | 1.50        | 1.42     |
| 6   | G     | 123  | GLY  | N-CA    | 5.65  | 1.54        | 1.46     |
| 2   | A     | 2170 | A    | C5-C4   | 5.65  | 1.42        | 1.38     |
| 2   | A     | 2098 | U    | N1-C2   | -5.65 | 1.33        | 1.38     |
| 3   | E     | 23   | G    | O3'-P   | -5.65 | 1.54        | 1.61     |
| 2   | A     | 2147 | A    | O3'-P   | -5.65 | 1.54        | 1.61     |
| 2   | A     | 2106 | U    | P-O5'   | -5.64 | 1.54        | 1.59     |
| 1   | B     | 1239 | A    | N9-C8   | 5.64  | 1.42        | 1.37     |
| 2   | A     | 1898 | U    | P-O5'   | -5.64 | 1.54        | 1.59     |
| 3   | E     | 35   | C    | C2-O2   | 5.64  | 1.29        | 1.24     |
| 2   | A     | 1852 | U    | C1'-N1  | -5.64 | 1.39        | 1.46     |
| 3   | E     | 70   | C    | P-O5'   | -5.63 | 1.54        | 1.59     |
| 2   | A     | 2130 | U    | C4'-C3' | 5.63  | 1.59        | 1.53     |
| 2   | A     | 1897 | G    | O4'-C1' | 5.60  | 1.49        | 1.41     |
| 2   | A     | 1892 | C    | N3-C4   | 5.60  | 1.37        | 1.33     |
| 2   | A     | 2163 | A    | N9-C8   | 5.60  | 1.42        | 1.37     |
| 2   | A     | 2189 | U    | O3'-P   | -5.60 | 1.54        | 1.61     |
| 2   | A     | 2118 | U    | C2-N3   | 5.60  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 2164 | C    | O3'-P   | -5.60 | 1.54        | 1.61     |
| 2   | A     | 2183 | A    | N9-C8   | -5.60 | 1.33        | 1.37     |
| 3   | E     | 33   | C    | P-O5'   | -5.60 | 1.54        | 1.59     |
| 2   | A     | 2126 | A    | C5-C4   | -5.59 | 1.34        | 1.38     |
| 2   | A     | 1906 | G    | C2-N2   | -5.58 | 1.28        | 1.34     |
| 2   | A     | 2120 | G    | C3'-O3' | 5.58  | 1.50        | 1.42     |
| 3   | E     | 28   | U    | N3-C4   | 5.58  | 1.43        | 1.38     |
| 2   | A     | 2134 | A    | N1-C2   | 5.57  | 1.39        | 1.34     |
| 2   | A     | 2125 | G    | C3'-C2' | -5.57 | 1.46        | 1.52     |
| 3   | E     | 70   | C    | N1-C6   | -5.56 | 1.33        | 1.37     |
| 2   | A     | 2117 | A    | C2'-C1' | -5.56 | 1.47        | 1.53     |
| 2   | A     | 2192 | U    | C4'-O4' | 5.56  | 1.52        | 1.45     |
| 4   | D     | 89   | SER  | CA-CB   | 5.56  | 1.61        | 1.52     |
| 6   | G     | 10   | GLU  | CB-CG   | 5.55  | 1.62        | 1.52     |
| 2   | A     | 1881 | C    | C2'-C1' | -5.55 | 1.47        | 1.53     |
| 2   | A     | 1834 | U    | C4-C5   | 5.55  | 1.48        | 1.43     |
| 3   | E     | 10   | G    | C2-N3   | 5.54  | 1.37        | 1.32     |
| 2   | A     | 2123 | G    | N7-C5   | 5.54  | 1.42        | 1.39     |
| 2   | A     | 2175 | C    | C2-N3   | -5.54 | 1.31        | 1.35     |
| 1   | B     | 1237 | C    | N1-C6   | -5.54 | 1.33        | 1.37     |
| 3   | E     | 7    | G    | C8-N7   | -5.54 | 1.27        | 1.30     |
| 3   | E     | 22   | A    | O3'-P   | -5.54 | 1.54        | 1.61     |
| 2   | A     | 2134 | A    | C6-N1   | 5.53  | 1.39        | 1.35     |
| 2   | A     | 2182 | U    | C1'-N1  | 5.52  | 1.57        | 1.48     |
| 3   | E     | 48   | U    | C4'-O4' | 5.52  | 1.52        | 1.45     |
| 2   | A     | 1850 | G    | C1'-N9  | 5.52  | 1.57        | 1.48     |
| 2   | A     | 1877 | A    | N7-C5   | 5.52  | 1.42        | 1.39     |
| 2   | A     | 2179 | C    | C2'-O2' | 5.51  | 1.48        | 1.41     |
| 1   | B     | 1237 | C    | C5'-C4' | 5.51  | 1.57        | 1.51     |
| 3   | E     | 5    | G    | N1-C2   | 5.51  | 1.42        | 1.37     |
| 5   | F     | 68   | GLY  | N-CA    | -5.50 | 1.37        | 1.46     |
| 4   | D     | 37   | VAL  | CB-CG1  | 5.50  | 1.64        | 1.52     |
| 1   | B     | 1237 | C    | C4'-C3' | 5.50  | 1.59        | 1.53     |
| 2   | A     | 2127 | G    | N3-C4   | -5.50 | 1.31        | 1.35     |
| 2   | A     | 2131 | U    | C4'-C3' | 5.50  | 1.59        | 1.53     |
| 2   | A     | 1889 | A    | C6-N1   | -5.49 | 1.31        | 1.35     |
| 2   | A     | 2099 | U    | C5-C6   | 5.49  | 1.39        | 1.34     |
| 2   | A     | 2183 | A    | C8-N7   | -5.49 | 1.27        | 1.31     |
| 1   | B     | 1238 | A    | N3-C4   | -5.49 | 1.31        | 1.34     |
| 2   | A     | 2112 | G    | N9-C8   | 5.49  | 1.41        | 1.37     |
| 2   | A     | 2130 | U    | C2-N3   | -5.48 | 1.33        | 1.37     |
| 2   | A     | 2114 | A    | C3'-C2' | -5.48 | 1.46        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | B     | 1294 | G    | C5-C4   | -5.48 | 1.34        | 1.38     |
| 2   | A     | 2171 | A    | N1-C2   | -5.48 | 1.29        | 1.34     |
| 5   | F     | 151  | GLU  | CD-OE1  | 5.47  | 1.31        | 1.25     |
| 2   | A     | 1863 | G    | C5-C4   | 5.47  | 1.42        | 1.38     |
| 2   | A     | 1907 | G    | C5-C4   | -5.47 | 1.34        | 1.38     |
| 3   | E     | 54   | G    | N1-C2   | -5.47 | 1.33        | 1.37     |
| 4   | D     | 188  | GLU  | CD-OE1  | 5.47  | 1.31        | 1.25     |
| 3   | E     | 4    | G    | P-O5'   | -5.46 | 1.54        | 1.59     |
| 2   | A     | 2147 | A    | C4'-C3' | -5.46 | 1.47        | 1.52     |
| 2   | A     | 1850 | G    | C3'-C2' | -5.46 | 1.46        | 1.52     |
| 2   | A     | 1844 | C    | O3'-P   | -5.46 | 1.54        | 1.61     |
| 2   | A     | 1886 | U    | C2'-C1' | -5.46 | 1.47        | 1.53     |
| 3   | E     | 74   | A    | N7-C5   | -5.46 | 1.35        | 1.39     |
| 1   | B     | 1336 | C    | C3'-O3' | 5.45  | 1.49        | 1.42     |
| 3   | E     | 11   | A    | N9-C8   | 5.45  | 1.42        | 1.37     |
| 8   | I     | 102  | TRP  | CZ3-CH2 | 5.45  | 1.48        | 1.40     |
| 2   | A     | 2106 | U    | C3'-O3' | 5.45  | 1.49        | 1.42     |
| 1   | B     | 1239 | A    | C3'-O3' | 5.44  | 1.49        | 1.42     |
| 4   | D     | 316  | GLY  | N-CA    | 5.44  | 1.54        | 1.46     |
| 3   | E     | 8    | U    | C5'-C4' | 5.44  | 1.57        | 1.51     |
| 3   | E     | 38   | A    | C8-N7   | -5.43 | 1.27        | 1.31     |
| 2   | A     | 1858 | A    | C3'-O3' | 5.43  | 1.49        | 1.42     |
| 2   | A     | 1857 | G    | O3'-P   | -5.43 | 1.54        | 1.61     |
| 3   | E     | 2    | G    | N9-C4   | -5.43 | 1.33        | 1.38     |
| 3   | E     | 18   | U    | C3'-C2' | 5.43  | 1.58        | 1.52     |
| 4   | D     | 271  | LYS  | CD-CE   | 5.43  | 1.64        | 1.51     |
| 1   | B     | 1301 | U    | O3'-P   | -5.42 | 1.54        | 1.61     |
| 2   | A     | 2177 | C    | P-O5'   | -5.42 | 1.54        | 1.59     |
| 2   | A     | 1838 | C    | C4'-C3' | 5.42  | 1.59        | 1.53     |
| 1   | B     | 1236 | A    | C8-N7   | -5.42 | 1.27        | 1.31     |
| 3   | E     | 5    | G    | C5'-C4' | 5.41  | 1.57        | 1.51     |
| 3   | E     | 58   | A    | C5'-C4' | 5.41  | 1.57        | 1.51     |
| 2   | A     | 1845 | G    | C2-N2   | -5.40 | 1.29        | 1.34     |
| 3   | E     | 16   | C    | C4'-O4' | 5.40  | 1.52        | 1.45     |
| 3   | E     | 59   | A    | N9-C8   | 5.39  | 1.42        | 1.37     |
| 2   | A     | 1892 | C    | C5-C6   | -5.39 | 1.30        | 1.34     |
| 3   | E     | 25   | U    | C4'-O4' | 5.39  | 1.52        | 1.45     |
| 3   | E     | 77   | A    | C6-N1   | 5.39  | 1.39        | 1.35     |
| 2   | A     | 2188 | U    | C2-N3   | 5.39  | 1.41        | 1.37     |
| 2   | A     | 1866 | A    | N7-C5   | 5.38  | 1.42        | 1.39     |
| 2   | A     | 2188 | U    | N3-C4   | -5.38 | 1.33        | 1.38     |
| 2   | A     | 1853 | A    | N7-C5   | -5.37 | 1.36        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6   | G     | 176  | PHE  | CG-CD2  | 5.37  | 1.46        | 1.38     |
| 1   | B     | 1297 | G    | C2-N3   | 5.37  | 1.37        | 1.32     |
| 3   | E     | 51   | U    | C1'-N1  | 5.37  | 1.56        | 1.48     |
| 1   | B     | 1334 | G    | C6-N1   | 5.36  | 1.43        | 1.39     |
| 2   | A     | 1899 | A    | C5-C4   | -5.36 | 1.34        | 1.38     |
| 3   | E     | 34   | U    | N3-C4   | -5.36 | 1.33        | 1.38     |
| 2   | A     | 2113 | U    | C5'-C4' | 5.36  | 1.57        | 1.51     |
| 1   | B     | 1241 | G    | C2-N3   | -5.35 | 1.28        | 1.32     |
| 2   | A     | 1870 | C    | N1-C6   | -5.35 | 1.33        | 1.37     |
| 2   | A     | 1900 | A    | N3-C4   | -5.35 | 1.31        | 1.34     |
| 3   | E     | 49   | C    | N3-C4   | 5.35  | 1.37        | 1.33     |
| 1   | B     | 1302 | C    | C2'-C1' | -5.35 | 1.47        | 1.53     |
| 2   | A     | 2116 | G    | N7-C5   | 5.35  | 1.42        | 1.39     |
| 2   | A     | 2141 | G    | N9-C8   | 5.35  | 1.41        | 1.37     |
| 3   | E     | 47   | G    | C4'-C3' | 5.35  | 1.59        | 1.53     |
| 4   | D     | 242  | GLY  | CA-C    | -5.35 | 1.43        | 1.51     |
| 2   | A     | 2107 | G    | O3'-P   | -5.35 | 1.54        | 1.61     |
| 2   | A     | 1871 | A    | N1-C2   | 5.34  | 1.39        | 1.34     |
| 2   | A     | 2135 | A    | C5-C4   | -5.34 | 1.35        | 1.38     |
| 3   | E     | 4    | G    | C4'-C3' | 5.34  | 1.59        | 1.53     |
| 2   | A     | 1856 | U    | C2-N3   | 5.34  | 1.41        | 1.37     |
| 2   | A     | 1905 | C    | C5'-C4' | 5.33  | 1.57        | 1.51     |
| 4   | D     | 30   | PHE  | CE1-CZ  | 5.33  | 1.47        | 1.37     |
| 1   | B     | 1295 | U    | C4'-O4' | 5.33  | 1.52        | 1.45     |
| 2   | A     | 2119 | A    | C4'-C3' | 5.33  | 1.59        | 1.53     |
| 3   | E     | 68   | C    | C4-N4   | 5.32  | 1.38        | 1.33     |
| 2   | A     | 2173 | A    | O4'-C1' | 5.31  | 1.48        | 1.41     |
| 2   | A     | 2138 | G    | N7-C5   | 5.31  | 1.42        | 1.39     |
| 2   | A     | 2171 | A    | C5-C4   | -5.30 | 1.35        | 1.38     |
| 2   | A     | 1856 | U    | C2'-O2' | 5.30  | 1.48        | 1.41     |
| 2   | A     | 2142 | A    | C5'-C4' | 5.30  | 1.57        | 1.51     |
| 3   | E     | 24   | C    | C4'-O4' | 5.30  | 1.52        | 1.45     |
| 3   | E     | 61   | U    | C4'-C3' | 5.30  | 1.58        | 1.53     |
| 3   | E     | 43   | G    | N9-C4   | -5.30 | 1.33        | 1.38     |
| 6   | G     | 98   | PHE  | CA-CB   | 5.29  | 1.65        | 1.53     |
| 2   | A     | 1839 | G    | N9-C8   | 5.29  | 1.41        | 1.37     |
| 2   | A     | 2103 | C    | O3'-P   | -5.29 | 1.54        | 1.61     |
| 2   | A     | 2162 | G    | C3'-C2' | -5.29 | 1.47        | 1.52     |
| 3   | E     | 29   | C    | C1'-N1  | 5.29  | 1.56        | 1.48     |
| 2   | A     | 1866 | A    | C3'-O3' | 5.29  | 1.49        | 1.42     |
| 3   | E     | 77   | A    | C4'-C3' | 5.28  | 1.58        | 1.53     |
| 2   | A     | 2105 | U    | C3'-C2' | 5.27  | 1.58        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | D     | 231  | GLU  | CG-CD   | -5.27 | 1.44        | 1.51     |
| 3   | E     | 62   | C    | N1-C6   | 5.27  | 1.40        | 1.37     |
| 2   | A     | 1898 | U    | C2'-C1' | 5.27  | 1.59        | 1.53     |
| 3   | E     | 10   | G    | C2'-C1' | -5.27 | 1.47        | 1.53     |
| 2   | A     | 2106 | U    | C5'-C4' | 5.26  | 1.57        | 1.51     |
| 1   | B     | 1332 | A    | N7-C5   | -5.26 | 1.36        | 1.39     |
| 2   | A     | 2160 | C    | C3'-C2' | 5.26  | 1.58        | 1.52     |
| 3   | E     | 44   | A    | N7-C5   | -5.26 | 1.36        | 1.39     |
| 2   | A     | 1886 | U    | C2-N3   | -5.25 | 1.34        | 1.37     |
| 2   | A     | 1840 | G    | C1'-N9  | -5.24 | 1.39        | 1.46     |
| 2   | A     | 1873 | G    | N3-C4   | 5.24  | 1.39        | 1.35     |
| 3   | E     | 32   | G    | C4'-O4' | 5.23  | 1.52        | 1.45     |
| 2   | A     | 2141 | G    | C3'-O3' | 5.23  | 1.49        | 1.42     |
| 2   | A     | 1834 | U    | C3'-C2' | 5.23  | 1.58        | 1.52     |
| 4   | D     | 56   | ASP  | CA-CB   | 5.23  | 1.65        | 1.53     |
| 2   | A     | 1865 | U    | C5-C6   | -5.23 | 1.29        | 1.34     |
| 2   | A     | 2152 | G    | C8-N7   | -5.22 | 1.27        | 1.30     |
| 3   | E     | 21   | U    | N1-C2   | -5.22 | 1.33        | 1.38     |
| 3   | E     | 51   | U    | C3'-O3' | 5.22  | 1.49        | 1.42     |
| 2   | A     | 2146 | C    | N1-C6   | 5.22  | 1.40        | 1.37     |
| 3   | E     | 20   | G    | C2'-C1' | -5.21 | 1.47        | 1.53     |
| 2   | A     | 1858 | A    | N9-C8   | -5.21 | 1.33        | 1.37     |
| 2   | A     | 2112 | G    | C3'-C2' | -5.21 | 1.47        | 1.52     |
| 3   | E     | 66   | C    | C4-C5   | 5.21  | 1.47        | 1.43     |
| 8   | I     | 128  | GLU  | CD-OE1  | 5.21  | 1.31        | 1.25     |
| 2   | A     | 2128 | G    | N3-C4   | 5.20  | 1.39        | 1.35     |
| 3   | E     | 58   | A    | N9-C4   | -5.19 | 1.34        | 1.37     |
| 1   | B     | 1240 | U    | C3'-C2' | 5.19  | 1.58        | 1.52     |
| 2   | A     | 1883 | U    | C2'-C1' | -5.19 | 1.47        | 1.53     |
| 2   | A     | 1838 | C    | C2'-C1' | -5.19 | 1.47        | 1.53     |
| 3   | E     | 53   | G    | C6-O6   | -5.19 | 1.19        | 1.24     |
| 2   | A     | 1866 | A    | C4'-C3' | -5.19 | 1.47        | 1.52     |
| 1   | B     | 1298 | U    | P-O5'   | -5.19 | 1.54        | 1.59     |
| 2   | A     | 1904 | G    | C5'-C4' | 5.19  | 1.57        | 1.51     |
| 3   | E     | 46   | G    | N3-C4   | -5.19 | 1.31        | 1.35     |
| 2   | A     | 2138 | G    | C2-N2   | -5.18 | 1.29        | 1.34     |
| 2   | A     | 1876 | A    | N1-C2   | 5.18  | 1.39        | 1.34     |
| 2   | A     | 2163 | A    | C4'-O4' | 5.18  | 1.52        | 1.45     |
| 3   | E     | 66   | C    | C3'-C2' | -5.18 | 1.47        | 1.52     |
| 3   | E     | 6    | G    | C3'-O3' | 5.18  | 1.49        | 1.42     |
| 3   | E     | 23   | G    | C2-N3   | -5.17 | 1.28        | 1.32     |
| 2   | A     | 2107 | G    | C2-N2   | -5.17 | 1.29        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | B     | 1334 | G    | N9-C8   | 5.17  | 1.41        | 1.37     |
| 3   | E     | 16   | C    | C2'-C1' | -5.16 | 1.47        | 1.53     |
| 2   | A     | 2176 | A    | O3'-P   | -5.16 | 1.54        | 1.61     |
| 2   | A     | 2166 | U    | C4'-C3' | 5.16  | 1.58        | 1.53     |
| 2   | A     | 2123 | G    | C4'-C3' | 5.16  | 1.58        | 1.53     |
| 2   | A     | 1901 | A    | N3-C4   | -5.15 | 1.31        | 1.34     |
| 2   | A     | 2188 | U    | C3'-O3' | 5.14  | 1.49        | 1.42     |
| 2   | A     | 2186 | G    | N9-C4   | 5.14  | 1.42        | 1.38     |
| 2   | A     | 2119 | A    | N1-C2   | 5.14  | 1.39        | 1.34     |
| 2   | A     | 2157 | G    | N7-C5   | 5.13  | 1.42        | 1.39     |
| 2   | A     | 2191 | A    | C5'-C4' | 5.13  | 1.57        | 1.51     |
| 2   | A     | 2193 | G    | C3'-O3' | 5.13  | 1.49        | 1.42     |
| 2   | A     | 2173 | A    | N1-C2   | 5.12  | 1.39        | 1.34     |
| 3   | E     | 44   | A    | N9-C4   | -5.12 | 1.34        | 1.37     |
| 3   | E     | 77   | A    | C2-N3   | -5.12 | 1.28        | 1.33     |
| 2   | A     | 1860 | G    | N9-C4   | 5.12  | 1.42        | 1.38     |
| 2   | A     | 2096 | C    | C4-C5   | -5.12 | 1.38        | 1.43     |
| 2   | A     | 1837 | C    | C5-C6   | -5.11 | 1.30        | 1.34     |
| 2   | A     | 2129 | C    | C4'-C3' | 5.11  | 1.58        | 1.53     |
| 2   | A     | 2158 | A    | C5-C6   | -5.11 | 1.36        | 1.41     |
| 1   | B     | 1236 | A    | N7-C5   | -5.10 | 1.36        | 1.39     |
| 2   | A     | 1853 | A    | O3'-P   | -5.10 | 1.55        | 1.61     |
| 2   | A     | 2148 | G    | N9-C4   | 5.10  | 1.42        | 1.38     |
| 4   | D     | 73   | TYR  | CZ-OH   | 5.10  | 1.46        | 1.37     |
| 4   | D     | 127  | ARG  | CD-NE   | 5.10  | 1.55        | 1.46     |
| 2   | A     | 1895 | C    | N3-C4   | 5.09  | 1.37        | 1.33     |
| 2   | A     | 1903 | G    | C2-N2   | -5.09 | 1.29        | 1.34     |
| 2   | A     | 2182 | U    | C4'-O4' | -5.09 | 1.39        | 1.45     |
| 3   | E     | 33   | C    | C5'-C4' | 5.09  | 1.57        | 1.51     |
| 4   | D     | 370  | SER  | CB-OG   | 5.09  | 1.48        | 1.42     |
| 3   | E     | 51   | U    | C2-N3   | -5.09 | 1.34        | 1.37     |
| 2   | A     | 2125 | G    | C5'-C4' | -5.08 | 1.45        | 1.51     |
| 3   | E     | 19   | G    | O3'-P   | -5.08 | 1.55        | 1.61     |
| 3   | E     | 45   | A    | C6-N6   | 5.08  | 1.38        | 1.33     |
| 1   | B     | 1289 | A    | C5-C6   | 5.07  | 1.45        | 1.41     |
| 1   | B     | 1244 | G    | P-O5'   | -5.07 | 1.54        | 1.59     |
| 2   | A     | 1872 | A    | C6-N1   | 5.07  | 1.39        | 1.35     |
| 2   | A     | 2104 | C    | N3-C4   | -5.07 | 1.30        | 1.33     |
| 1   | B     | 1244 | G    | C2-N3   | 5.06  | 1.36        | 1.32     |
| 2   | A     | 2171 | A    | C4'-C3' | 5.06  | 1.58        | 1.53     |
| 2   | A     | 1849 | G    | C2'-C1' | -5.06 | 1.47        | 1.53     |
| 2   | A     | 2159 | G    | C1'-N9  | 5.06  | 1.56        | 1.48     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | F     | 96   | GLY  | N-CA    | 5.06  | 1.53        | 1.46     |
| 3   | E     | 58   | A    | N3-C4   | -5.05 | 1.31        | 1.34     |
| 2   | A     | 2162 | G    | C6-N1   | 5.05  | 1.43        | 1.39     |
| 2   | A     | 1893 | C    | C2-N3   | 5.05  | 1.39        | 1.35     |
| 2   | A     | 2105 | U    | N1-C2   | -5.05 | 1.34        | 1.38     |
| 3   | E     | 5    | G    | N3-C4   | 5.05  | 1.39        | 1.35     |
| 3   | E     | 72   | C    | C5'-C4' | -5.05 | 1.45        | 1.51     |
| 6   | G     | 160  | LYS  | N-CA    | -5.05 | 1.36        | 1.46     |
| 2   | A     | 1891 | G    | N3-C4   | 5.04  | 1.39        | 1.35     |
| 2   | A     | 1869 | G    | C2-N2   | -5.04 | 1.29        | 1.34     |
| 3   | E     | 36   | A    | N9-C8   | 5.04  | 1.41        | 1.37     |
| 4   | D     | 514  | TYR  | CG-CD2  | 5.04  | 1.45        | 1.39     |
| 3   | E     | 17   | C    | N1-C2   | 5.04  | 1.45        | 1.40     |
| 3   | E     | 40   | C    | C3'-C2' | 5.04  | 1.58        | 1.52     |
| 2   | A     | 1901 | A    | N9-C8   | -5.03 | 1.33        | 1.37     |
| 3   | E     | 42   | C    | C4-N4   | 5.03  | 1.38        | 1.33     |
| 6   | G     | 132  | ARG  | CD-NE   | 5.03  | 1.54        | 1.46     |
| 3   | E     | 26   | C    | C3'-O3' | 5.03  | 1.49        | 1.42     |
| 2   | A     | 2149 | U    | O3'-P   | -5.03 | 1.55        | 1.61     |
| 3   | E     | 22   | A    | N1-C2   | 5.03  | 1.38        | 1.34     |
| 2   | A     | 2178 | C    | C2-N3   | 5.02  | 1.39        | 1.35     |
| 3   | E     | 8    | U    | C3'-O3' | 5.02  | 1.49        | 1.42     |
| 4   | D     | 64   | ARG  | CD-NE   | 5.02  | 1.54        | 1.46     |
| 5   | F     | 53   | ARG  | CD-NE   | 5.02  | 1.54        | 1.46     |
| 8   | I     | 44   | SER  | CA-CB   | 5.02  | 1.60        | 1.52     |
| 1   | B     | 1302 | C    | C4-C5   | -5.02 | 1.39        | 1.43     |
| 1   | B     | 1299 | A    | C1'-N9  | 5.02  | 1.56        | 1.48     |
| 2   | A     | 2138 | G    | C2-N3   | 5.01  | 1.36        | 1.32     |
| 3   | E     | 7    | G    | N7-C5   | 5.01  | 1.42        | 1.39     |
| 2   | A     | 2126 | A    | C8-N7   | -5.01 | 1.28        | 1.31     |
| 4   | D     | 46   | SER  | CA-CB   | 5.01  | 1.60        | 1.52     |
| 2   | A     | 2100 | G    | C2-N2   | -5.01 | 1.29        | 1.34     |
| 7   | H     | 48   | TYR  | N-CA    | -5.01 | 1.36        | 1.46     |
| 3   | E     | 45   | A    | C2'-C1' | -5.00 | 1.47        | 1.53     |
| 2   | A     | 2165 | C    | C5'-C4' | 5.00  | 1.57        | 1.51     |
| 3   | E     | 40   | C    | C2'-C1' | -5.00 | 1.47        | 1.53     |

All (1480) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 8   | I     | 91  | ARG  | NE-CZ-NH2 | -25.82 | 107.39      | 120.30   |
| 4   | D     | 430 | ARG  | NE-CZ-NH1 | 23.11  | 131.85      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | B     | 1236 | A    | N1-C6-N6   | 19.82  | 130.49      | 118.60   |
| 1   | B     | 1334 | G    | C5-C6-O6   | -18.89 | 117.27      | 128.60   |
| 1   | B     | 1334 | G    | N1-C6-O6   | 17.55  | 130.43      | 119.90   |
| 2   | A     | 1871 | A    | P-O3'-C3'  | 17.40  | 140.58      | 119.70   |
| 3   | E     | 20   | G    | C5-C6-O6   | -16.97 | 118.42      | 128.60   |
| 2   | A     | 2123 | G    | C5-C6-O6   | -16.71 | 118.57      | 128.60   |
| 8   | I     | 137  | ARG  | NE-CZ-NH1  | 16.70  | 128.65      | 120.30   |
| 3   | E     | 20   | G    | N1-C6-O6   | 16.07  | 129.54      | 119.90   |
| 8   | I     | 43   | TYR  | CB-CG-CD1  | 15.88  | 130.53      | 121.00   |
| 8   | I     | 95   | ARG  | NE-CZ-NH1  | 15.41  | 128.00      | 120.30   |
| 3   | E     | 59   | A    | N9-C4-C5   | 15.24  | 111.89      | 105.80   |
| 3   | E     | 10   | G    | C5-C6-O6   | -15.12 | 119.53      | 128.60   |
| 4   | D     | 283  | ARG  | NE-CZ-NH1  | 14.93  | 127.77      | 120.30   |
| 2   | A     | 1903 | G    | N1-C6-O6   | 14.91  | 128.85      | 119.90   |
| 2   | A     | 1904 | G    | C5-C6-O6   | -14.80 | 119.72      | 128.60   |
| 2   | A     | 2103 | C    | N3-C4-C5   | 14.69  | 127.78      | 121.90   |
| 3   | E     | 10   | G    | N1-C6-O6   | 14.60  | 128.66      | 119.90   |
| 2   | A     | 2158 | A    | P-O3'-C3'  | 14.51  | 137.11      | 119.70   |
| 6   | G     | 94   | ARG  | NE-CZ-NH2  | -14.35 | 113.12      | 120.30   |
| 2   | A     | 1869 | G    | C5-C6-O6   | -14.28 | 120.03      | 128.60   |
| 3   | E     | 2    | G    | N1-C6-O6   | 14.27  | 128.46      | 119.90   |
| 4   | D     | 168  | ARG  | NE-CZ-NH1  | 14.24  | 127.42      | 120.30   |
| 2   | A     | 1860 | G    | C5-C6-O6   | -13.94 | 120.24      | 128.60   |
| 4   | D     | 19   | ARG  | NE-CZ-NH2  | -13.92 | 113.34      | 120.30   |
| 4   | D     | 87   | ARG  | NE-CZ-NH1  | 13.86  | 127.23      | 120.30   |
| 4   | D     | 108  | TYR  | CB-CG-CD2  | -13.78 | 112.73      | 121.00   |
| 4   | D     | 152  | ARG  | NE-CZ-NH2  | -13.62 | 113.49      | 120.30   |
| 2   | A     | 1906 | G    | N1-C6-O6   | 13.56  | 128.04      | 119.90   |
| 2   | A     | 2153 | C    | C6-N1-C2   | -13.54 | 114.88      | 120.30   |
| 4   | D     | 481  | ARG  | NE-CZ-NH1  | 13.53  | 127.06      | 120.30   |
| 2   | A     | 2175 | C    | C6-N1-C2   | -13.48 | 114.91      | 120.30   |
| 2   | A     | 2118 | U    | N1-C2-O2   | 13.47  | 132.23      | 122.80   |
| 3   | E     | 30   | G    | C4-C5-N7   | 13.44  | 116.18      | 110.80   |
| 3   | E     | 57   | C    | C6-N1-C2   | -13.44 | 114.92      | 120.30   |
| 3   | E     | 3    | C    | C6-N1-C2   | -13.42 | 114.93      | 120.30   |
| 8   | I     | 52   | ARG  | NE-CZ-NH1  | 13.41  | 127.00      | 120.30   |
| 8   | I     | 4    | ARG  | NE-CZ-NH2  | -13.34 | 113.63      | 120.30   |
| 2   | A     | 1891 | G    | C2-N3-C4   | -13.22 | 105.29      | 111.90   |
| 2   | A     | 1892 | C    | O4'-C1'-N1 | 13.21  | 118.77      | 108.20   |
| 2   | A     | 2148 | G    | N1-C6-O6   | 13.13  | 127.78      | 119.90   |
| 2   | A     | 2130 | U    | C5-C6-N1   | 13.12  | 129.26      | 122.70   |
| 2   | A     | 2187 | U    | O4'-C1'-N1 | 13.06  | 118.65      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 2   | A     | 1904 | G    | N1-C6-O6   | 12.99  | 127.69      | 119.90   |
| 8   | I     | 91   | ARG  | NE-CZ-NH1  | 12.90  | 126.75      | 120.30   |
| 2   | A     | 2128 | G    | C5-C6-O6   | -12.75 | 120.95      | 128.60   |
| 3   | E     | 48   | U    | P-O3'-C3'  | 12.68  | 134.91      | 119.70   |
| 3   | E     | 65   | G    | N1-C6-O6   | 12.67  | 127.50      | 119.90   |
| 4   | D     | 395  | ARG  | NE-CZ-NH2  | -12.61 | 113.99      | 120.30   |
| 2   | A     | 1860 | G    | N1-C6-O6   | 12.54  | 127.42      | 119.90   |
| 1   | B     | 1241 | G    | N1-C6-O6   | 12.31  | 127.28      | 119.90   |
| 1   | B     | 1236 | A    | C5-C6-N6   | -12.27 | 113.88      | 123.70   |
| 2   | A     | 2169 | A    | O4'-C1'-N9 | 12.20  | 117.96      | 108.20   |
| 2   | A     | 2109 | U    | O4'-C1'-N1 | 12.08  | 117.86      | 108.20   |
| 3   | E     | 52   | C    | N3-C4-N4   | -11.98 | 109.61      | 118.00   |
| 4   | D     | 152  | ARG  | NE-CZ-NH1  | 11.97  | 126.28      | 120.30   |
| 1   | B     | 1290 | G    | O4'-C1'-N9 | 11.81  | 117.65      | 108.20   |
| 3   | E     | 64   | G    | N1-C6-O6   | -11.77 | 112.84      | 119.90   |
| 2   | A     | 2110 | G    | C4-C5-N7   | 11.76  | 115.50      | 110.80   |
| 2   | A     | 2110 | G    | C5-C6-N1   | 11.76  | 117.38      | 111.50   |
| 6   | G     | 91   | ARG  | NE-CZ-NH1  | -11.75 | 114.42      | 120.30   |
| 1   | B     | 1333 | A    | N9-C4-C5   | 11.69  | 110.47      | 105.80   |
| 2   | A     | 2102 | G    | N1-C6-O6   | 11.68  | 126.91      | 119.90   |
| 3   | E     | 17   | C    | C6-N1-C2   | -11.63 | 115.65      | 120.30   |
| 8   | I     | 137  | ARG  | NE-CZ-NH2  | -11.63 | 114.49      | 120.30   |
| 1   | B     | 1238 | A    | N1-C6-N6   | -11.57 | 111.66      | 118.60   |
| 2   | A     | 1874 | C    | O4'-C1'-N1 | 11.55  | 117.44      | 108.20   |
| 3   | E     | 32   | G    | N1-C6-O6   | 11.46  | 126.77      | 119.90   |
| 2   | A     | 2107 | G    | C6-N1-C2   | -11.44 | 118.23      | 125.10   |
| 2   | A     | 2135 | A    | N1-C6-N6   | -11.39 | 111.77      | 118.60   |
| 3   | E     | 22   | A    | C8-N9-C4   | 11.36  | 110.35      | 105.80   |
| 2   | A     | 2177 | C    | O4'-C1'-N1 | 11.36  | 117.28      | 108.20   |
| 3   | E     | 69   | C    | C6-N1-C2   | -11.34 | 115.76      | 120.30   |
| 1   | B     | 1290 | G    | C4-C5-N7   | -11.32 | 106.27      | 110.80   |
| 2   | A     | 2164 | C    | N3-C4-C5   | 11.32  | 126.43      | 121.90   |
| 3   | E     | 41   | C    | C6-N1-C2   | -11.19 | 115.83      | 120.30   |
| 2   | A     | 1907 | G    | N1-C6-O6   | -11.15 | 113.21      | 119.90   |
| 2   | A     | 2178 | C    | P-O3'-C3'  | 11.15  | 133.08      | 119.70   |
| 4   | D     | 506  | ARG  | NE-CZ-NH2  | -11.11 | 114.75      | 120.30   |
| 3   | E     | 49   | C    | C5-C6-N1   | 11.06  | 126.53      | 121.00   |
| 6   | G     | 29   | ARG  | NE-CZ-NH1  | 11.02  | 125.81      | 120.30   |
| 4   | D     | 175  | ARG  | NE-CZ-NH2  | -10.94 | 114.83      | 120.30   |
| 3   | E     | 38   | A    | C4-C5-N7   | -10.89 | 105.25      | 110.70   |
| 1   | B     | 1302 | C    | C6-N1-C2   | -10.89 | 115.94      | 120.30   |
| 2   | A     | 2101 | A    | N1-C6-N6   | 10.87  | 125.12      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 2   | A     | 2120 | G    | C5-C6-O6    | -10.87 | 122.08      | 128.60   |
| 2   | A     | 1906 | G    | C5-C6-O6    | -10.86 | 122.08      | 128.60   |
| 2   | A     | 2115 | G    | O4'-C1'-N9  | 10.86  | 116.89      | 108.20   |
| 2   | A     | 1843 | C    | O4'-C1'-N1  | 10.82  | 116.86      | 108.20   |
| 5   | F     | 7    | ARG  | NE-CZ-NH2   | -10.81 | 114.89      | 120.30   |
| 4   | D     | 530  | TYR  | CB-CG-CD2   | -10.81 | 114.52      | 121.00   |
| 2   | A     | 2094 | A    | C8-N9-C4    | 10.80  | 110.12      | 105.80   |
| 6   | G     | 109  | ARG  | NE-CZ-NH1   | -10.79 | 114.91      | 120.30   |
| 3   | E     | 65   | G    | C5-C6-O6    | -10.77 | 122.14      | 128.60   |
| 2   | A     | 1861 | G    | C5-C6-O6    | -10.75 | 122.15      | 128.60   |
| 3   | E     | 43   | G    | C5-C6-O6    | 10.75  | 135.05      | 128.60   |
| 2   | A     | 1860 | G    | O4'-C1'-N9  | 10.74  | 116.79      | 108.20   |
| 2   | A     | 2120 | G    | N3-C4-C5    | -10.72 | 123.24      | 128.60   |
| 2   | A     | 1850 | G    | N7-C8-N9    | -10.71 | 107.74      | 113.10   |
| 5   | F     | 9    | ARG  | NE-CZ-NH1   | 10.69  | 125.64      | 120.30   |
| 2   | A     | 2101 | A    | N9-C4-C5    | -10.68 | 101.53      | 105.80   |
| 1   | B     | 1294 | G    | N1-C6-O6    | 10.68  | 126.31      | 119.90   |
| 4   | D     | 108  | TYR  | CB-CG-CD1   | 10.65  | 127.39      | 121.00   |
| 1   | B     | 1333 | A    | C4-C5-N7    | -10.64 | 105.38      | 110.70   |
| 2   | A     | 2110 | G    | C5-N7-C8    | -10.62 | 98.99       | 104.30   |
| 2   | A     | 1901 | A    | N1-C6-N6    | -10.62 | 112.23      | 118.60   |
| 6   | G     | 94   | ARG  | NE-CZ-NH1   | 10.58  | 125.59      | 120.30   |
| 4   | D     | 506  | ARG  | NE-CZ-NH1   | 10.58  | 125.59      | 120.30   |
| 3   | E     | 10   | G    | N7-C8-N9    | -10.54 | 107.83      | 113.10   |
| 2   | A     | 2165 | C    | O4'-C1'-N1  | 10.54  | 116.63      | 108.20   |
| 4   | D     | 514  | TYR  | CB-CG-CD2   | -10.54 | 114.68      | 121.00   |
| 2   | A     | 2126 | A    | N1-C6-N6    | 10.50  | 124.90      | 118.60   |
| 4   | D     | 522  | PHE  | CB-CG-CD2   | -10.48 | 113.47      | 120.80   |
| 2   | A     | 1873 | G    | N9-C4-C5    | -10.46 | 101.22      | 105.40   |
| 3   | E     | 27   | G    | N1-C6-O6    | 10.43  | 126.16      | 119.90   |
| 2   | A     | 2103 | C    | C2-N3-C4    | -10.42 | 114.69      | 119.90   |
| 5   | F     | 53   | ARG  | NE-CZ-NH2   | -10.39 | 115.11      | 120.30   |
| 2   | A     | 2183 | A    | O4'-C1'-N9  | 10.39  | 116.51      | 108.20   |
| 3   | E     | 35   | C    | C1'-O4'-C4' | 10.35  | 118.18      | 109.90   |
| 2   | A     | 2110 | G    | C4-C5-C6    | -10.32 | 112.61      | 118.80   |
| 2   | A     | 2153 | C    | O4'-C1'-N1  | 10.29  | 116.43      | 108.20   |
| 2   | A     | 2095 | A    | C5-C6-N1    | -10.28 | 112.56      | 117.70   |
| 3   | E     | 68   | C    | N3-C4-C5    | -10.24 | 117.81      | 121.90   |
| 2   | A     | 2123 | G    | C5-C6-N1    | 10.21  | 116.61      | 111.50   |
| 2   | A     | 2169 | A    | C5-C6-N1    | 10.20  | 122.80      | 117.70   |
| 8   | I     | 77   | ARG  | NE-CZ-NH1   | 10.19  | 125.40      | 120.30   |
| 8   | I     | 110  | ARG  | NE-CZ-NH2   | 10.19  | 125.40      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 2   | A     | 1881 | C    | O4'-C1'-N1 | 10.16  | 116.33      | 108.20   |
| 3   | E     | 44   | A    | O4'-C1'-N9 | 10.16  | 116.33      | 108.20   |
| 4   | D     | 395  | ARG  | NE-CZ-NH1  | 10.14  | 125.37      | 120.30   |
| 5   | F     | 180  | PHE  | CB-CG-CD2  | -10.14 | 113.70      | 120.80   |
| 2   | A     | 1877 | A    | C5-C6-N1   | -10.10 | 112.65      | 117.70   |
| 2   | A     | 2190 | G    | O4'-C1'-N9 | 10.08  | 116.27      | 108.20   |
| 2   | A     | 1851 | U    | O4'-C1'-N1 | 10.08  | 116.26      | 108.20   |
| 3   | E     | 2    | G    | C8-N9-C4   | 10.08  | 110.43      | 106.40   |
| 2   | A     | 2122 | U    | O4'-C1'-N1 | 10.07  | 116.25      | 108.20   |
| 1   | B     | 1297 | G    | N1-C6-O6   | 10.06  | 125.94      | 119.90   |
| 2   | A     | 2164 | C    | C4-C5-C6   | -10.04 | 112.38      | 117.40   |
| 2   | A     | 2181 | U    | O4'-C1'-N1 | 10.02  | 116.22      | 108.20   |
| 1   | B     | 1292 | G    | N9-C4-C5   | -10.02 | 101.39      | 105.40   |
| 2   | A     | 2139 | U    | O4'-C1'-N1 | 10.01  | 116.21      | 108.20   |
| 3   | E     | 25   | U    | N3-C4-O4   | 10.01  | 126.41      | 119.40   |
| 2   | A     | 2157 | G    | P-O3'-C3'  | 9.99   | 131.69      | 119.70   |
| 3   | E     | 16   | C    | C6-N1-C2   | 9.99   | 124.30      | 120.30   |
| 2   | A     | 1906 | G    | C2-N3-C4   | 9.89   | 116.85      | 111.90   |
| 1   | B     | 1297 | G    | C6-C5-N7   | -9.85  | 124.49      | 130.40   |
| 3   | E     | 69   | C    | C5-C6-N1   | 9.85   | 125.92      | 121.00   |
| 2   | A     | 2128 | G    | O4'-C1'-N9 | 9.84   | 116.08      | 108.20   |
| 2   | A     | 2190 | G    | C5-C6-O6   | -9.84  | 122.70      | 128.60   |
| 3   | E     | 77   | A    | C8-N9-C4   | -9.83  | 101.87      | 105.80   |
| 1   | B     | 1333 | A    | C2-N3-C4   | 9.80   | 115.50      | 110.60   |
| 4   | D     | 50   | ARG  | NE-CZ-NH1  | 9.79   | 125.19      | 120.30   |
| 4   | D     | 254  | ARG  | NE-CZ-NH1  | 9.77   | 125.19      | 120.30   |
| 2   | A     | 2144 | G    | N3-C2-N2   | -9.76  | 113.07      | 119.90   |
| 3   | E     | 3    | C    | C5-C6-N1   | 9.75   | 125.88      | 121.00   |
| 4   | D     | 219  | ARG  | NE-CZ-NH2  | 9.75   | 125.18      | 120.30   |
| 1   | B     | 1298 | U    | C5-C4-O4   | -9.74  | 120.05      | 125.90   |
| 7   | H     | 19   | PHE  | CB-CG-CD2  | 9.73   | 127.61      | 120.80   |
| 2   | A     | 1860 | G    | N3-C2-N2   | 9.73   | 126.71      | 119.90   |
| 8   | I     | 4    | ARG  | NE-CZ-NH1  | 9.73   | 125.16      | 120.30   |
| 3   | E     | 7    | G    | N1-C6-O6   | 9.72   | 125.73      | 119.90   |
| 4   | D     | 234  | ARG  | NE-CZ-NH1  | 9.72   | 125.16      | 120.30   |
| 2   | A     | 1844 | C    | N3-C4-C5   | 9.72   | 125.79      | 121.90   |
| 3   | E     | 2    | G    | C5-C6-O6   | -9.70  | 122.78      | 128.60   |
| 2   | A     | 1844 | C    | C4-C5-C6   | -9.68  | 112.56      | 117.40   |
| 2   | A     | 1903 | G    | C5-C6-O6   | -9.68  | 122.79      | 128.60   |
| 2   | A     | 2144 | G    | N1-C6-O6   | 9.67   | 125.70      | 119.90   |
| 3   | E     | 72   | C    | N3-C4-C5   | -9.67  | 118.03      | 121.90   |
| 2   | A     | 1887 | C    | C5-C6-N1   | -9.66  | 116.17      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | B     | 1242 | G    | N3-C4-C5    | 9.66  | 133.43      | 128.60   |
| 1   | B     | 1304 | G    | C5-C6-O6    | -9.61 | 122.83      | 128.60   |
| 2   | A     | 2154 | A    | N1-C6-N6    | -9.57 | 112.86      | 118.60   |
| 2   | A     | 2136 | G    | N9-C4-C5    | 9.56  | 109.22      | 105.40   |
| 4   | D     | 6    | TYR  | CB-CG-CD2   | 9.56  | 126.73      | 121.00   |
| 3   | E     | 42   | C    | O4'-C1'-N1  | 9.54  | 115.83      | 108.20   |
| 7   | H     | 43   | ARG  | NE-CZ-NH2   | 9.54  | 125.07      | 120.30   |
| 3   | E     | 23   | G    | N3-C4-C5    | 9.54  | 133.37      | 128.60   |
| 2   | A     | 2179 | C    | O4'-C1'-N1  | 9.53  | 115.82      | 108.20   |
| 2   | A     | 2191 | A    | C5-N7-C8    | -9.52 | 99.14       | 103.90   |
| 4   | D     | 136  | ASP  | CB-CG-OD1   | 9.52  | 126.87      | 118.30   |
| 2   | A     | 1872 | A    | N1-C2-N3    | 9.51  | 134.05      | 129.30   |
| 2   | A     | 2136 | G    | C8-N9-C4    | -9.50 | 102.60      | 106.40   |
| 3   | E     | 1    | C    | C4-C5-C6    | 9.49  | 122.15      | 117.40   |
| 2   | A     | 2095 | A    | C8-N9-C4    | -9.48 | 102.01      | 105.80   |
| 2   | A     | 2167 | U    | P-O5'-C5'   | 9.47  | 136.06      | 120.90   |
| 2   | A     | 1884 | G    | O4'-C1'-N9  | 9.47  | 115.78      | 108.20   |
| 2   | A     | 2180 | U    | O4'-C1'-N1  | 9.46  | 115.77      | 108.20   |
| 4   | D     | 425  | ARG  | NE-CZ-NH2   | -9.46 | 115.57      | 120.30   |
| 2   | A     | 2112 | G    | O4'-C1'-N9  | 9.45  | 115.76      | 108.20   |
| 3   | E     | 30   | G    | C5-N7-C8    | -9.45 | 99.58       | 104.30   |
| 2   | A     | 2167 | U    | O4'-C1'-N1  | 9.44  | 115.75      | 108.20   |
| 2   | A     | 2110 | G    | P-O3'-C3'   | 9.44  | 131.03      | 119.70   |
| 4   | D     | 136  | ASP  | CB-CG-OD2   | -9.44 | 109.81      | 118.30   |
| 3   | E     | 17   | C    | C2-N1-C1'   | 9.44  | 129.18      | 118.80   |
| 1   | B     | 1245 | C    | O4'-C1'-N1  | 9.43  | 115.74      | 108.20   |
| 2   | A     | 2144 | G    | C5-C6-O6    | -9.42 | 122.95      | 128.60   |
| 3   | E     | 77   | A    | N9-C4-C5    | 9.41  | 109.57      | 105.80   |
| 1   | B     | 1292 | G    | O4'-C1'-N9  | 9.39  | 115.71      | 108.20   |
| 2   | A     | 2180 | U    | C5-C6-N1    | -9.38 | 118.01      | 122.70   |
| 6   | G     | 173  | ASP  | CB-CG-OD2   | 9.38  | 126.74      | 118.30   |
| 3   | E     | 64   | G    | C5-C6-O6    | 9.37  | 134.22      | 128.60   |
| 8   | I     | 9    | ARG  | NE-CZ-NH2   | -9.36 | 115.62      | 120.30   |
| 2   | A     | 2126 | A    | N1-C2-N3    | -9.35 | 124.62      | 129.30   |
| 2   | A     | 2148 | G    | C5-C6-O6    | -9.35 | 122.99      | 128.60   |
| 2   | A     | 2152 | G    | P-O3'-C3'   | 9.34  | 130.91      | 119.70   |
| 3   | E     | 11   | A    | C2-N3-C4    | -9.33 | 105.93      | 110.60   |
| 2   | A     | 2137 | U    | N3-C4-C5    | -9.33 | 109.00      | 114.60   |
| 2   | A     | 2105 | U    | C4'-C3'-C2' | -9.33 | 93.27       | 102.60   |
| 2   | A     | 2097 | A    | C8-N9-C4    | -9.33 | 102.07      | 105.80   |
| 2   | A     | 2116 | G    | C5-C6-N1    | -9.32 | 106.84      | 111.50   |
| 2   | A     | 1861 | G    | N1-C6-O6    | 9.32  | 125.49      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 2    | G    | C6-N1-C2    | 9.31  | 130.69      | 125.10   |
| 4   | D     | 430  | ARG  | NE-CZ-NH2   | -9.30 | 115.65      | 120.30   |
| 3   | E     | 76   | C    | P-O3'-C3'   | 9.30  | 130.86      | 119.70   |
| 3   | E     | 56   | U    | N1-C2-N3    | 9.29  | 120.48      | 114.90   |
| 3   | E     | 70   | C    | N3-C4-C5    | 9.29  | 125.61      | 121.90   |
| 3   | E     | 63   | C    | O4'-C1'-N1  | 9.28  | 115.63      | 108.20   |
| 2   | A     | 1894 | C    | N3-C4-C5    | -9.28 | 118.19      | 121.90   |
| 3   | E     | 36   | A    | C4-C5-C6    | -9.26 | 112.37      | 117.00   |
| 2   | A     | 2133 | G    | C4-C5-N7    | 9.25  | 114.50      | 110.80   |
| 2   | A     | 1846 | G    | O4'-C1'-N9  | 9.25  | 115.60      | 108.20   |
| 2   | A     | 2124 | G    | C8-N9-C4    | 9.22  | 110.09      | 106.40   |
| 2   | A     | 2189 | U    | N3-C4-O4    | 9.19  | 125.83      | 119.40   |
| 2   | A     | 1836 | C    | C5-C6-N1    | -9.16 | 116.42      | 121.00   |
| 3   | E     | 31   | G    | C5-C6-N1    | 9.16  | 116.08      | 111.50   |
| 8   | I     | 43   | TYR  | CB-CG-CD2   | -9.15 | 115.51      | 121.00   |
| 3   | E     | 9    | G    | N1-C6-O6    | 9.12  | 125.37      | 119.90   |
| 2   | A     | 1868 | C    | C6-N1-C2    | -9.11 | 116.66      | 120.30   |
| 2   | A     | 2105 | U    | O4'-C1'-N1  | 9.11  | 115.49      | 108.20   |
| 2   | A     | 1872 | A    | P-O3'-C3'   | 9.10  | 130.62      | 119.70   |
| 3   | E     | 54   | G    | O4'-C1'-N9  | 9.05  | 115.44      | 108.20   |
| 6   | G     | 6    | TYR  | CB-CG-CD1   | 9.04  | 126.42      | 121.00   |
| 3   | E     | 59   | A    | C8-N9-C4    | -9.03 | 102.19      | 105.80   |
| 3   | E     | 58   | A    | C1'-O4'-C4' | -9.02 | 102.69      | 109.90   |
| 2   | A     | 2123 | G    | C4'-C3'-C2' | -9.01 | 93.59       | 102.60   |
| 3   | E     | 33   | C    | C5-C4-N4    | -9.00 | 113.90      | 120.20   |
| 2   | A     | 2128 | G    | N1-C6-O6    | 8.99  | 125.29      | 119.90   |
| 5   | F     | 75   | VAL  | CG1-CB-CG2  | -8.95 | 96.59       | 110.90   |
| 3   | E     | 9    | G    | O4'-C1'-N9  | 8.94  | 115.35      | 108.20   |
| 1   | B     | 1294 | G    | C5-C6-O6    | -8.94 | 123.24      | 128.60   |
| 3   | E     | 22   | A    | N9-C4-C5    | -8.92 | 102.23      | 105.80   |
| 2   | A     | 2150 | C    | C6-N1-C2    | -8.90 | 116.74      | 120.30   |
| 3   | E     | 74   | A    | N1-C6-N6    | -8.89 | 113.26      | 118.60   |
| 2   | A     | 2160 | C    | C6-N1-C1'   | -8.88 | 110.14      | 120.80   |
| 3   | E     | 72   | C    | C4-C5-C6    | 8.88  | 121.84      | 117.40   |
| 2   | A     | 2178 | C    | O4'-C1'-N1  | 8.88  | 115.30      | 108.20   |
| 3   | E     | 47   | G    | C4'-C3'-C2' | -8.87 | 93.73       | 102.60   |
| 2   | A     | 2157 | G    | C2'-C3'-O3' | 8.87  | 129.01      | 109.50   |
| 2   | A     | 2106 | U    | C5-C6-N1    | 8.87  | 127.13      | 122.70   |
| 3   | E     | 17   | C    | O4'-C1'-N1  | 8.85  | 115.28      | 108.20   |
| 3   | E     | 69   | C    | N3-C4-C5    | -8.85 | 118.36      | 121.90   |
| 6   | G     | 91   | ARG  | NE-CZ-NH2   | 8.85  | 124.72      | 120.30   |
| 2   | A     | 2101 | A    | C8-N9-C4    | 8.84  | 109.34      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | B     | 1332 | A    | C8-N9-C4    | -8.81 | 102.28      | 105.80   |
| 2   | A     | 2156 | G    | N1-C6-O6    | 8.81  | 125.19      | 119.90   |
| 8   | I     | 101  | ARG  | NE-CZ-NH2   | -8.80 | 115.90      | 120.30   |
| 3   | E     | 6    | G    | N3-C4-C5    | 8.79  | 133.00      | 128.60   |
| 2   | A     | 2132 | U    | N3-C4-O4    | 8.77  | 125.54      | 119.40   |
| 2   | A     | 1848 | A    | C5-C6-N1    | -8.74 | 113.33      | 117.70   |
| 3   | E     | 23   | G    | O4'-C1'-N9  | 8.72  | 115.17      | 108.20   |
| 2   | A     | 2172 | U    | N3-C4-O4    | 8.70  | 125.49      | 119.40   |
| 2   | A     | 1901 | A    | C5-C6-N6    | 8.68  | 130.64      | 123.70   |
| 6   | G     | 109  | ARG  | NE-CZ-NH2   | 8.67  | 124.63      | 120.30   |
| 3   | E     | 66   | C    | N3-C4-C5    | -8.65 | 118.44      | 121.90   |
| 2   | A     | 2163 | A    | N1-C2-N3    | 8.65  | 133.62      | 129.30   |
| 2   | A     | 2183 | A    | C4-C5-N7    | -8.65 | 106.38      | 110.70   |
| 3   | E     | 34   | U    | C1'-O4'-C4' | -8.64 | 102.99      | 109.90   |
| 5   | F     | 1    | MET  | CG-SD-CE    | -8.64 | 86.37       | 100.20   |
| 2   | A     | 2123 | G    | N7-C8-N9    | 8.64  | 117.42      | 113.10   |
| 3   | E     | 33   | C    | O4'-C1'-N1  | 8.62  | 115.10      | 108.20   |
| 4   | D     | 4    | PHE  | CB-CG-CD2   | 8.60  | 126.82      | 120.80   |
| 1   | B     | 1296 | C    | C5-C6-N1    | -8.60 | 116.70      | 121.00   |
| 2   | A     | 1847 | A    | N1-C6-N6    | 8.60  | 123.76      | 118.60   |
| 2   | A     | 2143 | C    | O4'-C1'-N1  | 8.59  | 115.07      | 108.20   |
| 5   | F     | 208  | TYR  | CB-CG-CD1   | -8.59 | 115.85      | 121.00   |
| 2   | A     | 2193 | G    | N1-C6-O6    | 8.58  | 125.05      | 119.90   |
| 3   | E     | 2    | G    | N7-C8-N9    | -8.57 | 108.81      | 113.10   |
| 2   | A     | 1878 | G    | C8-N9-C4    | -8.56 | 102.98      | 106.40   |
| 2   | A     | 2132 | U    | C5-C4-O4    | -8.56 | 120.77      | 125.90   |
| 3   | E     | 37   | U    | N1-C2-O2    | -8.54 | 116.82      | 122.80   |
| 2   | A     | 1891 | G    | O4'-C1'-N9  | 8.53  | 115.02      | 108.20   |
| 3   | E     | 26   | C    | N3-C4-C5    | -8.52 | 118.49      | 121.90   |
| 4   | D     | 441  | ARG  | NE-CZ-NH2   | 8.52  | 124.56      | 120.30   |
| 5   | F     | 180  | PHE  | CB-CG-CD1   | 8.49  | 126.75      | 120.80   |
| 3   | E     | 43   | G    | C8-N9-C4    | 8.48  | 109.79      | 106.40   |
| 3   | E     | 71   | G    | N3-C4-C5    | -8.48 | 124.36      | 128.60   |
| 3   | E     | 31   | G    | N1-C6-O6    | -8.46 | 114.83      | 119.90   |
| 2   | A     | 2164 | C    | P-O3'-C3'   | 8.45  | 129.84      | 119.70   |
| 6   | G     | 19   | PHE  | CB-CG-CD1   | -8.45 | 114.89      | 120.80   |
| 2   | A     | 2152 | G    | N1-C2-N3    | -8.44 | 118.84      | 123.90   |
| 3   | E     | 30   | G    | N9-C4-C5    | -8.44 | 102.03      | 105.40   |
| 2   | A     | 2103 | C    | O4'-C1'-N1  | 8.43  | 114.94      | 108.20   |
| 2   | A     | 2128 | G    | C8-N9-C4    | 8.42  | 109.77      | 106.40   |
| 3   | E     | 74   | A    | C5-C6-N1    | 8.41  | 121.91      | 117.70   |
| 1   | B     | 1289 | A    | N1-C2-N3    | -8.41 | 125.10      | 129.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | B     | 1332 | A    | N1-C6-N6    | 8.41  | 123.64      | 118.60   |
| 3   | E     | 58   | A    | O4'-C1'-N9  | 8.41  | 114.93      | 108.20   |
| 2   | A     | 2109 | U    | C5'-C4'-O4' | 8.40  | 119.19      | 109.10   |
| 2   | A     | 2186 | G    | C2-N3-C4    | -8.38 | 107.71      | 111.90   |
| 3   | E     | 70   | C    | O4'-C1'-N1  | 8.38  | 114.91      | 108.20   |
| 2   | A     | 1899 | A    | C5-N7-C8    | -8.38 | 99.71       | 103.90   |
| 2   | A     | 1869 | G    | N1-C6-O6    | 8.36  | 124.92      | 119.90   |
| 6   | G     | 99   | PHE  | CB-CG-CD2   | -8.35 | 114.95      | 120.80   |
| 2   | A     | 2141 | G    | C5-N7-C8    | 8.35  | 108.47      | 104.30   |
| 2   | A     | 1842 | G    | C4-C5-N7    | -8.34 | 107.46      | 110.80   |
| 2   | A     | 2133 | G    | O4'-C1'-N9  | 8.33  | 114.86      | 108.20   |
| 4   | D     | 146  | ARG  | NE-CZ-NH1   | 8.33  | 124.47      | 120.30   |
| 2   | A     | 2145 | C    | P-O3'-C3'   | -8.32 | 109.72      | 119.70   |
| 5   | F     | 134  | ARG  | NE-CZ-NH2   | 8.32  | 124.46      | 120.30   |
| 2   | A     | 2145 | C    | C4'-C3'-C2' | -8.31 | 94.29       | 102.60   |
| 3   | E     | 9    | G    | C5-C6-O6    | -8.31 | 123.61      | 128.60   |
| 2   | A     | 1840 | G    | N1-C6-O6    | 8.31  | 124.89      | 119.90   |
| 2   | A     | 2108 | A    | N1-C6-N6    | 8.30  | 123.58      | 118.60   |
| 2   | A     | 2120 | G    | N3-C2-N2    | -8.30 | 114.09      | 119.90   |
| 3   | E     | 38   | A    | C2-N3-C4    | -8.30 | 106.45      | 110.60   |
| 2   | A     | 1849 | G    | N9-C4-C5    | -8.29 | 102.08      | 105.40   |
| 2   | A     | 2129 | C    | C2-N1-C1'   | 8.29  | 127.92      | 118.80   |
| 2   | A     | 2182 | U    | C5-C6-N1    | -8.29 | 118.56      | 122.70   |
| 1   | B     | 1295 | U    | N1-C2-O2    | -8.28 | 117.01      | 122.80   |
| 5   | F     | 71   | ARG  | NE-CZ-NH1   | 8.27  | 124.44      | 120.30   |
| 3   | E     | 21   | U    | C5-C6-N1    | 8.27  | 126.83      | 122.70   |
| 3   | E     | 32   | G    | C5-C6-O6    | -8.26 | 123.64      | 128.60   |
| 3   | E     | 57   | C    | N3-C4-C5    | 8.24  | 125.20      | 121.90   |
| 1   | B     | 1242 | G    | C5-C6-O6    | -8.23 | 123.66      | 128.60   |
| 2   | A     | 2189 | U    | O4'-C1'-N1  | 8.23  | 114.78      | 108.20   |
| 7   | H     | 5    | ARG  | NE-CZ-NH1   | 8.22  | 124.41      | 120.30   |
| 2   | A     | 2190 | G    | C8-N9-C4    | -8.21 | 103.11      | 106.40   |
| 4   | D     | 496  | VAL  | CG1-CB-CG2  | -8.21 | 97.76       | 110.90   |
| 3   | E     | 39   | A    | C2-N3-C4    | 8.21  | 114.70      | 110.60   |
| 3   | E     | 41   | C    | C5-C6-N1    | 8.20  | 125.10      | 121.00   |
| 3   | E     | 7    | G    | C5-C6-O6    | -8.19 | 123.69      | 128.60   |
| 3   | E     | 49   | C    | C6-N1-C2    | -8.18 | 117.03      | 120.30   |
| 2   | A     | 2120 | G    | C6-N1-C2    | -8.17 | 120.20      | 125.10   |
| 1   | B     | 1332 | A    | C4-C5-C6    | 8.16  | 121.08      | 117.00   |
| 2   | A     | 1858 | A    | C2-N3-C4    | -8.16 | 106.52      | 110.60   |
| 1   | B     | 1299 | A    | N9-C4-C5    | 8.15  | 109.06      | 105.80   |
| 2   | A     | 2162 | G    | C2-N3-C4    | 8.15  | 115.98      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 1895 | C    | N1-C2-O2    | 8.15  | 123.79      | 118.90   |
| 2   | A     | 1867 | G    | N3-C2-N2    | 8.14  | 125.60      | 119.90   |
| 2   | A     | 2110 | G    | C6-N1-C2    | -8.14 | 120.22      | 125.10   |
| 2   | A     | 2133 | G    | N9-C4-C5    | -8.12 | 102.15      | 105.40   |
| 2   | A     | 2171 | A    | N9-C4-C5    | 8.12  | 109.05      | 105.80   |
| 4   | D     | 441  | ARG  | NE-CZ-NH1   | 8.11  | 124.35      | 120.30   |
| 3   | E     | 73   | A    | C3'-C2'-C1' | 8.10  | 107.98      | 101.50   |
| 2   | A     | 1846 | G    | C5-N7-C8    | -8.10 | 100.25      | 104.30   |
| 2   | A     | 1852 | U    | C6-N1-C2    | -8.10 | 116.14      | 121.00   |
| 3   | E     | 62   | C    | O4'-C1'-N1  | 8.09  | 114.67      | 108.20   |
| 6   | G     | 19   | PHE  | CB-CG-CD2   | 8.08  | 126.46      | 120.80   |
| 3   | E     | 58   | A    | N1-C2-N3    | -8.08 | 125.26      | 129.30   |
| 2   | A     | 2120 | G    | N1-C6-O6    | 8.07  | 124.74      | 119.90   |
| 2   | A     | 2161 | C    | O4'-C1'-N1  | 8.05  | 114.64      | 108.20   |
| 2   | A     | 1859 | U    | O4'-C1'-N1  | 8.04  | 114.63      | 108.20   |
| 2   | A     | 1850 | G    | O4'-C1'-N9  | 8.02  | 114.62      | 108.20   |
| 3   | E     | 31   | G    | C4-C5-N7    | 8.02  | 114.01      | 110.80   |
| 6   | G     | 177  | ARG  | NE-CZ-NH2   | -8.02 | 116.29      | 120.30   |
| 2   | A     | 1876 | A    | C6-N1-C2    | -8.02 | 113.79      | 118.60   |
| 3   | E     | 5    | G    | N1-C6-O6    | 8.01  | 124.71      | 119.90   |
| 1   | B     | 1292 | G    | C4-C5-N7    | 8.00  | 114.00      | 110.80   |
| 2   | A     | 2102 | G    | C5-C6-N1    | -8.00 | 107.50      | 111.50   |
| 2   | A     | 1855 | U    | N1-C2-O2    | 7.99  | 128.40      | 122.80   |
| 3   | E     | 23   | G    | N1-C6-O6    | 7.99  | 124.69      | 119.90   |
| 1   | B     | 1243 | C    | C5-C4-N4    | -7.96 | 114.62      | 120.20   |
| 3   | E     | 57   | C    | N1-C2-O2    | -7.95 | 114.13      | 118.90   |
| 2   | A     | 2123 | G    | N1-C6-O6    | 7.94  | 124.67      | 119.90   |
| 2   | A     | 2172 | U    | N1-C2-O2    | -7.94 | 117.24      | 122.80   |
| 2   | A     | 2095 | A    | N1-C6-N6    | 7.94  | 123.36      | 118.60   |
| 2   | A     | 1838 | C    | N1-C2-O2    | -7.93 | 114.14      | 118.90   |
| 2   | A     | 1867 | G    | O4'-C1'-N9  | 7.92  | 114.54      | 108.20   |
| 2   | A     | 1901 | A    | N1-C2-N3    | 7.91  | 133.25      | 129.30   |
| 2   | A     | 2176 | A    | C1'-O4'-C4' | 7.90  | 116.22      | 109.90   |
| 2   | A     | 1847 | A    | N1-C2-N3    | 7.89  | 133.25      | 129.30   |
| 3   | E     | 29   | C    | C6-N1-C2    | -7.89 | 117.14      | 120.30   |
| 1   | B     | 1304 | G    | C4-C5-N7    | 7.88  | 113.95      | 110.80   |
| 1   | B     | 1245 | C    | C5-C6-N1    | 7.88  | 124.94      | 121.00   |
| 3   | E     | 69   | C    | O4'-C1'-N1  | 7.88  | 114.50      | 108.20   |
| 2   | A     | 2144 | G    | N1-C2-N2    | 7.87  | 123.29      | 116.20   |
| 2   | A     | 1905 | C    | O4'-C1'-N1  | 7.87  | 114.49      | 108.20   |
| 2   | A     | 1845 | G    | C4-C5-N7    | -7.85 | 107.66      | 110.80   |
| 2   | A     | 2168 | G    | N9-C4-C5    | -7.85 | 102.26      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | D     | 367  | ARG  | NE-CZ-NH1   | 7.83  | 124.21      | 120.30   |
| 5   | F     | 37   | LYS  | CB-CA-C     | 7.83  | 126.05      | 110.40   |
| 2   | A     | 1894 | C    | N3-C4-N4    | 7.81  | 123.47      | 118.00   |
| 1   | B     | 1238 | A    | C5-C6-N6    | 7.81  | 129.95      | 123.70   |
| 3   | E     | 52   | C    | C5-C4-N4    | 7.81  | 125.67      | 120.20   |
| 3   | E     | 15   | G    | C6-C5-N7    | 7.81  | 135.08      | 130.40   |
| 2   | A     | 1883 | U    | C5-C6-N1    | 7.80  | 126.60      | 122.70   |
| 4   | D     | 441  | ARG  | NH1-CZ-NH2  | -7.78 | 110.84      | 119.40   |
| 3   | E     | 6    | G    | C4-C5-C6    | -7.78 | 114.13      | 118.80   |
| 2   | A     | 1835 | G    | P-O5'-C5'   | 7.77  | 133.34      | 120.90   |
| 3   | E     | 62   | C    | P-O3'-C3'   | -7.77 | 110.37      | 119.70   |
| 2   | A     | 2103 | C    | N3-C4-N4    | -7.76 | 112.56      | 118.00   |
| 3   | E     | 3    | C    | N3-C4-C5    | -7.76 | 118.80      | 121.90   |
| 2   | A     | 2154 | A    | O4'-C1'-N9  | 7.76  | 114.41      | 108.20   |
| 2   | A     | 1838 | C    | C2-N3-C4    | -7.75 | 116.02      | 119.90   |
| 1   | B     | 1243 | C    | C6-N1-C2    | 7.74  | 123.40      | 120.30   |
| 3   | E     | 57   | C    | C5-C6-N1    | 7.74  | 124.87      | 121.00   |
| 2   | A     | 2102 | G    | C4-C5-N7    | -7.74 | 107.70      | 110.80   |
| 2   | A     | 2152 | G    | C4-C5-N7    | 7.74  | 113.89      | 110.80   |
| 2   | A     | 1850 | G    | C8-N9-C4    | 7.73  | 109.49      | 106.40   |
| 2   | A     | 1868 | C    | C5-C4-N4    | 7.72  | 125.61      | 120.20   |
| 2   | A     | 2178 | C    | N3-C4-C5    | 7.72  | 124.99      | 121.90   |
| 2   | A     | 1896 | G    | C2-N3-C4    | 7.72  | 115.76      | 111.90   |
| 2   | A     | 1906 | G    | N3-C4-C5    | -7.72 | 124.74      | 128.60   |
| 2   | A     | 2130 | U    | C6-N1-C2    | -7.72 | 116.37      | 121.00   |
| 1   | B     | 1304 | G    | P-O3'-C3'   | 7.71  | 128.96      | 119.70   |
| 1   | B     | 1242 | G    | N9-C4-C5    | -7.71 | 102.32      | 105.40   |
| 1   | B     | 1245 | C    | C2-N3-C4    | 7.71  | 123.75      | 119.90   |
| 2   | A     | 2126 | A    | P-O3'-C3'   | 7.69  | 128.93      | 119.70   |
| 5   | F     | 97   | MET  | CG-SD-CE    | -7.68 | 87.91       | 100.20   |
| 3   | E     | 66   | C    | C6-N1-C2    | -7.67 | 117.23      | 120.30   |
| 1   | B     | 1290 | G    | N9-C4-C5    | 7.67  | 108.47      | 105.40   |
| 2   | A     | 2127 | G    | C4-C5-N7    | 7.67  | 113.87      | 110.80   |
| 1   | B     | 1245 | C    | C4-C5-C6    | -7.67 | 113.57      | 117.40   |
| 3   | E     | 57   | C    | N1-C2-N3    | 7.67  | 124.57      | 119.20   |
| 2   | A     | 1854 | A    | N1-C2-N3    | 7.65  | 133.12      | 129.30   |
| 2   | A     | 2166 | U    | C4'-C3'-C2' | -7.64 | 94.96       | 102.60   |
| 2   | A     | 2193 | G    | C5-C6-N1    | -7.63 | 107.68      | 111.50   |
| 2   | A     | 2169 | A    | C4-C5-C6    | -7.63 | 113.18      | 117.00   |
| 2   | A     | 2135 | A    | O4'-C1'-N9  | 7.63  | 114.30      | 108.20   |
| 8   | I     | 22   | LEU  | CB-CG-CD2   | 7.62  | 123.95      | 111.00   |
| 3   | E     | 15   | G    | N3-C2-N2    | 7.62  | 125.23      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2124 | G    | N7-C8-N9    | -7.61 | 109.30      | 113.10   |
| 3   | E     | 29   | C    | C2-N3-C4    | -7.60 | 116.10      | 119.90   |
| 3   | E     | 76   | C    | C5-C4-N4    | -7.60 | 114.88      | 120.20   |
| 4   | D     | 405  | TRP  | CB-CG-CD1   | 7.60  | 136.87      | 127.00   |
| 2   | A     | 2131 | U    | P-O3'-C3'   | 7.59  | 128.81      | 119.70   |
| 6   | G     | 101  | ARG  | NE-CZ-NH1   | -7.59 | 116.50      | 120.30   |
| 2   | A     | 1868 | C    | O4'-C1'-N1  | 7.58  | 114.27      | 108.20   |
| 2   | A     | 2145 | C    | C1'-O4'-C4' | -7.58 | 103.83      | 109.90   |
| 2   | A     | 2191 | A    | N1-C6-N6    | 7.58  | 123.15      | 118.60   |
| 3   | E     | 49   | C    | P-O3'-C3'   | 7.58  | 128.80      | 119.70   |
| 3   | E     | 75   | C    | C4-C5-C6    | 7.58  | 121.19      | 117.40   |
| 2   | A     | 2133 | G    | P-O3'-C3'   | 7.58  | 128.79      | 119.70   |
| 5   | F     | 99   | ASP  | CB-CG-OD2   | 7.57  | 125.12      | 118.30   |
| 2   | A     | 1883 | U    | C4-C5-C6    | -7.57 | 115.16      | 119.70   |
| 2   | A     | 2130 | U    | P-O3'-C3'   | -7.57 | 110.62      | 119.70   |
| 1   | B     | 1332 | A    | O4'-C1'-N9  | 7.56  | 114.25      | 108.20   |
| 3   | E     | 37   | U    | C4-C5-C6    | 7.56  | 124.23      | 119.70   |
| 1   | B     | 1333 | A    | N3-C4-C5    | -7.55 | 121.51      | 126.80   |
| 2   | A     | 2120 | G    | N3-C4-N9    | 7.55  | 130.53      | 126.00   |
| 2   | A     | 2155 | U    | O4'-C1'-N1  | 7.55  | 114.24      | 108.20   |
| 1   | B     | 1292 | G    | P-O3'-C3'   | 7.54  | 128.75      | 119.70   |
| 2   | A     | 2141 | G    | C3'-C2'-C1' | -7.53 | 95.48       | 101.50   |
| 2   | A     | 1907 | G    | C5-C6-N1    | 7.51  | 115.26      | 111.50   |
| 8   | I     | 110  | ARG  | NH1-CZ-NH2  | -7.51 | 111.14      | 119.40   |
| 2   | A     | 2147 | A    | O4'-C1'-N9  | 7.50  | 114.20      | 108.20   |
| 6   | G     | 6    | TYR  | CB-CG-CD2   | -7.50 | 116.50      | 121.00   |
| 2   | A     | 2110 | G    | C3'-C2'-C1' | -7.49 | 95.51       | 101.50   |
| 7   | H     | 43   | ARG  | NE-CZ-NH1   | -7.48 | 116.56      | 120.30   |
| 4   | D     | 390  | SER  | N-CA-CB     | 7.47  | 121.71      | 110.50   |
| 2   | A     | 2192 | U    | O4'-C1'-N1  | 7.47  | 114.18      | 108.20   |
| 1   | B     | 1244 | G    | C4-C5-N7    | 7.46  | 113.78      | 110.80   |
| 2   | A     | 1892 | C    | C5-C6-N1    | 7.44  | 124.72      | 121.00   |
| 2   | A     | 2168 | G    | C4-C5-N7    | 7.43  | 113.77      | 110.80   |
| 1   | B     | 1290 | G    | C4-C5-C6    | 7.43  | 123.26      | 118.80   |
| 2   | A     | 1906 | G    | C6-C5-N7    | -7.43 | 125.94      | 130.40   |
| 4   | D     | 220  | TYR  | CB-CG-CD2   | 7.42  | 125.45      | 121.00   |
| 2   | A     | 2108 | A    | C5-C6-N6    | -7.41 | 117.77      | 123.70   |
| 1   | B     | 1238 | A    | C6-N1-C2    | -7.41 | 114.16      | 118.60   |
| 2   | A     | 2111 | U    | O3'-P-O5'   | -7.41 | 89.93       | 104.00   |
| 2   | A     | 2178 | C    | OP1-P-OP2   | -7.41 | 108.49      | 119.60   |
| 2   | A     | 2144 | G    | C4-C5-N7    | -7.40 | 107.84      | 110.80   |
| 2   | A     | 2118 | U    | N3-C2-O2    | -7.39 | 117.03      | 122.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | B     | 1304 | G    | N1-C6-O6    | 7.38  | 124.33      | 119.90   |
| 1   | B     | 1292 | G    | C8-N9-C4    | 7.38  | 109.35      | 106.40   |
| 2   | A     | 1893 | C    | O4'-C1'-N1  | 7.37  | 114.10      | 108.20   |
| 3   | E     | 76   | C    | N3-C4-N4    | 7.37  | 123.16      | 118.00   |
| 1   | B     | 1305 | G    | C8-N9-C4    | 7.36  | 109.34      | 106.40   |
| 3   | E     | 4    | G    | C5-N7-C8    | -7.36 | 100.62      | 104.30   |
| 3   | E     | 6    | G    | C5-C6-O6    | -7.35 | 124.19      | 128.60   |
| 4   | D     | 200  | TRP  | CH2-CZ2-CE2 | 7.35  | 124.75      | 117.40   |
| 2   | A     | 2148 | G    | P-O3'-C3'   | 7.34  | 128.51      | 119.70   |
| 3   | E     | 35   | C    | O4'-C1'-N1  | 7.34  | 114.08      | 108.20   |
| 6   | G     | 172  | PHE  | CB-CG-CD2   | -7.34 | 115.66      | 120.80   |
| 2   | A     | 1865 | U    | C4-C5-C6    | 7.34  | 124.10      | 119.70   |
| 3   | E     | 43   | G    | C1'-O4'-C4' | -7.33 | 104.03      | 109.90   |
| 2   | A     | 2180 | U    | C2-N3-C4    | 7.33  | 131.40      | 127.00   |
| 3   | E     | 30   | G    | O4'-C1'-N9  | 7.33  | 114.06      | 108.20   |
| 5   | F     | 162  | ARG  | CA-CB-CG    | 7.32  | 129.51      | 113.40   |
| 5   | F     | 9    | ARG  | NE-CZ-NH2   | -7.32 | 116.64      | 120.30   |
| 2   | A     | 2162 | G    | P-O3'-C3'   | -7.31 | 110.93      | 119.70   |
| 2   | A     | 1899 | A    | N1-C6-N6    | -7.30 | 114.22      | 118.60   |
| 2   | A     | 1855 | U    | C2-N3-C4    | 7.30  | 131.38      | 127.00   |
| 2   | A     | 2110 | G    | N9-C4-C5    | -7.29 | 102.48      | 105.40   |
| 2   | A     | 2174 | C    | C6-N1-C2    | 7.29  | 123.22      | 120.30   |
| 2   | A     | 1878 | G    | C2-N3-C4    | -7.29 | 108.25      | 111.90   |
| 3   | E     | 11   | A    | C8-N9-C4    | -7.29 | 102.89      | 105.80   |
| 3   | E     | 40   | C    | O4'-C1'-N1  | 7.28  | 114.03      | 108.20   |
| 2   | A     | 2127 | G    | O4'-C1'-N9  | 7.28  | 114.02      | 108.20   |
| 2   | A     | 2168 | G    | O4'-C1'-N9  | 7.26  | 114.01      | 108.20   |
| 8   | I     | 17   | PHE  | CB-CG-CD1   | -7.25 | 115.72      | 120.80   |
| 3   | E     | 9    | G    | C5-N7-C8    | -7.25 | 100.67      | 104.30   |
| 2   | A     | 1840 | G    | N9-C4-C5    | 7.25  | 108.30      | 105.40   |
| 2   | A     | 1861 | G    | C4-C5-N7    | -7.25 | 107.90      | 110.80   |
| 3   | E     | 29   | C    | N3-C4-C5    | 7.25  | 124.80      | 121.90   |
| 2   | A     | 2161 | C    | C2-N3-C4    | -7.24 | 116.28      | 119.90   |
| 3   | E     | 17   | C    | N3-C2-O2    | -7.24 | 116.83      | 121.90   |
| 2   | A     | 2141 | G    | C4-C5-N7    | -7.24 | 107.91      | 110.80   |
| 2   | A     | 1847 | A    | C6-N1-C2    | -7.22 | 114.27      | 118.60   |
| 2   | A     | 2113 | U    | N1-C2-N3    | 7.22  | 119.23      | 114.90   |
| 3   | E     | 66   | C    | N3-C4-N4    | 7.22  | 123.06      | 118.00   |
| 2   | A     | 1900 | A    | C6-C5-N7    | 7.19  | 137.33      | 132.30   |
| 2   | A     | 1836 | C    | N3-C2-O2    | -7.16 | 116.89      | 121.90   |
| 2   | A     | 2112 | G    | C8-N9-C4    | -7.16 | 103.54      | 106.40   |
| 3   | E     | 44   | A    | N1-C6-N6    | 7.16  | 122.89      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | G     | 99   | PHE  | CB-CG-CD1   | 7.16  | 125.81      | 120.80   |
| 2   | A     | 2137 | U    | N1-C2-N3    | -7.15 | 110.61      | 114.90   |
| 2   | A     | 1863 | G    | N1-C6-O6    | -7.15 | 115.61      | 119.90   |
| 1   | B     | 1305 | G    | N1-C6-O6    | -7.13 | 115.62      | 119.90   |
| 1   | B     | 1298 | U    | C2-N1-C1'   | 7.13  | 126.26      | 117.70   |
| 2   | A     | 2147 | A    | C5-C6-N1    | -7.13 | 114.14      | 117.70   |
| 1   | B     | 1297 | G    | C5-C6-O6    | -7.13 | 124.33      | 128.60   |
| 3   | E     | 71   | G    | N3-C4-N9    | 7.12  | 130.28      | 126.00   |
| 3   | E     | 33   | C    | N3-C4-N4    | 7.12  | 122.99      | 118.00   |
| 3   | E     | 59   | A    | P-O5'-C5'   | 7.12  | 132.30      | 120.90   |
| 2   | A     | 1869 | G    | O4'-C1'-N9  | 7.12  | 113.89      | 108.20   |
| 2   | A     | 2160 | C    | C2-N3-C4    | -7.12 | 116.34      | 119.90   |
| 2   | A     | 1896 | G    | N3-C4-N9    | 7.12  | 130.27      | 126.00   |
| 3   | E     | 69   | C    | N3-C4-N4    | 7.11  | 122.98      | 118.00   |
| 1   | B     | 1237 | C    | C2-N3-C4    | 7.10  | 123.45      | 119.90   |
| 2   | A     | 2114 | A    | P-O3'-C3'   | -7.09 | 111.19      | 119.70   |
| 4   | D     | 547  | ARG  | NE-CZ-NH1   | 7.09  | 123.84      | 120.30   |
| 4   | D     | 469  | ASP  | CB-CG-OD1   | 7.08  | 124.67      | 118.30   |
| 2   | A     | 1891 | G    | N1-C2-N3    | 7.08  | 128.15      | 123.90   |
| 1   | B     | 1241 | G    | C5-C6-N1    | -7.07 | 107.96      | 111.50   |
| 2   | A     | 2102 | G    | C6-N1-C2    | 7.06  | 129.34      | 125.10   |
| 3   | E     | 25   | U    | N3-C4-C5    | -7.06 | 110.36      | 114.60   |
| 3   | E     | 58   | A    | C5-C6-N1    | -7.06 | 114.17      | 117.70   |
| 4   | D     | 514  | TYR  | CB-CG-CD1   | 7.06  | 125.23      | 121.00   |
| 2   | A     | 2173 | A    | C5-N7-C8    | 7.05  | 107.43      | 103.90   |
| 3   | E     | 34   | U    | C5-C6-N1    | -7.05 | 119.17      | 122.70   |
| 3   | E     | 74   | A    | N9-C4-C5    | -7.05 | 102.98      | 105.80   |
| 3   | E     | 46   | G    | C5-C6-O6    | -7.04 | 124.37      | 128.60   |
| 2   | A     | 2176 | A    | C4'-C3'-C2' | 7.04  | 109.64      | 102.60   |
| 3   | E     | 46   | G    | C5-C6-N1    | 7.03  | 115.02      | 111.50   |
| 2   | A     | 2172 | U    | N3-C4-C5    | -7.03 | 110.38      | 114.60   |
| 3   | E     | 57   | C    | C2-N3-C4    | -7.03 | 116.39      | 119.90   |
| 2   | A     | 2121 | G    | N1-C6-O6    | 7.02  | 124.11      | 119.90   |
| 2   | A     | 1847 | A    | C4-C5-N7    | -7.02 | 107.19      | 110.70   |
| 2   | A     | 2110 | G    | C5-C6-O6    | -7.01 | 124.39      | 128.60   |
| 3   | E     | 43   | G    | N7-C8-N9    | -7.01 | 109.59      | 113.10   |
| 2   | A     | 2186 | G    | N1-C6-O6    | -7.01 | 115.69      | 119.90   |
| 2   | A     | 1836 | C    | C4-C5-C6    | 7.01  | 120.90      | 117.40   |
| 4   | D     | 530  | TYR  | CB-CG-CD1   | 7.00  | 125.20      | 121.00   |
| 4   | D     | 481  | ARG  | NH1-CZ-NH2  | -6.99 | 111.71      | 119.40   |
| 2   | A     | 1900 | A    | O4'-C1'-N9  | -6.99 | 102.61      | 108.20   |
| 2   | A     | 1897 | G    | O4'-C1'-N9  | 6.97  | 113.78      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | D     | 127  | ARG  | NE-CZ-NH1   | 6.97  | 123.79      | 120.30   |
| 2   | A     | 1863 | G    | C5-C6-O6    | 6.97  | 132.78      | 128.60   |
| 4   | D     | 144  | LEU  | CB-CG-CD1   | 6.96  | 122.84      | 111.00   |
| 1   | B     | 1242 | G    | N1-C2-N3    | -6.96 | 119.72      | 123.90   |
| 4   | D     | 336  | ARG  | NE-CZ-NH2   | -6.96 | 116.82      | 120.30   |
| 1   | B     | 1336 | C    | C4-C5-C6    | 6.96  | 120.88      | 117.40   |
| 3   | E     | 54   | G    | N3-C2-N2    | 6.96  | 124.77      | 119.90   |
| 3   | E     | 43   | G    | C5-C6-N1    | -6.95 | 108.02      | 111.50   |
| 3   | E     | 25   | U    | C2-N3-C4    | 6.95  | 131.17      | 127.00   |
| 2   | A     | 1889 | A    | N1-C6-N6    | -6.95 | 114.43      | 118.60   |
| 3   | E     | 4    | G    | O4'-C1'-N9  | 6.94  | 113.75      | 108.20   |
| 3   | E     | 37   | U    | C6-N1-C2    | -6.94 | 116.84      | 121.00   |
| 2   | A     | 2171 | A    | C6-C5-N7    | 6.94  | 137.16      | 132.30   |
| 2   | A     | 2118 | U    | N1-C2-N3    | -6.94 | 110.74      | 114.90   |
| 2   | A     | 2119 | A    | N1-C2-N3    | -6.94 | 125.83      | 129.30   |
| 4   | D     | 244  | TYR  | CB-CG-CD2   | -6.93 | 116.84      | 121.00   |
| 2   | A     | 2125 | G    | C5-C6-O6    | 6.93  | 132.76      | 128.60   |
| 1   | B     | 1241 | G    | C5-C6-O6    | -6.93 | 124.44      | 128.60   |
| 2   | A     | 1901 | A    | C2-N3-C4    | -6.92 | 107.14      | 110.60   |
| 2   | A     | 2172 | U    | N1-C2-N3    | 6.92  | 119.05      | 114.90   |
| 2   | A     | 2161 | C    | C5-C6-N1    | -6.92 | 117.54      | 121.00   |
| 3   | E     | 58   | A    | C2-N3-C4    | 6.91  | 114.06      | 110.60   |
| 2   | A     | 2110 | G    | N7-C8-N9    | 6.91  | 116.55      | 113.10   |
| 1   | B     | 1332 | A    | C5-C6-N1    | -6.90 | 114.25      | 117.70   |
| 2   | A     | 2139 | U    | C5-C4-O4    | -6.90 | 121.76      | 125.90   |
| 2   | A     | 2119 | A    | C5'-C4'-C3' | 6.90  | 127.03      | 116.00   |
| 5   | F     | 164  | ARG  | NE-CZ-NH2   | 6.90  | 123.75      | 120.30   |
| 2   | A     | 1847 | A    | C5-C6-N6    | -6.89 | 118.19      | 123.70   |
| 2   | A     | 1899 | A    | C5-C6-N6    | 6.89  | 129.21      | 123.70   |
| 6   | G     | 82   | TYR  | CB-CG-CD1   | -6.89 | 116.86      | 121.00   |
| 3   | E     | 19   | G    | C3'-C2'-C1' | 6.89  | 107.01      | 101.50   |
| 3   | E     | 16   | C    | C5-C6-N1    | -6.88 | 117.56      | 121.00   |
| 2   | A     | 2141 | G    | N7-C8-N9    | -6.88 | 109.66      | 113.10   |
| 8   | I     | 26   | VAL  | CA-CB-CG2   | 6.88  | 121.22      | 110.90   |
| 2   | A     | 1839 | G    | N3-C4-C5    | -6.88 | 125.16      | 128.60   |
| 2   | A     | 1878 | G    | C5-N7-C8    | -6.88 | 100.86      | 104.30   |
| 2   | A     | 2123 | G    | C4-C5-C6    | -6.88 | 114.67      | 118.80   |
| 2   | A     | 2172 | U    | C4-C5-C6    | 6.87  | 123.82      | 119.70   |
| 3   | E     | 54   | G    | C5-C6-O6    | -6.87 | 124.48      | 128.60   |
| 7   | H     | 48   | TYR  | CB-CG-CD1   | -6.87 | 116.88      | 121.00   |
| 2   | A     | 1888 | G    | N3-C2-N2    | 6.87  | 124.70      | 119.90   |
| 1   | B     | 1335 | U    | C5'-C4'-O4' | 6.86  | 117.33      | 109.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2133 | G    | N3-C4-C5    | 6.86  | 132.03      | 128.60   |
| 3   | E     | 24   | C    | N3-C4-C5    | -6.86 | 119.16      | 121.90   |
| 2   | A     | 2173 | A    | N1-C6-N6    | -6.85 | 114.49      | 118.60   |
| 4   | D     | 405  | TRP  | CB-CG-CD2   | -6.85 | 117.69      | 126.60   |
| 2   | A     | 1889 | A    | C5-C6-N6    | 6.85  | 129.18      | 123.70   |
| 2   | A     | 2153 | C    | C5'-C4'-C3' | -6.85 | 105.04      | 116.00   |
| 3   | E     | 5    | G    | C8-N9-C4    | 6.85  | 109.14      | 106.40   |
| 2   | A     | 1904 | G    | O4'-C1'-N9  | 6.84  | 113.67      | 108.20   |
| 2   | A     | 1868 | C    | N3-C2-O2    | -6.84 | 117.11      | 121.90   |
| 3   | E     | 38   | A    | C4-N9-C1'   | 6.84  | 138.60      | 126.30   |
| 5   | F     | 38   | PHE  | CB-CG-CD2   | -6.83 | 116.02      | 120.80   |
| 2   | A     | 2151 | U    | N3-C2-O2    | -6.83 | 117.42      | 122.20   |
| 2   | A     | 2175 | C    | C2-N1-C1'   | 6.83  | 126.31      | 118.80   |
| 3   | E     | 59   | A    | O5'-P-OP2   | -6.83 | 99.56       | 105.70   |
| 3   | E     | 19   | G    | O4'-C4'-C3' | 6.83  | 111.56      | 106.10   |
| 1   | B     | 1242 | G    | O4'-C1'-N9  | 6.83  | 113.66      | 108.20   |
| 2   | A     | 1866 | A    | C8-N9-C4    | -6.83 | 103.07      | 105.80   |
| 1   | B     | 1304 | G    | C2-N3-C4    | -6.82 | 108.49      | 111.90   |
| 3   | E     | 10   | G    | N3-C4-C5    | 6.82  | 132.01      | 128.60   |
| 1   | B     | 1297 | G    | N7-C8-N9    | -6.82 | 109.69      | 113.10   |
| 1   | B     | 1334 | G    | N9-C4-C5    | -6.82 | 102.67      | 105.40   |
| 2   | A     | 2112 | G    | C5-C6-O6    | -6.81 | 124.51      | 128.60   |
| 3   | E     | 72   | C    | C1'-O4'-C4' | -6.81 | 104.45      | 109.90   |
| 1   | B     | 1295 | U    | C5-C4-O4    | -6.81 | 121.81      | 125.90   |
| 4   | D     | 399  | ASP  | CB-CG-OD2   | 6.81  | 124.43      | 118.30   |
| 2   | A     | 2137 | U    | O4'-C1'-N1  | 6.81  | 113.65      | 108.20   |
| 4   | D     | 476  | ASP  | CB-CG-OD2   | 6.80  | 124.42      | 118.30   |
| 3   | E     | 70   | C    | C2-N3-C4    | -6.80 | 116.50      | 119.90   |
| 2   | A     | 2173 | A    | C5-C6-N6    | 6.80  | 129.14      | 123.70   |
| 3   | E     | 36   | A    | C6-C5-N7    | 6.79  | 137.06      | 132.30   |
| 1   | B     | 1296 | C    | O4'-C1'-N1  | 6.79  | 113.63      | 108.20   |
| 3   | E     | 30   | G    | C5-C6-O6    | -6.79 | 124.53      | 128.60   |
| 2   | A     | 1869 | G    | C5-N7-C8    | -6.79 | 100.91      | 104.30   |
| 2   | A     | 2158 | A    | N9-C4-C5    | 6.79  | 108.52      | 105.80   |
| 3   | E     | 49   | C    | O4'-C1'-N1  | 6.78  | 113.62      | 108.20   |
| 3   | E     | 57   | C    | C4-C5-C6    | -6.77 | 114.01      | 117.40   |
| 2   | A     | 1878 | G    | N9-C4-C5    | 6.77  | 108.11      | 105.40   |
| 4   | D     | 333  | TYR  | CG-CD2-CE2  | 6.77  | 126.72      | 121.30   |
| 2   | A     | 2104 | C    | C5-C4-N4    | -6.76 | 115.47      | 120.20   |
| 2   | A     | 2129 | C    | C6-N1-C1'   | -6.75 | 112.69      | 120.80   |
| 2   | A     | 2138 | G    | N1-C2-N3    | -6.74 | 119.85      | 123.90   |
| 3   | E     | 74   | A    | P-O3'-C3'   | 6.74  | 127.79      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 1849 | G    | N3-C4-N9    | 6.74  | 130.04      | 126.00   |
| 4   | D     | 425  | ARG  | NE-CZ-NH1   | 6.74  | 123.67      | 120.30   |
| 2   | A     | 2136 | G    | C2-N3-C4    | 6.72  | 115.26      | 111.90   |
| 2   | A     | 1852 | U    | N3-C4-C5    | 6.72  | 118.63      | 114.60   |
| 1   | B     | 1295 | U    | N3-C2-O2    | 6.72  | 126.90      | 122.20   |
| 3   | E     | 50   | G    | C6-C5-N7    | 6.72  | 134.43      | 130.40   |
| 5   | F     | 179  | ASP  | CB-CG-OD2   | 6.71  | 124.34      | 118.30   |
| 2   | A     | 1877 | A    | C5-C6-N6    | 6.71  | 129.07      | 123.70   |
| 2   | A     | 2158 | A    | N1-C6-N6    | -6.71 | 114.57      | 118.60   |
| 2   | A     | 2157 | G    | O4'-C1'-N9  | 6.70  | 113.56      | 108.20   |
| 2   | A     | 1851 | U    | C3'-C2'-C1' | -6.70 | 96.14       | 101.50   |
| 2   | A     | 2131 | U    | C3'-C2'-C1' | -6.70 | 96.14       | 101.50   |
| 2   | A     | 2146 | C    | O4'-C1'-N1  | 6.70  | 113.56      | 108.20   |
| 1   | B     | 1290 | G    | C8-N9-C4    | -6.69 | 103.72      | 106.40   |
| 3   | E     | 43   | G    | C4'-C3'-C2' | -6.69 | 95.91       | 102.60   |
| 6   | G     | 7    | TYR  | CB-CG-CD1   | -6.68 | 116.99      | 121.00   |
| 4   | D     | 103  | ARG  | NE-CZ-NH2   | -6.68 | 116.96      | 120.30   |
| 2   | A     | 2147 | A    | P-O3'-C3'   | 6.68  | 127.72      | 119.70   |
| 2   | A     | 2161 | C    | C6-N1-C2    | 6.67  | 122.97      | 120.30   |
| 2   | A     | 2116 | G    | C4'-C3'-C2' | -6.67 | 95.94       | 102.60   |
| 2   | A     | 1897 | G    | C5-N7-C8    | -6.66 | 100.97      | 104.30   |
| 6   | G     | 29   | ARG  | NE-CZ-NH2   | -6.65 | 116.97      | 120.30   |
| 2   | A     | 1900 | A    | C6-N1-C2    | -6.65 | 114.61      | 118.60   |
| 3   | E     | 75   | C    | O4'-C1'-N1  | 6.65  | 113.52      | 108.20   |
| 1   | B     | 1241 | G    | C2-N3-C4    | 6.65  | 115.22      | 111.90   |
| 2   | A     | 2118 | U    | O4'-C1'-N1  | 6.64  | 113.52      | 108.20   |
| 8   | I     | 84   | TYR  | CB-CG-CD2   | -6.64 | 117.02      | 121.00   |
| 2   | A     | 2160 | C    | C5-C4-N4    | -6.64 | 115.55      | 120.20   |
| 3   | E     | 30   | G    | C4-C5-C6    | -6.64 | 114.82      | 118.80   |
| 5   | F     | 99   | ASP  | CB-CG-OD1   | -6.63 | 112.33      | 118.30   |
| 2   | A     | 1864 | U    | N1-C2-O2    | 6.63  | 127.44      | 122.80   |
| 4   | D     | 50   | ARG  | NE-CZ-NH2   | -6.63 | 116.99      | 120.30   |
| 4   | D     | 258  | GLU  | O-C-N       | -6.63 | 112.09      | 122.70   |
| 2   | A     | 2183 | A    | C5-C6-N1    | -6.62 | 114.39      | 117.70   |
| 2   | A     | 2191 | A    | N7-C8-N9    | 6.62  | 117.11      | 113.80   |
| 2   | A     | 2174 | C    | C5'-C4'-C3' | -6.62 | 105.41      | 116.00   |
| 2   | A     | 2104 | C    | O4'-C1'-N1  | 6.61  | 113.49      | 108.20   |
| 2   | A     | 2183 | A    | C5'-C4'-O4' | 6.61  | 117.03      | 109.10   |
| 2   | A     | 2190 | G    | N3-C2-N2    | 6.60  | 124.52      | 119.90   |
| 4   | D     | 2    | ALA  | N-CA-CB     | -6.60 | 100.86      | 110.10   |
| 2   | A     | 2175 | C    | P-O3'-C3'   | 6.60  | 127.62      | 119.70   |
| 1   | B     | 1294 | G    | C8-N9-C4    | -6.60 | 103.76      | 106.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 1840 | G    | C5-C6-O6    | -6.60 | 124.64      | 128.60   |
| 2   | A     | 2101 | A    | C4'-C3'-C2' | -6.59 | 96.01       | 102.60   |
| 2   | A     | 2100 | G    | N9-C1'-C2'  | -6.59 | 104.75      | 112.00   |
| 3   | E     | 74   | A    | N1-C2-N3    | 6.58  | 132.59      | 129.30   |
| 2   | A     | 2121 | G    | C4-C5-N7    | -6.58 | 108.17      | 110.80   |
| 2   | A     | 2136 | G    | C4'-C3'-C2' | -6.58 | 96.02       | 102.60   |
| 2   | A     | 2191 | A    | C5-C6-N6    | -6.58 | 118.43      | 123.70   |
| 2   | A     | 2171 | A    | C6-N1-C2    | -6.57 | 114.66      | 118.60   |
| 4   | D     | 4    | PHE  | CB-CG-CD1   | -6.57 | 116.20      | 120.80   |
| 2   | A     | 1859 | U    | N3-C2-O2    | 6.57  | 126.80      | 122.20   |
| 3   | E     | 7    | G    | P-O5'-C5'   | 6.56  | 131.40      | 120.90   |
| 1   | B     | 1296 | C    | N1-C2-N3    | -6.56 | 114.61      | 119.20   |
| 2   | A     | 2095 | A    | C6-N1-C2    | 6.55  | 122.53      | 118.60   |
| 2   | A     | 2131 | U    | C5-C4-O4    | -6.55 | 121.97      | 125.90   |
| 8   | I     | 2    | ARG  | NE-CZ-NH1   | 6.55  | 123.58      | 120.30   |
| 3   | E     | 74   | A    | O4'-C1'-N9  | 6.55  | 113.44      | 108.20   |
| 2   | A     | 2171 | A    | C1'-O4'-C4' | -6.55 | 104.66      | 109.90   |
| 2   | A     | 1878 | G    | N3-C4-N9    | -6.54 | 122.07      | 126.00   |
| 2   | A     | 2160 | C    | O4'-C1'-N1  | 6.54  | 113.43      | 108.20   |
| 2   | A     | 2110 | G    | N3-C2-N2    | -6.54 | 115.32      | 119.90   |
| 3   | E     | 24   | C    | C4-C5-C6    | 6.54  | 120.67      | 117.40   |
| 1   | B     | 1296 | C    | N3-C2-O2    | 6.53  | 126.47      | 121.90   |
| 2   | A     | 1872 | A    | N1-C6-N6    | -6.53 | 114.68      | 118.60   |
| 1   | B     | 1289 | A    | C2-N3-C4    | 6.53  | 113.86      | 110.60   |
| 2   | A     | 1878 | G    | N7-C8-N9    | 6.53  | 116.37      | 113.10   |
| 2   | A     | 2116 | G    | P-O5'-C5'   | 6.53  | 131.35      | 120.90   |
| 2   | A     | 1868 | C    | C3'-C2'-C1' | -6.53 | 96.28       | 101.50   |
| 2   | A     | 2101 | A    | O4'-C1'-N9  | 6.53  | 113.42      | 108.20   |
| 2   | A     | 1896 | G    | C5-C6-N1    | -6.52 | 108.24      | 111.50   |
| 5   | F     | 119  | ASP  | O-C-N       | -6.52 | 112.26      | 122.70   |
| 2   | A     | 2128 | G    | C6-C5-N7    | 6.52  | 134.31      | 130.40   |
| 3   | E     | 23   | G    | N1-C2-N2    | 6.52  | 122.07      | 116.20   |
| 3   | E     | 73   | A    | N1-C2-N3    | -6.51 | 126.04      | 129.30   |
| 3   | E     | 71   | G    | P-O3'-C3'   | 6.51  | 127.51      | 119.70   |
| 6   | G     | 124  | ARG  | NE-CZ-NH1   | 6.51  | 123.55      | 120.30   |
| 2   | A     | 2106 | U    | C6-N1-C2    | -6.51 | 117.10      | 121.00   |
| 2   | A     | 2125 | G    | OP2-P-O3'   | 6.51  | 119.52      | 105.20   |
| 3   | E     | 34   | U    | C4-C5-C6    | 6.51  | 123.60      | 119.70   |
| 2   | A     | 2131 | U    | C6-N1-C2    | 6.50  | 124.90      | 121.00   |
| 3   | E     | 15   | G    | C1'-O4'-C4' | 6.50  | 115.10      | 109.90   |
| 5   | F     | 202  | THR  | CA-CB-CG2   | -6.50 | 103.30      | 112.40   |
| 2   | A     | 2128 | G    | C4-C5-C6    | -6.50 | 114.90      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2164 | C    | O5'-C5'-C4' | -6.50 | 99.36       | 111.70   |
| 2   | A     | 1896 | G    | C6-N1-C2    | 6.50  | 129.00      | 125.10   |
| 3   | E     | 64   | G    | C8-N9-C4    | -6.49 | 103.81      | 106.40   |
| 4   | D     | 366  | PHE  | CB-CG-CD1   | 6.49  | 125.34      | 120.80   |
| 3   | E     | 2    | G    | P-O3'-C3'   | -6.48 | 111.92      | 119.70   |
| 4   | D     | 536  | ARG  | NE-CZ-NH1   | 6.48  | 123.54      | 120.30   |
| 2   | A     | 1840 | G    | N7-C8-N9    | 6.47  | 116.34      | 113.10   |
| 3   | E     | 37   | U    | N3-C4-C5    | -6.46 | 110.72      | 114.60   |
| 2   | A     | 1836 | C    | N1-C2-O2    | 6.46  | 122.78      | 118.90   |
| 2   | A     | 2151 | U    | O5'-P-OP1   | -6.46 | 99.89       | 105.70   |
| 2   | A     | 1857 | G    | P-O3'-C3'   | 6.45  | 127.44      | 119.70   |
| 5   | F     | 41   | SER  | N-CA-CB     | 6.45  | 120.17      | 110.50   |
| 1   | B     | 1290 | G    | N3-C4-C5    | -6.44 | 125.38      | 128.60   |
| 3   | E     | 5    | G    | C2-N3-C4    | -6.44 | 108.68      | 111.90   |
| 1   | B     | 1304 | G    | C5'-C4'-O4' | 6.44  | 116.82      | 109.10   |
| 2   | A     | 2164 | C    | C3'-C2'-C1' | 6.43  | 106.65      | 101.50   |
| 3   | E     | 4    | G    | N3-C4-C5    | -6.43 | 125.39      | 128.60   |
| 3   | E     | 52   | C    | N3-C4-C5    | 6.43  | 124.47      | 121.90   |
| 2   | A     | 1865 | U    | C6-N1-C2    | -6.42 | 117.15      | 121.00   |
| 2   | A     | 1894 | C    | O4'-C1'-N1  | 6.42  | 113.34      | 108.20   |
| 3   | E     | 46   | G    | C4-C5-C6    | -6.42 | 114.95      | 118.80   |
| 8   | I     | 25   | PHE  | CB-CG-CD1   | 6.42  | 125.29      | 120.80   |
| 3   | E     | 31   | G    | C4-C5-C6    | -6.42 | 114.95      | 118.80   |
| 1   | B     | 1336 | C    | C2-N1-C1'   | 6.41  | 125.85      | 118.80   |
| 2   | A     | 2168 | G    | C6-C5-N7    | -6.41 | 126.55      | 130.40   |
| 2   | A     | 2163 | A    | C6-N1-C2    | -6.41 | 114.75      | 118.60   |
| 2   | A     | 2190 | G    | C4-C5-N7    | -6.41 | 108.23      | 110.80   |
| 4   | D     | 430  | ARG  | NH1-CZ-NH2  | -6.41 | 112.35      | 119.40   |
| 2   | A     | 2141 | G    | P-O3'-C3'   | -6.41 | 112.01      | 119.70   |
| 2   | A     | 1859 | U    | C2-N3-C4    | -6.40 | 123.16      | 127.00   |
| 2   | A     | 1869 | G    | C4-C5-C6    | -6.40 | 114.96      | 118.80   |
| 2   | A     | 1866 | A    | N7-C8-N9    | 6.39  | 117.00      | 113.80   |
| 3   | E     | 16   | C    | C6-N1-C1'   | -6.39 | 113.13      | 120.80   |
| 2   | A     | 1853 | A    | O4'-C1'-N9  | 6.39  | 113.31      | 108.20   |
| 2   | A     | 1861 | G    | C4'-C3'-C2' | -6.38 | 96.22       | 102.60   |
| 3   | E     | 31   | G    | C5-N7-C8    | -6.38 | 101.11      | 104.30   |
| 3   | E     | 42   | C    | C5-C6-N1    | -6.38 | 117.81      | 121.00   |
| 2   | A     | 1842 | G    | C5-C6-O6    | 6.38  | 132.43      | 128.60   |
| 2   | A     | 2109 | U    | C4'-C3'-C2' | -6.38 | 96.22       | 102.60   |
| 2   | A     | 2189 | U    | N3-C4-C5    | -6.37 | 110.78      | 114.60   |
| 2   | A     | 1883 | U    | P-O3'-C3'   | 6.37  | 127.34      | 119.70   |
| 2   | A     | 2121 | G    | N3-C4-N9    | -6.37 | 122.18      | 126.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2176 | A    | OP1-P-OP2   | -6.37 | 110.05      | 119.60   |
| 2   | A     | 2126 | A    | C5-C6-N1    | -6.36 | 114.52      | 117.70   |
| 3   | E     | 42   | C    | N3-C4-C5    | -6.36 | 119.36      | 121.90   |
| 3   | E     | 74   | A    | C6-N1-C2    | -6.36 | 114.78      | 118.60   |
| 2   | A     | 1888 | G    | C3'-C2'-C1' | -6.36 | 96.41       | 101.50   |
| 3   | E     | 8    | U    | N1-C2-N3    | 6.36  | 118.72      | 114.90   |
| 3   | E     | 14   | A    | C4-C5-N7    | 6.36  | 113.88      | 110.70   |
| 3   | E     | 32   | G    | N9-C4-C5    | 6.35  | 107.94      | 105.40   |
| 5   | F     | 51   | ASP  | CB-CG-OD1   | 6.35  | 124.02      | 118.30   |
| 3   | E     | 1    | C    | C5-C6-N1    | -6.35 | 117.83      | 121.00   |
| 1   | B     | 1298 | U    | P-O3'-C3'   | 6.34  | 127.31      | 119.70   |
| 2   | A     | 2191 | A    | C3'-C2'-C1' | 6.34  | 106.57      | 101.50   |
| 2   | A     | 2116 | G    | C5-C6-O6    | 6.34  | 132.40      | 128.60   |
| 3   | E     | 20   | G    | C5'-C4'-C3' | -6.34 | 105.86      | 116.00   |
| 5   | F     | 144  | THR  | CA-CB-CG2   | 6.34  | 121.27      | 112.40   |
| 4   | D     | 19   | ARG  | NE-CZ-NH1   | 6.33  | 123.47      | 120.30   |
| 2   | A     | 1895 | C    | N3-C2-O2    | -6.33 | 117.47      | 121.90   |
| 2   | A     | 1835 | G    | C2-N3-C4    | 6.33  | 115.06      | 111.90   |
| 2   | A     | 2186 | G    | N3-C2-N2    | 6.33  | 124.33      | 119.90   |
| 2   | A     | 2156 | G    | C5-C6-N1    | -6.32 | 108.34      | 111.50   |
| 3   | E     | 6    | G    | O4'-C1'-N9  | 6.32  | 113.26      | 108.20   |
| 2   | A     | 1877 | A    | N7-C8-N9    | 6.32  | 116.96      | 113.80   |
| 8   | I     | 110  | ARG  | NE-CZ-NH1   | 6.32  | 123.46      | 120.30   |
| 3   | E     | 46   | G    | N9-C4-C5    | -6.32 | 102.87      | 105.40   |
| 4   | D     | 187  | ASP  | CB-CG-OD2   | -6.32 | 112.62      | 118.30   |
| 2   | A     | 2096 | C    | C6-N1-C2    | -6.31 | 117.78      | 120.30   |
| 2   | A     | 2123 | G    | C5-N7-C8    | -6.31 | 101.14      | 104.30   |
| 2   | A     | 2162 | G    | N1-C2-N3    | -6.31 | 120.11      | 123.90   |
| 1   | B     | 1305 | G    | N9-C4-C5    | -6.31 | 102.88      | 105.40   |
| 2   | A     | 2183 | A    | C4-C5-C6    | 6.31  | 120.15      | 117.00   |
| 2   | A     | 2113 | U    | C6-N1-C2    | -6.30 | 117.22      | 121.00   |
| 3   | E     | 77   | A    | N1-C2-N3    | 6.30  | 132.45      | 129.30   |
| 2   | A     | 2158 | A    | C5-C6-N1    | 6.29  | 120.84      | 117.70   |
| 3   | E     | 6    | G    | C5-C6-N1    | 6.29  | 114.64      | 111.50   |
| 1   | B     | 1305 | G    | C5-C6-N1    | 6.28  | 114.64      | 111.50   |
| 2   | A     | 1857 | G    | C4'-C3'-C2' | -6.28 | 96.32       | 102.60   |
| 2   | A     | 1903 | G    | C5-C6-N1    | -6.28 | 108.36      | 111.50   |
| 6   | G     | 21   | TYR  | CB-CG-CD1   | 6.28  | 124.77      | 121.00   |
| 3   | E     | 12   | G    | N1-C6-O6    | 6.28  | 123.67      | 119.90   |
| 3   | E     | 72   | C    | C5'-C4'-O4' | -6.28 | 101.57      | 109.10   |
| 3   | E     | 77   | A    | C4-C5-N7    | -6.27 | 107.56      | 110.70   |
| 3   | E     | 77   | A    | C6-N1-C2    | -6.27 | 114.84      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2190 | G    | C5'-C4'-C3' | -6.27 | 105.97      | 116.00   |
| 3   | E     | 63   | C    | C5-C4-N4    | -6.27 | 115.81      | 120.20   |
| 2   | A     | 2158 | A    | C6-N1-C2    | -6.27 | 114.84      | 118.60   |
| 4   | D     | 168  | ARG  | NE-CZ-NH2   | -6.27 | 117.17      | 120.30   |
| 5   | F     | 122  | ARG  | NE-CZ-NH2   | -6.27 | 117.17      | 120.30   |
| 1   | B     | 1300 | G    | C4-C5-N7    | -6.26 | 108.30      | 110.80   |
| 3   | E     | 11   | A    | N1-C2-N3    | 6.26  | 132.43      | 129.30   |
| 2   | A     | 2174 | C    | C2-N1-C1'   | -6.25 | 111.92      | 118.80   |
| 2   | A     | 2121 | G    | P-O3'-C3'   | -6.25 | 112.20      | 119.70   |
| 1   | B     | 1240 | U    | C5'-C4'-C3' | -6.25 | 106.00      | 116.00   |
| 5   | F     | 174  | THR  | CA-CB-CG2   | -6.25 | 103.66      | 112.40   |
| 2   | A     | 2117 | A    | C2-N3-C4    | 6.24  | 113.72      | 110.60   |
| 3   | E     | 59   | A    | N1-C2-N3    | -6.24 | 126.18      | 129.30   |
| 3   | E     | 2    | G    | N3-C2-N2    | 6.23  | 124.26      | 119.90   |
| 2   | A     | 1888 | G    | C8-N9-C1'   | 6.23  | 135.10      | 127.00   |
| 2   | A     | 2131 | U    | N1-C2-N3    | -6.23 | 111.16      | 114.90   |
| 1   | B     | 1240 | U    | C5-C4-O4    | -6.22 | 122.17      | 125.90   |
| 3   | E     | 6    | G    | N9-C4-C5    | -6.22 | 102.91      | 105.40   |
| 3   | E     | 50   | G    | C5-C6-N1    | 6.22  | 114.61      | 111.50   |
| 8   | I     | 108  | ARG  | CG-CD-NE    | -6.22 | 98.73       | 111.80   |
| 3   | E     | 59   | A    | C5-C6-N1    | 6.22  | 120.81      | 117.70   |
| 8   | I     | 95   | ARG  | CD-NE-CZ    | 6.22  | 132.31      | 123.60   |
| 2   | A     | 1897 | G    | N1-C2-N2    | -6.21 | 110.61      | 116.20   |
| 2   | A     | 1901 | A    | C8-N9-C4    | 6.21  | 108.28      | 105.80   |
| 2   | A     | 2165 | C    | C6-N1-C2    | -6.20 | 117.82      | 120.30   |
| 3   | E     | 38   | A    | N1-C2-N3    | 6.20  | 132.40      | 129.30   |
| 1   | B     | 1296 | C    | C6-N1-C2    | 6.20  | 122.78      | 120.30   |
| 4   | D     | 536  | ARG  | NE-CZ-NH2   | -6.19 | 117.20      | 120.30   |
| 8   | I     | 95   | ARG  | NH1-CZ-NH2  | -6.19 | 112.59      | 119.40   |
| 2   | A     | 2117 | A    | C5'-C4'-C3' | 6.19  | 125.90      | 116.00   |
| 2   | A     | 2118 | U    | C6-N1-C1'   | -6.19 | 112.54      | 121.20   |
| 2   | A     | 2185 | U    | O4'-C1'-N1  | 6.19  | 113.15      | 108.20   |
| 2   | A     | 2137 | U    | C2-N3-C4    | 6.19  | 130.71      | 127.00   |
| 4   | D     | 363  | SER  | N-CA-CB     | 6.19  | 119.78      | 110.50   |
| 6   | G     | 114  | ARG  | NE-CZ-NH1   | -6.19 | 117.21      | 120.30   |
| 2   | A     | 1905 | C    | C3'-C2'-C1' | 6.18  | 106.45      | 101.50   |
| 2   | A     | 2176 | A    | C5-C6-N6    | -6.18 | 118.75      | 123.70   |
| 3   | E     | 73   | A    | C6-N1-C2    | 6.18  | 122.31      | 118.60   |
| 2   | A     | 1901 | A    | N9-C4-C5    | -6.18 | 103.33      | 105.80   |
| 2   | A     | 1867 | G    | N1-C2-N2    | -6.17 | 110.65      | 116.20   |
| 1   | B     | 1241 | G    | C8-N9-C4    | -6.17 | 103.93      | 106.40   |
| 2   | A     | 1906 | G    | P-O5'-C5'   | -6.17 | 111.03      | 120.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 38   | A    | C6-C5-N7    | 6.16  | 136.62      | 132.30   |
| 2   | A     | 1885 | A    | C5-N7-C8    | 6.16  | 106.98      | 103.90   |
| 2   | A     | 1866 | A    | C5-N7-C8    | -6.16 | 100.82      | 103.90   |
| 2   | A     | 1887 | C    | N3-C4-C5    | 6.16  | 124.36      | 121.90   |
| 7   | H     | 39   | ASP  | O-C-N       | -6.16 | 109.41      | 121.10   |
| 2   | A     | 2148 | G    | C4-C5-N7    | 6.15  | 113.26      | 110.80   |
| 5   | F     | 7    | ARG  | CB-CA-C     | -6.15 | 98.10       | 110.40   |
| 5   | F     | 208  | TYR  | CG-CD2-CE2  | -6.15 | 116.38      | 121.30   |
| 1   | B     | 1242 | G    | C4-C5-C6    | -6.15 | 115.11      | 118.80   |
| 2   | A     | 2184 | A    | O4'-C1'-N9  | 6.15  | 113.12      | 108.20   |
| 3   | E     | 73   | A    | N9-C4-C5    | -6.15 | 103.34      | 105.80   |
| 2   | A     | 1899 | A    | N7-C8-N9    | 6.15  | 116.87      | 113.80   |
| 2   | A     | 1895 | C    | O4'-C1'-N1  | 6.14  | 113.11      | 108.20   |
| 3   | E     | 47   | G    | C5-N7-C8    | -6.14 | 101.23      | 104.30   |
| 4   | D     | 68   | ASP  | CB-CG-OD2   | 6.14  | 123.83      | 118.30   |
| 2   | A     | 2112 | G    | C5'-C4'-C3' | -6.14 | 106.18      | 116.00   |
| 2   | A     | 2156 | G    | N1-C2-N3    | -6.14 | 120.22      | 123.90   |
| 2   | A     | 2167 | U    | C2-N3-C4    | 6.13  | 130.68      | 127.00   |
| 2   | A     | 2146 | C    | N1-C2-O2    | 6.13  | 122.58      | 118.90   |
| 2   | A     | 2171 | A    | N7-C8-N9    | -6.13 | 110.74      | 113.80   |
| 3   | E     | 38   | A    | N7-C8-N9    | 6.13  | 116.86      | 113.80   |
| 5   | F     | 17   | ALA  | N-CA-CB     | -6.13 | 101.52      | 110.10   |
| 2   | A     | 2125 | G    | C1'-O4'-C4' | -6.12 | 105.00      | 109.90   |
| 2   | A     | 2102 | G    | C5-C6-O6    | -6.12 | 124.93      | 128.60   |
| 2   | A     | 1880 | U    | O4'-C1'-N1  | 6.12  | 113.09      | 108.20   |
| 2   | A     | 1900 | A    | C4-C5-C6    | -6.12 | 113.94      | 117.00   |
| 1   | B     | 1242 | G    | N1-C6-O6    | 6.12  | 123.57      | 119.90   |
| 2   | A     | 1847 | A    | P-O3'-C3'   | 6.12  | 127.04      | 119.70   |
| 1   | B     | 1291 | U    | C3'-C2'-C1' | 6.11  | 106.39      | 101.50   |
| 2   | A     | 1837 | C    | P-O5'-C5'   | -6.11 | 111.12      | 120.90   |
| 4   | D     | 111  | TYR  | CB-CG-CD1   | -6.11 | 117.33      | 121.00   |
| 3   | E     | 5    | G    | N7-C8-N9    | -6.11 | 110.05      | 113.10   |
| 2   | A     | 2169 | A    | C5-C6-N6    | -6.10 | 118.82      | 123.70   |
| 8   | I     | 94   | ARG  | NE-CZ-NH1   | 6.10  | 123.35      | 120.30   |
| 2   | A     | 2101 | A    | C5-C6-N6    | -6.10 | 118.82      | 123.70   |
| 3   | E     | 34   | U    | O4'-C1'-N1  | 6.10  | 113.08      | 108.20   |
| 3   | E     | 64   | G    | O4'-C1'-N9  | 6.10  | 113.08      | 108.20   |
| 2   | A     | 2100 | G    | OP1-P-OP2   | -6.09 | 110.46      | 119.60   |
| 3   | E     | 24   | C    | N3-C4-N4    | 6.09  | 122.26      | 118.00   |
| 2   | A     | 2128 | G    | N9-C4-C5    | -6.09 | 102.96      | 105.40   |
| 1   | B     | 1241 | G    | C4-N9-C1'   | 6.09  | 134.41      | 126.50   |
| 2   | A     | 2116 | G    | C8-N9-C4    | 6.09  | 108.83      | 106.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 14   | A    | C8-N9-C1'   | -6.08 | 116.75      | 127.70   |
| 3   | E     | 31   | G    | N9-C4-C5    | -6.08 | 102.97      | 105.40   |
| 2   | A     | 1884 | G    | P-O5'-C5'   | 6.08  | 130.63      | 120.90   |
| 3   | E     | 4    | G    | N1-C6-O6    | -6.07 | 116.26      | 119.90   |
| 2   | A     | 1869 | G    | C5-C6-N1    | 6.07  | 114.53      | 111.50   |
| 3   | E     | 48   | U    | O4'-C1'-N1  | 6.07  | 113.06      | 108.20   |
| 2   | A     | 2103 | C    | C6-N1-C2    | -6.07 | 117.87      | 120.30   |
| 2   | A     | 1858 | A    | C4-C5-N7    | -6.06 | 107.67      | 110.70   |
| 3   | E     | 69   | C    | C4'-C3'-C2' | -6.06 | 96.54       | 102.60   |
| 5   | F     | 21   | TYR  | CB-CG-CD1   | -6.06 | 117.37      | 121.00   |
| 2   | A     | 1844 | C    | C5-C4-N4    | -6.05 | 115.96      | 120.20   |
| 2   | A     | 1840 | G    | O4'-C1'-N9  | 6.05  | 113.04      | 108.20   |
| 2   | A     | 2140 | G    | C5-N7-C8    | -6.05 | 101.28      | 104.30   |
| 2   | A     | 2161 | C    | C5-C4-N4    | -6.05 | 115.97      | 120.20   |
| 2   | A     | 1907 | G    | C6-N1-C2    | -6.05 | 121.47      | 125.10   |
| 1   | B     | 1290 | G    | C5-N7-C8    | 6.04  | 107.32      | 104.30   |
| 1   | B     | 1298 | U    | N3-C4-O4    | 6.04  | 123.63      | 119.40   |
| 3   | E     | 66   | C    | C4-C5-C6    | 6.03  | 120.42      | 117.40   |
| 3   | E     | 23   | G    | C5-C6-O6    | -6.03 | 124.98      | 128.60   |
| 3   | E     | 16   | C    | C3'-C2'-C1' | 6.03  | 106.32      | 101.50   |
| 2   | A     | 1899 | A    | C6-C5-N7    | -6.03 | 128.08      | 132.30   |
| 4   | D     | 360  | ALA  | N-CA-CB     | -6.03 | 101.66      | 110.10   |
| 2   | A     | 2157 | G    | C5-C6-O6    | -6.03 | 124.98      | 128.60   |
| 2   | A     | 2160 | C    | N3-C4-C5    | 6.03  | 124.31      | 121.90   |
| 1   | B     | 1244 | G    | C5-N7-C8    | -6.02 | 101.29      | 104.30   |
| 5   | F     | 68   | GLY  | C-N-CA      | 6.02  | 136.75      | 121.70   |
| 4   | D     | 395  | ARG  | CG-CD-NE    | -6.02 | 99.16       | 111.80   |
| 3   | E     | 21   | U    | C4-C5-C6    | -6.01 | 116.09      | 119.70   |
| 4   | D     | 293  | ARG  | N-CA-CB     | 6.01  | 121.42      | 110.60   |
| 2   | A     | 2177 | C    | C5'-C4'-O4' | 6.01  | 116.31      | 109.10   |
| 3   | E     | 26   | C    | C5-C4-N4    | 6.01  | 124.41      | 120.20   |
| 2   | A     | 2140 | G    | N1-C2-N3    | -6.01 | 120.30      | 123.90   |
| 3   | E     | 4    | G    | C5-C6-O6    | 6.01  | 132.20      | 128.60   |
| 2   | A     | 2135 | A    | N7-C8-N9    | -6.00 | 110.80      | 113.80   |
| 2   | A     | 1849 | G    | O4'-C1'-N9  | 6.00  | 113.00      | 108.20   |
| 3   | E     | 14   | A    | P-O3'-C3'   | -5.99 | 112.51      | 119.70   |
| 3   | E     | 39   | A    | N1-C6-N6    | 5.99  | 122.20      | 118.60   |
| 2   | A     | 2121 | G    | O4'-C1'-N9  | 5.99  | 112.99      | 108.20   |
| 3   | E     | 62   | C    | C5-C4-N4    | -5.99 | 116.01      | 120.20   |
| 3   | E     | 60   | A    | C5-C6-N1    | 5.99  | 120.69      | 117.70   |
| 2   | A     | 2097 | A    | N9-C4-C5    | 5.99  | 108.19      | 105.80   |
| 2   | A     | 1859 | U    | C5'-C4'-C3' | -5.98 | 106.43      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 1896 | G    | N1-C2-N3    | -5.98 | 120.31      | 123.90   |
| 3   | E     | 50   | G    | O4'-C1'-N9  | 5.98  | 112.99      | 108.20   |
| 2   | A     | 1840 | G    | P-O3'-C3'   | 5.98  | 126.88      | 119.70   |
| 2   | A     | 1905 | C    | C2-N3-C4    | -5.98 | 116.91      | 119.90   |
| 2   | A     | 1862 | G    | C5'-C4'-C3' | -5.97 | 106.44      | 116.00   |
| 2   | A     | 1886 | U    | O4'-C1'-C2' | -5.97 | 99.83       | 105.80   |
| 3   | E     | 5    | G    | C5-C6-O6    | -5.97 | 125.02      | 128.60   |
| 2   | A     | 2159 | G    | C4-C5-N7    | 5.97  | 113.19      | 110.80   |
| 2   | A     | 2165 | C    | C2-N1-C1'   | 5.97  | 125.36      | 118.80   |
| 3   | E     | 39   | A    | N7-C8-N9    | 5.97  | 116.78      | 113.80   |
| 2   | A     | 1903 | G    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 7   | H     | 48   | TYR  | CG-CD2-CE2  | -5.96 | 116.53      | 121.30   |
| 4   | D     | 170  | ARG  | NE-CZ-NH1   | 5.95  | 123.28      | 120.30   |
| 2   | A     | 2119 | A    | N9-C1'-C2'  | -5.95 | 105.46      | 112.00   |
| 2   | A     | 2157 | G    | C5'-C4'-O4' | 5.95  | 116.24      | 109.10   |
| 4   | D     | 149  | ASP  | CB-CG-OD2   | 5.95  | 123.65      | 118.30   |
| 1   | B     | 1293 | C    | O4'-C1'-N1  | 5.95  | 112.96      | 108.20   |
| 4   | D     | 440  | LYS  | CB-CG-CD    | 5.94  | 127.05      | 111.60   |
| 3   | E     | 60   | A    | C6-N1-C2    | -5.94 | 115.04      | 118.60   |
| 2   | A     | 2140 | G    | C4'-C3'-C2' | -5.94 | 96.66       | 102.60   |
| 4   | D     | 151  | LEU  | C-N-CA      | 5.94  | 136.54      | 121.70   |
| 2   | A     | 2169 | A    | C6-N1-C2    | -5.93 | 115.04      | 118.60   |
| 4   | D     | 290  | ARG  | NE-CZ-NH1   | -5.93 | 117.33      | 120.30   |
| 2   | A     | 1904 | G    | C6-C5-N7    | 5.93  | 133.96      | 130.40   |
| 1   | B     | 1239 | A    | C4-C5-N7    | 5.92  | 113.66      | 110.70   |
| 4   | D     | 28   | SER  | O-C-N       | -5.92 | 113.22      | 122.70   |
| 6   | G     | 96   | TRP  | CH2-CZ2-CE2 | 5.92  | 123.33      | 117.40   |
| 3   | E     | 45   | A    | C8-N9-C4    | -5.92 | 103.43      | 105.80   |
| 1   | B     | 1243 | C    | O4'-C1'-N1  | 5.92  | 112.93      | 108.20   |
| 2   | A     | 2120 | G    | C6-C5-N7    | -5.92 | 126.85      | 130.40   |
| 2   | A     | 1873 | G    | C1'-O4'-C4' | -5.91 | 105.17      | 109.90   |
| 2   | A     | 2144 | G    | O4'-C1'-N9  | 5.91  | 112.93      | 108.20   |
| 2   | A     | 2118 | U    | OP1-P-OP2   | -5.91 | 110.73      | 119.60   |
| 2   | A     | 2110 | G    | O4'-C1'-N9  | 5.91  | 112.93      | 108.20   |
| 2   | A     | 2152 | G    | O4'-C1'-N9  | 5.91  | 112.93      | 108.20   |
| 4   | D     | 527  | PHE  | CB-CG-CD2   | -5.91 | 116.66      | 120.80   |
| 4   | D     | 294  | PHE  | CD1-CE1-CZ  | 5.91  | 127.19      | 120.10   |
| 2   | A     | 2148 | G    | C4'-C3'-C2' | -5.91 | 96.69       | 102.60   |
| 3   | E     | 54   | G    | N1-C2-N2    | -5.90 | 110.89      | 116.20   |
| 5   | F     | 201  | PRO  | N-CA-CB     | 5.90  | 110.38      | 103.30   |
| 8   | I     | 108  | ARG  | NE-CZ-NH2   | 5.89  | 123.25      | 120.30   |
| 1   | B     | 1236 | A    | C2-N3-C4    | -5.89 | 107.66      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2128 | G    | N7-C8-N9    | -5.88 | 110.16      | 113.10   |
| 3   | E     | 53   | G    | N9-C4-C5    | -5.88 | 103.05      | 105.40   |
| 3   | E     | 59   | A    | O4'-C1'-N9  | 5.88  | 112.90      | 108.20   |
| 2   | A     | 2127 | G    | C5-C6-O6    | -5.87 | 125.08      | 128.60   |
| 2   | A     | 2172 | U    | C5'-C4'-O4' | -5.87 | 102.05      | 109.10   |
| 2   | A     | 1877 | A    | C6-N1-C2    | 5.87  | 122.12      | 118.60   |
| 2   | A     | 2106 | U    | C5'-C4'-O4' | 5.87  | 116.15      | 109.10   |
| 3   | E     | 37   | U    | N1-C2-N3    | 5.87  | 118.42      | 114.90   |
| 1   | B     | 1289 | A    | C3'-C2'-C1' | -5.87 | 96.81       | 101.50   |
| 1   | B     | 1303 | C    | C6-N1-C1'   | -5.87 | 113.76      | 120.80   |
| 2   | A     | 2191 | A    | C4-C5-C6    | -5.87 | 114.07      | 117.00   |
| 8   | I     | 108  | ARG  | NE-CZ-NH1   | 5.87  | 123.23      | 120.30   |
| 2   | A     | 2130 | U    | C4-C5-C6    | -5.87 | 116.18      | 119.70   |
| 3   | E     | 54   | G    | N1-C6-O6    | 5.87  | 123.42      | 119.90   |
| 2   | A     | 2141 | G    | C5-C6-O6    | 5.86  | 132.12      | 128.60   |
| 2   | A     | 1901 | A    | O4'-C1'-N9  | 5.86  | 112.89      | 108.20   |
| 8   | I     | 91   | ARG  | NH1-CZ-NH2  | 5.86  | 125.84      | 119.40   |
| 3   | E     | 23   | G    | N3-C4-N9    | -5.86 | 122.48      | 126.00   |
| 1   | B     | 1241 | G    | O4'-C1'-N9  | 5.86  | 112.89      | 108.20   |
| 1   | B     | 1303 | C    | C5-C6-N1    | -5.86 | 118.07      | 121.00   |
| 2   | A     | 1842 | G    | C2-N3-C4    | 5.86  | 114.83      | 111.90   |
| 2   | A     | 1881 | C    | C2-N1-C1'   | 5.86  | 125.24      | 118.80   |
| 3   | E     | 29   | C    | N1-C2-N3    | 5.85  | 123.29      | 119.20   |
| 2   | A     | 1837 | C    | O4'-C1'-N1  | 5.85  | 112.88      | 108.20   |
| 3   | E     | 10   | G    | C4-C5-N7    | 5.84  | 113.14      | 110.80   |
| 2   | A     | 2127 | G    | OP1-P-OP2   | -5.84 | 110.84      | 119.60   |
| 2   | A     | 1890 | A    | P-O3'-C3'   | -5.84 | 112.69      | 119.70   |
| 3   | E     | 68   | C    | C2-N3-C4    | 5.83  | 122.82      | 119.90   |
| 4   | D     | 234  | ARG  | NH1-CZ-NH2  | -5.83 | 112.98      | 119.40   |
| 3   | E     | 4    | G    | C6-C5-N7    | -5.83 | 126.90      | 130.40   |
| 3   | E     | 62   | C    | N3-C2-O2    | 5.83  | 125.98      | 121.90   |
| 2   | A     | 2134 | A    | O4'-C1'-N9  | 5.83  | 112.86      | 108.20   |
| 2   | A     | 2129 | C    | N3-C4-C5    | -5.83 | 119.57      | 121.90   |
| 3   | E     | 3    | C    | C5'-C4'-C3' | -5.83 | 106.67      | 116.00   |
| 4   | D     | 87   | ARG  | NH1-CZ-NH2  | -5.83 | 112.99      | 119.40   |
| 2   | A     | 1852 | U    | C4-C5-C6    | -5.83 | 116.20      | 119.70   |
| 3   | E     | 67   | C    | O4'-C1'-N1  | 5.83  | 112.86      | 108.20   |
| 4   | D     | 490  | PHE  | CG-CD2-CE2  | -5.82 | 114.40      | 120.80   |
| 2   | A     | 2099 | U    | C6-N1-C2    | -5.82 | 117.51      | 121.00   |
| 2   | A     | 2164 | C    | C5'-C4'-O4' | -5.82 | 102.12      | 109.10   |
| 3   | E     | 6    | G    | C4-C5-N7    | 5.82  | 113.13      | 110.80   |
| 2   | A     | 2169 | A    | C2-N3-C4    | 5.82  | 113.51      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | D     | 169  | ARG  | NE-CZ-NH1   | 5.82  | 123.21      | 120.30   |
| 2   | A     | 2127 | G    | N9-C1'-C2'  | -5.82 | 105.60      | 112.00   |
| 1   | B     | 1294 | G    | P-O5'-C5'   | 5.81  | 130.20      | 120.90   |
| 2   | A     | 1878 | G    | O4'-C1'-N9  | 5.81  | 112.85      | 108.20   |
| 3   | E     | 27   | G    | C5-C6-O6    | -5.81 | 125.12      | 128.60   |
| 4   | D     | 155  | ASP  | O-C-N       | -5.81 | 113.41      | 122.70   |
| 3   | E     | 5    | G    | P-O3'-C3'   | -5.80 | 112.74      | 119.70   |
| 2   | A     | 1896 | G    | N9-C4-C5    | -5.80 | 103.08      | 105.40   |
| 4   | D     | 135  | HIS  | CA-CB-CG    | -5.80 | 103.74      | 113.60   |
| 6   | G     | 70   | ARG  | O-C-N       | -5.80 | 113.42      | 122.70   |
| 4   | D     | 503  | PHE  | CB-CG-CD1   | -5.80 | 116.74      | 120.80   |
| 2   | A     | 2102 | G    | N9-C4-C5    | 5.79  | 107.72      | 105.40   |
| 2   | A     | 1848 | A    | O4'-C1'-N9  | 5.79  | 112.83      | 108.20   |
| 2   | A     | 2094 | A    | P-O5'-C5'   | 5.79  | 130.17      | 120.90   |
| 3   | E     | 10   | G    | C2-N3-C4    | -5.79 | 109.00      | 111.90   |
| 1   | B     | 1236 | A    | C3'-C2'-C1' | -5.79 | 96.87       | 101.50   |
| 2   | A     | 2111 | U    | OP2-P-O3'   | 5.79  | 117.93      | 105.20   |
| 2   | A     | 1884 | G    | N1-C6-O6    | 5.79  | 123.37      | 119.90   |
| 3   | E     | 59   | A    | N3-C4-N9    | -5.78 | 122.77      | 127.40   |
| 2   | A     | 2154 | A    | C5-C6-N1    | 5.78  | 120.59      | 117.70   |
| 2   | A     | 2147 | A    | C5-C6-N6    | 5.78  | 128.32      | 123.70   |
| 6   | G     | 141  | ASP  | CB-CG-OD1   | 5.77  | 123.50      | 118.30   |
| 2   | A     | 2186 | G    | C5-C6-N1    | 5.77  | 114.39      | 111.50   |
| 3   | E     | 2    | G    | C5-C6-N1    | -5.77 | 108.61      | 111.50   |
| 2   | A     | 2189 | U    | C6-N1-C2    | -5.77 | 117.54      | 121.00   |
| 2   | A     | 2153 | C    | C5-C6-N1    | 5.77  | 123.89      | 121.00   |
| 2   | A     | 1901 | A    | OP1-P-OP2   | -5.77 | 110.95      | 119.60   |
| 4   | D     | 431  | PHE  | CB-CG-CD2   | 5.77  | 124.84      | 120.80   |
| 1   | B     | 1336 | C    | C5-C6-N1    | -5.76 | 118.12      | 121.00   |
| 3   | E     | 38   | A    | P-O5'-C5'   | -5.76 | 111.68      | 120.90   |
| 2   | A     | 1907 | G    | C4-C5-N7    | 5.76  | 113.11      | 110.80   |
| 1   | B     | 1296 | C    | N3-C4-C5    | -5.76 | 119.60      | 121.90   |
| 3   | E     | 55   | U    | O4'-C1'-N1  | 5.76  | 112.81      | 108.20   |
| 2   | A     | 1880 | U    | C6-N1-C2    | -5.76 | 117.55      | 121.00   |
| 5   | F     | 102  | ASP  | CB-CG-OD2   | 5.76  | 123.48      | 118.30   |
| 2   | A     | 2171 | A    | C4-C5-N7    | -5.75 | 107.82      | 110.70   |
| 6   | G     | 148  | VAL  | CA-CB-CG1   | 5.75  | 119.53      | 110.90   |
| 1   | B     | 1300 | G    | N1-C2-N2    | 5.75  | 121.38      | 116.20   |
| 3   | E     | 15   | G    | C5-C6-O6    | -5.75 | 125.15      | 128.60   |
| 2   | A     | 1888 | G    | P-O5'-C5'   | 5.74  | 130.09      | 120.90   |
| 4   | D     | 204  | PHE  | CB-CG-CD2   | 5.74  | 124.82      | 120.80   |
| 2   | A     | 2163 | A    | N9-C1'-C2'  | -5.74 | 105.69      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2144 | G    | C8-N9-C1'   | -5.74 | 119.54      | 127.00   |
| 2   | A     | 2152 | G    | C5-C6-O6    | -5.74 | 125.16      | 128.60   |
| 2   | A     | 2186 | G    | N1-C2-N2    | -5.73 | 111.04      | 116.20   |
| 2   | A     | 2119 | A    | O4'-C1'-N9  | 5.73  | 112.78      | 108.20   |
| 1   | B     | 1241 | G    | C6-N1-C2    | 5.73  | 128.54      | 125.10   |
| 2   | A     | 1861 | G    | C5-N7-C8    | 5.73  | 107.16      | 104.30   |
| 2   | A     | 1902 | C    | O4'-C1'-N1  | 5.73  | 112.78      | 108.20   |
| 2   | A     | 2123 | G    | O4'-C1'-N9  | 5.73  | 112.78      | 108.20   |
| 2   | A     | 2190 | G    | C5-C6-N1    | 5.73  | 114.36      | 111.50   |
| 4   | D     | 522  | PHE  | CB-CG-CD1   | 5.72  | 124.80      | 120.80   |
| 2   | A     | 1888 | G    | N3-C4-C5    | -5.72 | 125.74      | 128.60   |
| 3   | E     | 19   | G    | N1-C2-N2    | -5.72 | 111.05      | 116.20   |
| 2   | A     | 1850 | G    | N3-C4-C5    | 5.72  | 131.46      | 128.60   |
| 2   | A     | 1891 | G    | P-O3'-C3'   | -5.71 | 112.84      | 119.70   |
| 6   | G     | 136  | ILE  | O-C-N       | -5.71 | 113.56      | 122.70   |
| 2   | A     | 1902 | C    | C4'-C3'-C2' | -5.71 | 96.89       | 102.60   |
| 3   | E     | 27   | G    | C5-C6-N1    | -5.71 | 108.65      | 111.50   |
| 1   | B     | 1333 | A    | N1-C2-N3    | -5.70 | 126.45      | 129.30   |
| 2   | A     | 2153 | C    | C2-N3-C4    | -5.70 | 117.05      | 119.90   |
| 2   | A     | 1859 | U    | N1-C2-O2    | -5.69 | 118.82      | 122.80   |
| 2   | A     | 1866 | A    | N9-C4-C5    | 5.69  | 108.08      | 105.80   |
| 3   | E     | 46   | G    | C2-N3-C4    | 5.69  | 114.75      | 111.90   |
| 5   | F     | 199  | ALA  | N-CA-CB     | -5.69 | 102.13      | 110.10   |
| 2   | A     | 1847 | A    | N9-C4-C5    | 5.69  | 108.08      | 105.80   |
| 2   | A     | 1855 | U    | C1'-O4'-C4' | 5.69  | 114.45      | 109.90   |
| 2   | A     | 1881 | C    | P-O5'-C5'   | 5.68  | 129.99      | 120.90   |
| 2   | A     | 1906 | G    | N1-C2-N3    | -5.68 | 120.49      | 123.90   |
| 2   | A     | 2098 | U    | N3-C4-C5    | -5.68 | 111.19      | 114.60   |
| 2   | A     | 1840 | G    | C8-N9-C4    | -5.68 | 104.13      | 106.40   |
| 2   | A     | 1860 | G    | N3-C4-C5    | 5.68  | 131.44      | 128.60   |
| 2   | A     | 2121 | G    | C5-C6-O6    | -5.68 | 125.19      | 128.60   |
| 8   | I     | 9    | ARG  | NE-CZ-NH1   | 5.67  | 123.14      | 120.30   |
| 6   | G     | 12   | VAL  | CG1-CB-CG2  | -5.67 | 101.83      | 110.90   |
| 2   | A     | 2107 | G    | N1-C2-N3    | 5.67  | 127.30      | 123.90   |
| 3   | E     | 38   | A    | C5'-C4'-O4' | 5.66  | 115.89      | 109.10   |
| 2   | A     | 2128 | G    | C5-N7-C8    | 5.66  | 107.13      | 104.30   |
| 2   | A     | 2164 | C    | C5-C6-N1    | 5.66  | 123.83      | 121.00   |
| 1   | B     | 1297 | G    | C4-C5-C6    | 5.66  | 122.19      | 118.80   |
| 2   | A     | 2193 | G    | C4-C5-N7    | -5.66 | 108.54      | 110.80   |
| 5   | F     | 56   | ASP  | CB-CG-OD1   | -5.66 | 113.21      | 118.30   |
| 1   | B     | 1242 | G    | C4'-C3'-C2' | -5.66 | 96.94       | 102.60   |
| 2   | A     | 1834 | U    | P-O5'-C5'   | 5.66  | 129.95      | 120.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 1872 | A    | C5-N7-C8    | -5.66 | 101.07      | 103.90   |
| 3   | E     | 44   | A    | N9-C4-C5    | -5.66 | 103.54      | 105.80   |
| 3   | E     | 3    | C    | C5-C4-N4    | 5.65  | 124.16      | 120.20   |
| 3   | E     | 36   | A    | N3-C4-N9    | -5.65 | 122.88      | 127.40   |
| 2   | A     | 1871 | A    | P-O5'-C5'   | -5.65 | 111.86      | 120.90   |
| 2   | A     | 2190 | G    | C5-N7-C8    | 5.65  | 107.13      | 104.30   |
| 4   | D     | 257  | GLN  | O-C-N       | -5.65 | 113.66      | 122.70   |
| 6   | G     | 121  | PHE  | CB-CG-CD1   | -5.64 | 116.85      | 120.80   |
| 2   | A     | 2158 | A    | N7-C8-N9    | -5.64 | 110.98      | 113.80   |
| 3   | E     | 8    | U    | OP1-P-OP2   | -5.64 | 111.14      | 119.60   |
| 1   | B     | 1237 | C    | C6-N1-C2    | 5.63  | 122.55      | 120.30   |
| 1   | B     | 1237 | C    | N3-C4-C5    | -5.63 | 119.65      | 121.90   |
| 1   | B     | 1291 | U    | O4'-C1'-N1  | 5.63  | 112.70      | 108.20   |
| 5   | F     | 219  | GLY  | N-CA-C      | -5.63 | 99.03       | 113.10   |
| 5   | F     | 78   | PHE  | CB-CG-CD1   | -5.63 | 116.86      | 120.80   |
| 2   | A     | 2156 | G    | C6-N1-C2    | 5.62  | 128.47      | 125.10   |
| 3   | E     | 38   | A    | C8-N9-C4    | -5.62 | 103.55      | 105.80   |
| 1   | B     | 1292 | G    | N3-C4-N9    | 5.62  | 129.37      | 126.00   |
| 4   | D     | 4    | PHE  | CB-CA-C     | -5.62 | 99.16       | 110.40   |
| 3   | E     | 72   | C    | C5-C6-N1    | -5.62 | 118.19      | 121.00   |
| 2   | A     | 2165 | C    | P-O3'-C3'   | -5.61 | 112.96      | 119.70   |
| 4   | D     | 219  | ARG  | NH1-CZ-NH2  | -5.61 | 113.22      | 119.40   |
| 2   | A     | 2149 | U    | N3-C4-O4    | -5.61 | 115.47      | 119.40   |
| 3   | E     | 48   | U    | C4-C5-C6    | -5.61 | 116.33      | 119.70   |
| 2   | A     | 2126 | A    | OP1-P-OP2   | -5.61 | 111.19      | 119.60   |
| 2   | A     | 2164 | C    | OP1-P-OP2   | -5.61 | 111.19      | 119.60   |
| 1   | B     | 1336 | C    | O4'-C1'-N1  | 5.61  | 112.69      | 108.20   |
| 8   | I     | 78   | ARG  | NE-CZ-NH1   | 5.60  | 123.10      | 120.30   |
| 2   | A     | 1897 | G    | C3'-C2'-C1' | -5.60 | 97.02       | 101.50   |
| 2   | A     | 1864 | U    | P-O3'-C3'   | 5.60  | 126.42      | 119.70   |
| 2   | A     | 1849 | G    | C4-C5-N7    | 5.59  | 113.04      | 110.80   |
| 2   | A     | 2144 | G    | N3-C4-C5    | -5.59 | 125.80      | 128.60   |
| 5   | F     | 12   | ARG  | NE-CZ-NH2   | -5.59 | 117.50      | 120.30   |
| 3   | E     | 61   | U    | C5'-C4'-O4' | 5.59  | 115.81      | 109.10   |
| 1   | B     | 1245 | C    | N3-C4-N4    | 5.59  | 121.91      | 118.00   |
| 2   | A     | 2135 | A    | C4-C5-C6    | -5.59 | 114.21      | 117.00   |
| 2   | A     | 2173 | A    | N7-C8-N9    | -5.59 | 111.01      | 113.80   |
| 3   | E     | 41   | C    | N3-C4-C5    | 5.59  | 124.13      | 121.90   |
| 4   | D     | 333  | TYR  | CB-CG-CD1   | -5.58 | 117.65      | 121.00   |
| 7   | H     | 36   | LYS  | O-C-N       | -5.57 | 113.79      | 122.70   |
| 6   | G     | 82   | TYR  | CG-CD1-CE1  | -5.57 | 116.85      | 121.30   |
| 2   | A     | 2138 | G    | N7-C8-N9    | 5.56  | 115.88      | 113.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | F     | 51   | ASP  | CB-CG-OD2   | -5.56 | 113.29      | 118.30   |
| 4   | D     | 172  | ALA  | CB-CA-C     | -5.56 | 101.76      | 110.10   |
| 8   | I     | 108  | ARG  | NH1-CZ-NH2  | -5.56 | 113.28      | 119.40   |
| 3   | E     | 16   | C    | N1-C2-N3    | -5.56 | 115.31      | 119.20   |
| 5   | F     | 177  | LYS  | N-CA-CB     | -5.56 | 100.59      | 110.60   |
| 3   | E     | 14   | A    | O4'-C1'-N9  | 5.55  | 112.64      | 108.20   |
| 2   | A     | 2174 | C    | C5'-C4'-O4' | 5.55  | 115.76      | 109.10   |
| 1   | B     | 1332 | A    | C6-C5-N7    | -5.55 | 128.42      | 132.30   |
| 3   | E     | 50   | G    | N9-C4-C5    | 5.55  | 107.62      | 105.40   |
| 2   | A     | 1856 | U    | C4-C5-C6    | 5.54  | 123.03      | 119.70   |
| 2   | A     | 2159 | G    | C5'-C4'-O4' | 5.54  | 115.75      | 109.10   |
| 2   | A     | 2176 | A    | C5-C6-N1    | 5.54  | 120.47      | 117.70   |
| 2   | A     | 2111 | U    | N3-C2-O2    | 5.53  | 126.07      | 122.20   |
| 2   | A     | 2143 | C    | N3-C4-C5    | -5.53 | 119.69      | 121.90   |
| 4   | D     | 408  | VAL  | O-C-N       | -5.53 | 113.86      | 122.70   |
| 1   | B     | 1244 | G    | C6-C5-N7    | -5.52 | 127.09      | 130.40   |
| 2   | A     | 1852 | U    | O4'-C1'-N1  | 5.52  | 112.62      | 108.20   |
| 4   | D     | 547  | ARG  | CD-NE-CZ    | 5.52  | 131.33      | 123.60   |
| 8   | I     | 101  | ARG  | NE-CZ-NH1   | 5.52  | 123.06      | 120.30   |
| 1   | B     | 1300 | G    | C1'-O4'-C4' | -5.52 | 105.49      | 109.90   |
| 3   | E     | 5    | G    | C4'-C3'-C2' | -5.52 | 97.08       | 102.60   |
| 2   | A     | 1872 | A    | C6-N1-C2    | -5.51 | 115.29      | 118.60   |
| 3   | E     | 38   | A    | C8-N9-C1'   | -5.51 | 117.78      | 127.70   |
| 1   | B     | 1244 | G    | N1-C6-O6    | -5.51 | 116.59      | 119.90   |
| 3   | E     | 30   | G    | C3'-C2'-C1' | -5.51 | 97.09       | 101.50   |
| 1   | B     | 1303 | C    | O4'-C1'-N1  | 5.51  | 112.61      | 108.20   |
| 2   | A     | 2145 | C    | C2'-C3'-O3' | 5.50  | 122.51      | 113.70   |
| 3   | E     | 68   | C    | N3-C4-N4    | 5.50  | 121.85      | 118.00   |
| 1   | B     | 1334 | G    | C5-N7-C8    | 5.50  | 107.05      | 104.30   |
| 2   | A     | 2137 | U    | N1-C2-O2    | 5.50  | 126.65      | 122.80   |
| 2   | A     | 1897 | G    | N3-C4-C5    | -5.50 | 125.85      | 128.60   |
| 2   | A     | 2152 | G    | C5'-C4'-O4' | 5.50  | 115.70      | 109.10   |
| 2   | A     | 1878 | G    | C3'-C2'-C1' | -5.50 | 97.10       | 101.50   |
| 2   | A     | 2171 | A    | C3'-C2'-C1' | -5.50 | 97.10       | 101.50   |
| 4   | D     | 209  | GLU  | C-N-CA      | 5.50  | 133.84      | 122.30   |
| 8   | I     | 116  | ALA  | CB-CA-C     | -5.50 | 101.86      | 110.10   |
| 2   | A     | 1903 | G    | C5-N7-C8    | 5.49  | 107.05      | 104.30   |
| 3   | E     | 18   | U    | C5-C6-N1    | -5.49 | 119.95      | 122.70   |
| 2   | A     | 2179 | C    | C2-N3-C4    | -5.49 | 117.16      | 119.90   |
| 2   | A     | 1904 | G    | C4-C5-N7    | -5.48 | 108.61      | 110.80   |
| 8   | I     | 63   | VAL  | O-C-N       | -5.48 | 113.93      | 122.70   |
| 2   | A     | 2185 | U    | C6-N1-C2    | -5.48 | 117.71      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2159 | G    | C5'-C4'-C3' | -5.48 | 107.24      | 116.00   |
| 2   | A     | 2186 | G    | O4'-C1'-N9  | 5.48  | 112.58      | 108.20   |
| 1   | B     | 1305 | G    | C4-C5-C6    | -5.47 | 115.52      | 118.80   |
| 4   | D     | 333  | TYR  | N-CA-CB     | 5.47  | 120.45      | 110.60   |
| 3   | E     | 12   | G    | O4'-C1'-N9  | 5.47  | 112.57      | 108.20   |
| 2   | A     | 1875 | G    | C5-C6-N1    | -5.46 | 108.77      | 111.50   |
| 2   | A     | 2159 | G    | C6-N1-C2    | -5.46 | 121.82      | 125.10   |
| 2   | A     | 2126 | A    | C2-N3-C4    | 5.46  | 113.33      | 110.60   |
| 4   | D     | 467  | LEU  | O-C-N       | -5.46 | 113.96      | 122.70   |
| 6   | G     | 111  | ARG  | NE-CZ-NH1   | 5.46  | 123.03      | 120.30   |
| 3   | E     | 2    | G    | N1-C2-N3    | -5.46 | 120.63      | 123.90   |
| 3   | E     | 24   | C    | N3-C2-O2    | -5.45 | 118.08      | 121.90   |
| 4   | D     | 83   | GLU  | O-C-N       | -5.45 | 113.98      | 122.70   |
| 6   | G     | 143  | ASP  | CB-CG-OD1   | 5.45  | 123.20      | 118.30   |
| 1   | B     | 1295 | U    | N3-C4-O4    | 5.45  | 123.21      | 119.40   |
| 4   | D     | 262  | GLU  | CA-CB-CG    | 5.44  | 125.38      | 113.40   |
| 2   | A     | 1863 | G    | C2-N3-C4    | 5.44  | 114.62      | 111.90   |
| 3   | E     | 19   | G    | C4-C5-N7    | -5.44 | 108.62      | 110.80   |
| 3   | E     | 23   | G    | P-O5'-C5'   | 5.44  | 129.60      | 120.90   |
| 4   | D     | 200  | TRP  | CZ3-CH2-CZ2 | -5.43 | 115.08      | 121.60   |
| 2   | A     | 1880 | U    | C5-C6-N1    | 5.43  | 125.42      | 122.70   |
| 4   | D     | 283  | ARG  | NH1-CZ-NH2  | -5.43 | 113.42      | 119.40   |
| 1   | B     | 1300 | G    | N1-C6-O6    | 5.43  | 123.16      | 119.90   |
| 3   | E     | 8    | U    | C5-C4-O4    | -5.43 | 122.64      | 125.90   |
| 2   | A     | 2125 | G    | C5-C6-N1    | -5.43 | 108.79      | 111.50   |
| 3   | E     | 39   | A    | C5-N7-C8    | -5.43 | 101.19      | 103.90   |
| 3   | E     | 1    | C    | N3-C4-C5    | -5.42 | 119.73      | 121.90   |
| 2   | A     | 1885 | A    | C8-N9-C4    | 5.42  | 107.97      | 105.80   |
| 3   | E     | 38   | A    | N9-C4-C5    | 5.42  | 107.97      | 105.80   |
| 1   | B     | 1300 | G    | P-O5'-C5'   | 5.42  | 129.57      | 120.90   |
| 2   | A     | 1887 | C    | C2-N3-C4    | -5.42 | 117.19      | 119.90   |
| 2   | A     | 2096 | C    | N3-C4-C5    | 5.42  | 124.07      | 121.90   |
| 2   | A     | 2121 | G    | N3-C2-N2    | 5.42  | 123.69      | 119.90   |
| 2   | A     | 2190 | G    | C6-C5-N7    | 5.41  | 133.65      | 130.40   |
| 8   | I     | 108  | ARG  | CD-NE-CZ    | -5.41 | 116.02      | 123.60   |
| 2   | A     | 2135 | A    | C5-C6-N1    | 5.41  | 120.40      | 117.70   |
| 3   | E     | 48   | U    | N1-C2-O2    | 5.41  | 126.58      | 122.80   |
| 2   | A     | 1854 | A    | C6-N1-C2    | -5.40 | 115.36      | 118.60   |
| 3   | E     | 48   | U    | C2'-C3'-O3' | 5.40  | 122.34      | 113.70   |
| 3   | E     | 52   | C    | P-O5'-C5'   | -5.40 | 112.26      | 120.90   |
| 5   | F     | 181  | ASP  | CB-CG-OD2   | -5.40 | 113.44      | 118.30   |
| 4   | D     | 52   | MET  | CG-SD-CE    | -5.40 | 91.57       | 100.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2153 | C    | N3-C2-O2    | -5.39 | 118.12      | 121.90   |
| 2   | A     | 1849 | G    | C5-N7-C8    | -5.39 | 101.60      | 104.30   |
| 3   | E     | 15   | G    | P-O3'-C3'   | 5.39  | 126.17      | 119.70   |
| 7   | H     | 42   | VAL  | C-N-CA      | 5.39  | 135.18      | 121.70   |
| 2   | A     | 2171 | A    | O4'-C1'-N9  | 5.39  | 112.51      | 108.20   |
| 3   | E     | 75   | C    | C5-C6-N1    | -5.39 | 118.31      | 121.00   |
| 4   | D     | 389  | ALA  | CB-CA-C     | 5.39  | 118.18      | 110.10   |
| 8   | I     | 52   | ARG  | NH1-CZ-NH2  | -5.39 | 113.47      | 119.40   |
| 3   | E     | 48   | U    | N3-C4-C5    | 5.38  | 117.83      | 114.60   |
| 6   | G     | 76   | PHE  | CB-CG-CD1   | -5.38 | 117.03      | 120.80   |
| 2   | A     | 1893 | C    | N1-C1'-C2'  | -5.38 | 106.08      | 112.00   |
| 3   | E     | 40   | C    | C5-C4-N4    | -5.38 | 116.43      | 120.20   |
| 3   | E     | 48   | U    | C2-N3-C4    | -5.38 | 123.77      | 127.00   |
| 2   | A     | 1854 | A    | C2-N3-C4    | -5.38 | 107.91      | 110.60   |
| 3   | E     | 24   | C    | C1'-O4'-C4' | -5.38 | 105.60      | 109.90   |
| 2   | A     | 2140 | G    | C2-N3-C4    | 5.37  | 114.59      | 111.90   |
| 3   | E     | 59   | A    | P-O3'-C3'   | -5.37 | 113.25      | 119.70   |
| 4   | D     | 68   | ASP  | CB-CG-OD1   | -5.37 | 113.47      | 118.30   |
| 4   | D     | 175  | ARG  | NE-CZ-NH1   | 5.37  | 122.98      | 120.30   |
| 3   | E     | 23   | G    | C4-C5-C6    | -5.37 | 115.58      | 118.80   |
| 8   | I     | 25   | PHE  | CD1-CG-CD2  | -5.36 | 111.33      | 118.30   |
| 2   | A     | 2106 | U    | O4'-C1'-N1  | 5.36  | 112.49      | 108.20   |
| 2   | A     | 2176 | A    | N9-C4-C5    | 5.36  | 107.94      | 105.80   |
| 8   | I     | 32   | ASP  | CB-CG-OD1   | 5.36  | 123.12      | 118.30   |
| 1   | B     | 1243 | C    | OP1-P-O3'   | 5.36  | 116.98      | 105.20   |
| 3   | E     | 62   | C    | N3-C4-N4    | 5.36  | 121.75      | 118.00   |
| 2   | A     | 1850 | G    | N1-C2-N3    | -5.35 | 120.69      | 123.90   |
| 3   | E     | 74   | A    | C4-C5-N7    | 5.35  | 113.38      | 110.70   |
| 1   | B     | 1300 | G    | C5'-C4'-C3' | -5.35 | 107.44      | 116.00   |
| 2   | A     | 1899 | A    | C4-C5-N7    | 5.35  | 113.37      | 110.70   |
| 1   | B     | 1236 | A    | N7-C8-N9    | 5.35  | 116.47      | 113.80   |
| 2   | A     | 1851 | U    | N1-C2-O2    | 5.35  | 126.54      | 122.80   |
| 2   | A     | 1857 | G    | C5-N7-C8    | -5.34 | 101.63      | 104.30   |
| 2   | A     | 2102 | G    | C5-N7-C8    | 5.34  | 106.97      | 104.30   |
| 8   | I     | 17   | PHE  | CB-CG-CD2   | 5.34  | 124.54      | 120.80   |
| 2   | A     | 1873 | G    | C4-C5-N7    | 5.34  | 112.94      | 110.80   |
| 2   | A     | 1872 | A    | N9-C1'-C2'  | -5.34 | 106.13      | 112.00   |
| 1   | B     | 1245 | C    | C4'-C3'-C2' | -5.34 | 97.26       | 102.60   |
| 2   | A     | 1881 | C    | N3-C2-O2    | -5.33 | 118.17      | 121.90   |
| 1   | B     | 1303 | C    | C2-N1-C1'   | 5.33  | 124.66      | 118.80   |
| 3   | E     | 5    | G    | P-O5'-C5'   | -5.33 | 112.38      | 120.90   |
| 2   | A     | 1888 | G    | N1-C2-N2    | -5.33 | 111.41      | 116.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 21   | U    | C6-N1-C2    | -5.33 | 117.80      | 121.00   |
| 2   | A     | 2147 | A    | N7-C8-N9    | 5.32  | 116.46      | 113.80   |
| 3   | E     | 15   | G    | C2-N3-C4    | 5.32  | 114.56      | 111.90   |
| 4   | D     | 228  | TRP  | CE2-CD2-CG  | -5.32 | 103.04      | 107.30   |
| 3   | E     | 56   | U    | N1-C2-O2    | -5.32 | 119.08      | 122.80   |
| 2   | A     | 2138 | G    | C2-N3-C4    | 5.32  | 114.56      | 111.90   |
| 2   | A     | 1857 | G    | N9-C4-C5    | 5.31  | 107.53      | 105.40   |
| 2   | A     | 1884 | G    | C5-C6-O6    | -5.31 | 125.41      | 128.60   |
| 4   | D     | 73   | TYR  | CG-CD2-CE2  | -5.31 | 117.05      | 121.30   |
| 6   | G     | 147  | ARG  | CG-CD-NE    | -5.31 | 100.65      | 111.80   |
| 1   | B     | 1239 | A    | C4-C5-C6    | -5.31 | 114.35      | 117.00   |
| 3   | E     | 4    | G    | P-O3'-C3'   | 5.31  | 126.07      | 119.70   |
| 5   | F     | 22   | ASP  | CB-CG-OD1   | 5.31  | 123.08      | 118.30   |
| 2   | A     | 2112 | G    | N3-C2-N2    | -5.30 | 116.19      | 119.90   |
| 2   | A     | 2173 | A    | C4-C5-N7    | -5.30 | 108.05      | 110.70   |
| 2   | A     | 2188 | U    | C5-C6-N1    | 5.30  | 125.35      | 122.70   |
| 3   | E     | 31   | G    | N1-C2-N3    | -5.30 | 120.72      | 123.90   |
| 2   | A     | 2109 | U    | C3'-C2'-C1' | 5.30  | 105.74      | 101.50   |
| 1   | B     | 1237 | C    | P-O3'-C3'   | 5.30  | 126.06      | 119.70   |
| 2   | A     | 1884 | G    | C4-C5-N7    | -5.30 | 108.68      | 110.80   |
| 2   | A     | 1906 | G    | C8-N9-C4    | -5.30 | 104.28      | 106.40   |
| 3   | E     | 8    | U    | C6-N1-C2    | -5.30 | 117.82      | 121.00   |
| 3   | E     | 43   | G    | N1-C6-O6    | -5.30 | 116.72      | 119.90   |
| 3   | E     | 66   | C    | N3-C2-O2    | -5.30 | 118.19      | 121.90   |
| 3   | E     | 70   | C    | C5-C4-N4    | -5.30 | 116.49      | 120.20   |
| 2   | A     | 1866 | A    | N1-C6-N6    | 5.29  | 121.77      | 118.60   |
| 2   | A     | 1890 | A    | N1-C2-N3    | -5.29 | 126.66      | 129.30   |
| 2   | A     | 1856 | U    | C2-N3-C4    | -5.29 | 123.83      | 127.00   |
| 3   | E     | 27   | G    | N3-C2-N2    | 5.29  | 123.60      | 119.90   |
| 3   | E     | 47   | G    | C5-C6-N1    | 5.28  | 114.14      | 111.50   |
| 3   | E     | 17   | C    | O5'-C5'-C4' | 5.28  | 121.73      | 111.70   |
| 2   | A     | 2123 | G    | C8-N9-C4    | -5.28 | 104.29      | 106.40   |
| 2   | A     | 2142 | A    | P-O5'-C5'   | -5.28 | 112.45      | 120.90   |
| 3   | E     | 15   | G    | C4-C5-C6    | -5.28 | 115.63      | 118.80   |
| 4   | D     | 461  | VAL  | CB-CA-C     | -5.28 | 101.38      | 111.40   |
| 1   | B     | 1298 | U    | C6-N1-C1'   | -5.27 | 113.82      | 121.20   |
| 2   | A     | 2160 | C    | C5-C6-N1    | -5.27 | 118.36      | 121.00   |
| 3   | E     | 52   | C    | N1-C2-N3    | -5.27 | 115.51      | 119.20   |
| 8   | I     | 69   | ARG  | NE-CZ-NH2   | -5.27 | 117.67      | 120.30   |
| 2   | A     | 1903 | G    | C6-N1-C2    | 5.26  | 128.26      | 125.10   |
| 2   | A     | 2189 | U    | C1'-O4'-C4' | 5.26  | 114.11      | 109.90   |
| 3   | E     | 17   | C    | N3-C4-N4    | 5.26  | 121.68      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2186 | G    | N7-C8-N9    | 5.26  | 115.73      | 113.10   |
| 2   | A     | 2113 | U    | N3-C2-O2    | -5.26 | 118.52      | 122.20   |
| 4   | D     | 99   | ASN  | CA-CB-CG    | -5.26 | 101.83      | 113.40   |
| 1   | B     | 1302 | C    | C2-N1-C1'   | 5.26  | 124.58      | 118.80   |
| 1   | B     | 1237 | C    | C5-C6-N1    | -5.25 | 118.37      | 121.00   |
| 6   | G     | 132  | ARG  | NE-CZ-NH2   | 5.25  | 122.93      | 120.30   |
| 2   | A     | 1905 | C    | C5'-C4'-O4' | 5.25  | 115.40      | 109.10   |
| 5   | F     | 112  | ASP  | CB-CG-OD1   | 5.25  | 123.03      | 118.30   |
| 2   | A     | 2127 | G    | C6-N1-C2    | -5.25 | 121.95      | 125.10   |
| 2   | A     | 1867 | G    | C4'-C3'-C2' | -5.25 | 97.35       | 102.60   |
| 3   | E     | 63   | C    | C4-C5-C6    | -5.25 | 114.78      | 117.40   |
| 2   | A     | 1887 | C    | OP2-P-O3'   | 5.24  | 116.74      | 105.20   |
| 6   | G     | 122  | ASP  | O-C-N       | -5.24 | 114.29      | 123.20   |
| 2   | A     | 1845 | G    | N9-C4-C5    | 5.24  | 107.50      | 105.40   |
| 2   | A     | 2132 | U    | C5-C6-N1    | -5.24 | 120.08      | 122.70   |
| 5   | F     | 151  | GLU  | CB-CA-C     | -5.23 | 99.93       | 110.40   |
| 2   | A     | 2166 | U    | C1'-O4'-C4' | -5.23 | 105.71      | 109.90   |
| 3   | E     | 26   | C    | C2-N3-C4    | 5.23  | 122.52      | 119.90   |
| 2   | A     | 1853 | A    | O3'-P-O5'   | 5.23  | 113.94      | 104.00   |
| 2   | A     | 1868 | C    | N3-C4-N4    | -5.23 | 114.34      | 118.00   |
| 2   | A     | 2127 | G    | C6-C5-N7    | -5.23 | 127.26      | 130.40   |
| 4   | D     | 434  | LYS  | O-C-N       | -5.23 | 114.31      | 123.20   |
| 2   | A     | 1840 | G    | N3-C4-N9    | -5.23 | 122.86      | 126.00   |
| 2   | A     | 1866 | A    | O5'-P-OP1   | -5.23 | 101.00      | 105.70   |
| 2   | A     | 2188 | U    | C4'-C3'-C2' | 5.23  | 107.83      | 102.60   |
| 1   | B     | 1303 | C    | P-O5'-C5'   | 5.22  | 129.26      | 120.90   |
| 3   | E     | 14   | A    | N9-C4-C5    | -5.22 | 103.71      | 105.80   |
| 1   | B     | 1332 | A    | N1-C2-N3    | -5.22 | 126.69      | 129.30   |
| 2   | A     | 1857 | G    | OP1-P-OP2   | -5.22 | 111.77      | 119.60   |
| 4   | D     | 376  | ASP  | CB-CG-OD2   | 5.22  | 123.00      | 118.30   |
| 8   | I     | 115  | MET  | O-C-N       | -5.22 | 114.35      | 122.70   |
| 3   | E     | 11   | A    | C5-C6-N6    | -5.22 | 119.53      | 123.70   |
| 5   | F     | 122  | ARG  | CD-NE-CZ    | 5.22  | 130.90      | 123.60   |
| 2   | A     | 2120 | G    | C2-N3-C4    | 5.21  | 114.51      | 111.90   |
| 2   | A     | 2121 | G    | C6-C5-N7    | 5.21  | 133.53      | 130.40   |
| 4   | D     | 66   | GLN  | CG-CD-OE1   | -5.21 | 111.17      | 121.60   |
| 3   | E     | 10   | G    | C5-N7-C8    | 5.21  | 106.91      | 104.30   |
| 3   | E     | 52   | C    | O4'-C1'-N1  | 5.21  | 112.37      | 108.20   |
| 4   | D     | 53   | ALA  | O-C-N       | -5.21 | 114.34      | 123.20   |
| 2   | A     | 2171 | A    | N1-C2-N3    | 5.21  | 131.90      | 129.30   |
| 4   | D     | 498  | SER  | CA-C-O      | 5.21  | 131.03      | 120.10   |
| 2   | A     | 2112 | G    | C2-N3-C4    | -5.21 | 109.30      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | D     | 494  | ALA  | N-CA-CB     | -5.21 | 102.81      | 110.10   |
| 2   | A     | 1842 | G    | C6-C5-N7    | 5.20  | 133.52      | 130.40   |
| 2   | A     | 1900 | A    | C4-C5-N7    | -5.20 | 108.10      | 110.70   |
| 2   | A     | 2159 | G    | N3-C2-N2    | -5.20 | 116.26      | 119.90   |
| 2   | A     | 1861 | G    | C6-N1-C2    | -5.20 | 121.98      | 125.10   |
| 2   | A     | 1864 | U    | OP1-P-OP2   | -5.20 | 111.80      | 119.60   |
| 2   | A     | 1902 | C    | C1'-O4'-C4' | -5.20 | 105.74      | 109.90   |
| 1   | B     | 1237 | C    | O4'-C1'-N1  | 5.19  | 112.35      | 108.20   |
| 3   | E     | 19   | G    | C4-C5-C6    | 5.19  | 121.91      | 118.80   |
| 5   | F     | 7    | ARG  | CG-CD-NE    | -5.19 | 100.91      | 111.80   |
| 3   | E     | 17   | C    | C5-C4-N4    | -5.18 | 116.57      | 120.20   |
| 2   | A     | 1866 | A    | C4-C5-C6    | 5.18  | 119.59      | 117.00   |
| 7   | H     | 35   | LEU  | CB-CA-C     | -5.18 | 100.35      | 110.20   |
| 2   | A     | 2118 | U    | N3-C4-O4    | 5.18  | 123.03      | 119.40   |
| 2   | A     | 2144 | G    | C4-N9-C1'   | 5.17  | 133.22      | 126.50   |
| 2   | A     | 2161 | C    | N3-C2-O2    | -5.17 | 118.28      | 121.90   |
| 4   | D     | 365  | LEU  | CB-CG-CD2   | -5.17 | 102.21      | 111.00   |
| 2   | A     | 2185 | U    | C5-C4-O4    | -5.17 | 122.80      | 125.90   |
| 3   | E     | 22   | A    | C5'-C4'-C3' | -5.17 | 107.73      | 116.00   |
| 4   | D     | 392  | ASP  | O-C-N       | -5.17 | 114.43      | 122.70   |
| 2   | A     | 1895 | C    | N3-C4-C5    | -5.16 | 119.83      | 121.90   |
| 2   | A     | 2120 | G    | P-O3'-C3'   | 5.16  | 125.89      | 119.70   |
| 3   | E     | 74   | A    | N3-C4-N9    | 5.16  | 131.53      | 127.40   |
| 4   | D     | 2    | ALA  | CB-CA-C     | 5.16  | 117.83      | 110.10   |
| 2   | A     | 2162 | G    | OP2-P-O3'   | 5.16  | 116.54      | 105.20   |
| 4   | D     | 246  | SER  | O-C-N       | -5.16 | 114.45      | 122.70   |
| 1   | B     | 1243 | C    | C2-N3-C4    | -5.15 | 117.32      | 119.90   |
| 2   | A     | 1851 | U    | N3-C4-C5    | 5.15  | 117.69      | 114.60   |
| 2   | A     | 2144 | G    | C5-N7-C8    | 5.15  | 106.88      | 104.30   |
| 2   | A     | 2190 | G    | N1-C2-N3    | -5.15 | 120.81      | 123.90   |
| 4   | D     | 138  | HIS  | N-CA-CB     | 5.15  | 119.87      | 110.60   |
| 2   | A     | 2104 | C    | C3'-C2'-C1' | 5.14  | 105.62      | 101.50   |
| 2   | A     | 1888 | G    | O4'-C1'-N9  | 5.14  | 112.31      | 108.20   |
| 2   | A     | 2094 | A    | N9-C4-C5    | -5.14 | 103.74      | 105.80   |
| 2   | A     | 2107 | G    | N1-C6-O6    | -5.14 | 116.82      | 119.90   |
| 2   | A     | 1902 | C    | N1-C2-O2    | 5.13  | 121.98      | 118.90   |
| 2   | A     | 2104 | C    | C2-N3-C4    | -5.13 | 117.33      | 119.90   |
| 3   | E     | 19   | G    | N9-C4-C5    | 5.13  | 107.45      | 105.40   |
| 4   | D     | 171  | VAL  | CB-CA-C     | -5.13 | 101.65      | 111.40   |
| 8   | I     | 80   | GLY  | N-CA-C      | -5.13 | 100.27      | 113.10   |
| 2   | A     | 1899 | A    | C8-N9-C4    | -5.13 | 103.75      | 105.80   |
| 1   | B     | 1297 | G    | C4-C5-N7    | 5.12  | 112.85      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2177 | C    | O5'-C5'-C4' | -5.12 | 101.96      | 111.70   |
| 3   | E     | 22   | A    | N7-C8-N9    | -5.12 | 111.24      | 113.80   |
| 2   | A     | 2101 | A    | N1-C2-N3    | 5.12  | 131.86      | 129.30   |
| 3   | E     | 16   | C    | OP1-P-OP2   | -5.12 | 111.92      | 119.60   |
| 3   | E     | 44   | A    | N3-C4-N9    | 5.12  | 131.50      | 127.40   |
| 2   | A     | 1871 | A    | N1-C6-N6    | 5.12  | 121.67      | 118.60   |
| 2   | A     | 1891 | G    | N1-C2-N2    | -5.12 | 111.59      | 116.20   |
| 2   | A     | 2126 | A    | C3'-C2'-C1' | 5.12  | 105.59      | 101.50   |
| 3   | E     | 26   | C    | N1-C1'-C2'  | -5.12 | 106.37      | 112.00   |
| 3   | E     | 53   | G    | P-O3'-C3'   | 5.11  | 125.83      | 119.70   |
| 1   | B     | 1294 | G    | O4'-C1'-N9  | 5.11  | 112.29      | 108.20   |
| 2   | A     | 1880 | U    | C2'-C3'-O3' | 5.11  | 121.87      | 113.70   |
| 2   | A     | 2167 | U    | N1-C2-N3    | -5.11 | 111.84      | 114.90   |
| 7   | H     | 42   | VAL  | O-C-N       | -5.11 | 114.53      | 122.70   |
| 1   | B     | 1301 | U    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 2   | A     | 2129 | C    | C1'-O4'-C4' | -5.10 | 105.82      | 109.90   |
| 3   | E     | 18   | U    | C4-C5-C6    | 5.10  | 122.76      | 119.70   |
| 3   | E     | 50   | G    | C4-C5-N7    | -5.10 | 108.76      | 110.80   |
| 1   | B     | 1302 | C    | C5-C6-N1    | 5.10  | 123.55      | 121.00   |
| 2   | A     | 1835 | G    | N3-C2-N2    | 5.10  | 123.47      | 119.90   |
| 3   | E     | 17   | C    | C6-N1-C1'   | -5.10 | 114.68      | 120.80   |
| 2   | A     | 1897 | G    | N3-C2-N2    | 5.10  | 123.47      | 119.90   |
| 4   | D     | 6    | TYR  | CB-CG-CD1   | -5.10 | 117.94      | 121.00   |
| 3   | E     | 18   | U    | N3-C4-C5    | -5.09 | 111.54      | 114.60   |
| 2   | A     | 1885 | A    | C5-C6-N1    | -5.09 | 115.15      | 117.70   |
| 4   | D     | 496  | VAL  | CA-CB-CG2   | 5.09  | 118.54      | 110.90   |
| 2   | A     | 1852 | U    | N3-C4-O4    | -5.09 | 115.84      | 119.40   |
| 3   | E     | 31   | G    | N3-C4-C5    | 5.09  | 131.15      | 128.60   |
| 2   | A     | 2107 | G    | OP2-P-O3'   | 5.09  | 116.39      | 105.20   |
| 1   | B     | 1297 | G    | C4'-C3'-C2' | 5.09  | 107.69      | 102.60   |
| 2   | A     | 2119 | A    | OP2-P-O3'   | 5.08  | 116.38      | 105.20   |
| 4   | D     | 200  | TRP  | CD1-NE1-CE2 | -5.08 | 104.42      | 109.00   |
| 2   | A     | 2173 | A    | C4'-C3'-C2' | 5.08  | 107.68      | 102.60   |
| 6   | G     | 96   | TRP  | CG-CD2-CE3  | -5.08 | 129.33      | 133.90   |
| 8   | I     | 115  | MET  | CG-SD-CE    | -5.08 | 92.07       | 100.20   |
| 1   | B     | 1244 | G    | O4'-C1'-C2' | 5.08  | 112.17      | 107.60   |
| 3   | E     | 50   | G    | C8-N9-C4    | -5.08 | 104.37      | 106.40   |
| 4   | D     | 275  | TRP  | CZ3-CH2-CZ2 | -5.08 | 115.51      | 121.60   |
| 2   | A     | 1867 | G    | N7-C8-N9    | -5.08 | 110.56      | 113.10   |
| 2   | A     | 2135 | A    | N1-C2-N3    | -5.07 | 126.76      | 129.30   |
| 4   | D     | 379  | THR  | N-CA-CB     | 5.07  | 119.94      | 110.30   |
| 8   | I     | 118  | ARG  | NE-CZ-NH2   | 5.07  | 122.84      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | B     | 1289 | A    | C8-N9-C4    | -5.07 | 103.77      | 105.80   |
| 2   | A     | 1858 | A    | C4'-C3'-C2' | -5.07 | 97.53       | 102.60   |
| 3   | E     | 47   | G    | P-O3'-C3'   | -5.07 | 113.61      | 119.70   |
| 2   | A     | 2109 | U    | C5'-C4'-C3' | -5.07 | 107.89      | 116.00   |
| 5   | F     | 181  | ASP  | CB-CG-OD1   | 5.07  | 122.86      | 118.30   |
| 6   | G     | 47   | LYS  | O-C-N       | -5.07 | 114.60      | 122.70   |
| 6   | G     | 7    | TYR  | CG-CD2-CE2  | -5.06 | 117.25      | 121.30   |
| 2   | A     | 2133 | G    | C8-N9-C4    | 5.06  | 108.42      | 106.40   |
| 2   | A     | 2182 | U    | O4'-C1'-N1  | 5.06  | 112.25      | 108.20   |
| 3   | E     | 12   | G    | C5-C6-O6    | -5.06 | 125.56      | 128.60   |
| 3   | E     | 74   | A    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 3   | E     | 27   | G    | C8-N9-C4    | -5.06 | 104.38      | 106.40   |
| 3   | E     | 14   | A    | C4-N9-C1'   | 5.05  | 135.40      | 126.30   |
| 4   | D     | 93   | ALA  | N-CA-CB     | 5.05  | 117.18      | 110.10   |
| 4   | D     | 294  | PHE  | CG-CD1-CE1  | -5.05 | 115.24      | 120.80   |
| 5   | F     | 148  | ASN  | N-CA-C      | -5.05 | 97.36       | 111.00   |
| 2   | A     | 1850 | G    | C6-N1-C2    | 5.05  | 128.13      | 125.10   |
| 5   | F     | 119  | ASP  | CA-C-O      | 5.05  | 130.70      | 120.10   |
| 3   | E     | 7    | G    | N3-C4-C5    | -5.05 | 126.08      | 128.60   |
| 1   | B     | 1333 | A    | C5-N7-C8    | 5.04  | 106.42      | 103.90   |
| 3   | E     | 4    | G    | N3-C4-N9    | 5.04  | 129.03      | 126.00   |
| 2   | A     | 1836 | C    | O4'-C1'-N1  | 5.04  | 112.23      | 108.20   |
| 3   | E     | 50   | G    | OP1-P-OP2   | -5.04 | 112.04      | 119.60   |
| 8   | I     | 94   | ARG  | NE-CZ-NH2   | -5.04 | 117.78      | 120.30   |
| 2   | A     | 1835 | G    | C5-C6-O6    | -5.04 | 125.58      | 128.60   |
| 2   | A     | 1875 | G    | N1-C2-N3    | -5.04 | 120.88      | 123.90   |
| 2   | A     | 2119 | A    | N7-C8-N9    | -5.04 | 111.28      | 113.80   |
| 3   | E     | 27   | G    | C4-C5-N7    | 5.04  | 112.81      | 110.80   |
| 3   | E     | 42   | C    | C4'-C3'-C2' | -5.04 | 97.56       | 102.60   |
| 2   | A     | 2175 | C    | N1-C2-N3    | 5.04  | 122.73      | 119.20   |
| 3   | E     | 25   | U    | N3-C2-O2    | 5.04  | 125.73      | 122.20   |
| 3   | E     | 49   | C    | C2-N3-C4    | -5.04 | 117.38      | 119.90   |
| 8   | I     | 134  | VAL  | CA-CB-CG2   | -5.04 | 103.35      | 110.90   |
| 1   | B     | 1303 | C    | C3'-C2'-C1' | -5.03 | 97.47       | 101.50   |
| 2   | A     | 1860 | G    | C4'-C3'-C2' | -5.03 | 97.57       | 102.60   |
| 2   | A     | 1901 | A    | C5'-C4'-O4' | 5.03  | 115.14      | 109.10   |
| 2   | A     | 2190 | G    | N1-C6-O6    | 5.03  | 122.92      | 119.90   |
| 2   | A     | 1897 | G    | P-O5'-C5'   | -5.03 | 112.86      | 120.90   |
| 2   | A     | 1857 | G    | N1-C6-O6    | 5.02  | 122.91      | 119.90   |
| 2   | A     | 1870 | C    | C1'-O4'-C4' | -5.02 | 105.88      | 109.90   |
| 8   | I     | 49   | LEU  | CB-CA-C     | 5.02  | 119.74      | 110.20   |
| 8   | I     | 25   | PHE  | CG-CD1-CE1  | 5.02  | 126.32      | 120.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | A     | 2189 | U    | N1-C2-O2   | -5.02 | 119.29      | 122.80   |
| 4   | D     | 420  | THR  | CB-CA-C    | -5.01 | 98.06       | 111.60   |
| 8   | I     | 25   | PHE  | CG-CD2-CE2 | 5.01  | 126.31      | 120.80   |
| 2   | A     | 2153 | C    | N3-C4-C5   | -5.01 | 119.90      | 121.90   |
| 2   | A     | 2174 | C    | OP1-P-OP2  | -5.01 | 112.09      | 119.60   |
| 3   | E     | 22   | A    | P-O3'-C3'  | 5.01  | 125.71      | 119.70   |
| 3   | E     | 1    | C    | O4'-C1'-N1 | 5.00  | 112.20      | 108.20   |
| 3   | E     | 60   | A    | C5-N7-C8   | 5.00  | 106.40      | 103.90   |

There are no chirality outliers.

All (178) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 2   | A     | 1835 | G    | Sidechain |
| 2   | A     | 1838 | C    | Sidechain |
| 2   | A     | 1839 | G    | Sidechain |
| 2   | A     | 1840 | G    | Sidechain |
| 2   | A     | 1842 | G    | Sidechain |
| 2   | A     | 1843 | C    | Sidechain |
| 2   | A     | 1845 | G    | Sidechain |
| 2   | A     | 1846 | G    | Sidechain |
| 2   | A     | 1850 | G    | Sidechain |
| 2   | A     | 1857 | G    | Sidechain |
| 2   | A     | 1858 | A    | Sidechain |
| 2   | A     | 1859 | U    | Sidechain |
| 2   | A     | 1862 | G    | Sidechain |
| 2   | A     | 1863 | G    | Sidechain |
| 2   | A     | 1865 | U    | Sidechain |
| 2   | A     | 1868 | C    | Sidechain |
| 2   | A     | 1869 | G    | Sidechain |
| 2   | A     | 1874 | C    | Sidechain |
| 2   | A     | 1876 | A    | Sidechain |
| 2   | A     | 1878 | G    | Sidechain |
| 2   | A     | 1882 | U    | Sidechain |
| 2   | A     | 1884 | G    | Sidechain |
| 2   | A     | 1886 | U    | Sidechain |
| 2   | A     | 1888 | G    | Sidechain |
| 2   | A     | 1889 | A    | Sidechain |
| 2   | A     | 1891 | G    | Sidechain |
| 2   | A     | 1894 | C    | Sidechain |
| 2   | A     | 1895 | C    | Sidechain |
| 2   | A     | 1896 | G    | Sidechain |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 2          | A            | 1900       | A           | Sidechain    |
| 2          | A            | 2094       | A           | Sidechain    |
| 2          | A            | 2095       | A           | Sidechain    |
| 2          | A            | 2102       | G           | Sidechain    |
| 2          | A            | 2103       | C           | Sidechain    |
| 2          | A            | 2104       | C           | Sidechain    |
| 2          | A            | 2106       | U           | Sidechain    |
| 2          | A            | 2109       | U           | Sidechain    |
| 2          | A            | 2110       | G           | Sidechain    |
| 2          | A            | 2111       | U           | Sidechain    |
| 2          | A            | 2112       | G           | Sidechain    |
| 2          | A            | 2114       | A           | Sidechain    |
| 2          | A            | 2115       | G           | Sidechain    |
| 2          | A            | 2116       | G           | Sidechain    |
| 2          | A            | 2120       | G           | Sidechain    |
| 2          | A            | 2123       | G           | Sidechain    |
| 2          | A            | 2124       | G           | Sidechain    |
| 2          | A            | 2125       | G           | Sidechain    |
| 2          | A            | 2127       | G           | Sidechain    |
| 2          | A            | 2128       | G           | Sidechain    |
| 2          | A            | 2129       | C           | Sidechain    |
| 2          | A            | 2130       | U           | Sidechain    |
| 2          | A            | 2132       | U           | Sidechain    |
| 2          | A            | 2133       | G           | Sidechain    |
| 2          | A            | 2135       | A           | Sidechain    |
| 2          | A            | 2136       | G           | Sidechain    |
| 2          | A            | 2137       | U           | Sidechain    |
| 2          | A            | 2138       | G           | Sidechain    |
| 2          | A            | 2141       | G           | Sidechain    |
| 2          | A            | 2144       | G           | Sidechain    |
| 2          | A            | 2147       | A           | Sidechain    |
| 2          | A            | 2148       | G           | Sidechain    |
| 2          | A            | 2152       | G           | Sidechain    |
| 2          | A            | 2153       | C           | Sidechain    |
| 2          | A            | 2154       | A           | Sidechain    |
| 2          | A            | 2156       | G           | Sidechain    |
| 2          | A            | 2157       | G           | Sidechain    |
| 2          | A            | 2158       | A           | Sidechain    |
| 2          | A            | 2159       | G           | Sidechain    |
| 2          | A            | 2160       | C           | Sidechain    |
| 2          | A            | 2161       | C           | Sidechain    |
| 2          | A            | 2164       | C           | Sidechain    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 2          | A            | 2165       | C           | Sidechain    |
| 2          | A            | 2166       | U           | Sidechain    |
| 2          | A            | 2168       | G           | Sidechain    |
| 2          | A            | 2176       | A           | Sidechain    |
| 2          | A            | 2177       | C           | Sidechain    |
| 2          | A            | 2179       | C           | Sidechain    |
| 2          | A            | 2184       | A           | Sidechain    |
| 2          | A            | 2186       | G           | Sidechain    |
| 2          | A            | 2187       | U           | Sidechain    |
| 2          | A            | 2189       | U           | Sidechain    |
| 2          | A            | 2190       | G           | Sidechain    |
| 2          | A            | 2191       | A           | Sidechain    |
| 2          | A            | 2192       | U           | Sidechain    |
| 1          | B            | 1239       | A           | Sidechain    |
| 1          | B            | 1242       | G           | Sidechain    |
| 1          | B            | 1243       | C           | Sidechain    |
| 1          | B            | 1290       | G           | Sidechain    |
| 1          | B            | 1295       | U           | Sidechain    |
| 1          | B            | 1296       | C           | Sidechain    |
| 1          | B            | 1301       | U           | Sidechain    |
| 1          | B            | 1302       | C           | Sidechain    |
| 1          | B            | 1304       | G           | Sidechain    |
| 1          | B            | 1332       | A           | Sidechain    |
| 1          | B            | 1334       | G           | Sidechain    |
| 1          | B            | 1336       | C           | Sidechain    |
| 4          | D            | 111        | TYR         | Sidechain    |
| 4          | D            | 181        | PRO         | Peptide      |
| 4          | D            | 186        | LEU         | Peptide      |
| 4          | D            | 19         | ARG         | Sidechain    |
| 4          | D            | 225        | VAL         | Peptide      |
| 4          | D            | 254        | ARG         | Sidechain    |
| 4          | D            | 290        | ARG         | Sidechain    |
| 4          | D            | 293        | ARG         | Sidechain    |
| 4          | D            | 316        | GLY         | Peptide      |
| 4          | D            | 318        | ARG         | Sidechain    |
| 4          | D            | 330        | ARG         | Sidechain    |
| 4          | D            | 333        | TYR         | Sidechain    |
| 4          | D            | 336        | ARG         | Sidechain    |
| 4          | D            | 366        | PHE         | Sidechain    |
| 4          | D            | 392        | ASP         | Peptide      |
| 4          | D            | 395        | ARG         | Sidechain    |
| 4          | D            | 427        | TYR         | Sidechain    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 4          | D            | 441        | ARG         | Sidechain    |
| 4          | D            | 481        | ARG         | Sidechain    |
| 4          | D            | 503        | PHE         | Sidechain    |
| 4          | D            | 508        | ALA         | Peptide      |
| 4          | D            | 530        | TYR         | Sidechain    |
| 4          | D            | 550        | TYR         | Sidechain    |
| 3          | E            | 1          | C           | Sidechain    |
| 3          | E            | 11         | A           | Sidechain    |
| 3          | E            | 12         | G           | Sidechain    |
| 3          | E            | 13         | C           | Sidechain    |
| 3          | E            | 15         | G           | Sidechain    |
| 3          | E            | 18         | U           | Sidechain    |
| 3          | E            | 19         | G           | Sidechain    |
| 3          | E            | 22         | A           | Sidechain    |
| 3          | E            | 23         | G           | Sidechain    |
| 3          | E            | 28         | U           | Sidechain    |
| 3          | E            | 29         | C           | Sidechain    |
| 3          | E            | 3          | C           | Sidechain    |
| 3          | E            | 30         | G           | Sidechain    |
| 3          | E            | 35         | C           | Sidechain    |
| 3          | E            | 36         | A           | Sidechain    |
| 3          | E            | 37         | U           | Sidechain    |
| 3          | E            | 38         | A           | Sidechain    |
| 3          | E            | 4          | G           | Sidechain    |
| 3          | E            | 40         | C           | Sidechain    |
| 3          | E            | 42         | C           | Sidechain    |
| 3          | E            | 44         | A           | Sidechain    |
| 3          | E            | 47         | G           | Sidechain    |
| 3          | E            | 5          | G           | Sidechain    |
| 3          | E            | 53         | G           | Sidechain    |
| 3          | E            | 59         | A           | Sidechain    |
| 3          | E            | 60         | A           | Sidechain    |
| 3          | E            | 61         | U           | Sidechain    |
| 3          | E            | 63         | C           | Sidechain    |
| 3          | E            | 64         | G           | Sidechain    |
| 3          | E            | 7          | G           | Sidechain    |
| 3          | E            | 73         | A           | Sidechain    |
| 3          | E            | 74         | A           | Sidechain    |
| 3          | E            | 8          | U           | Sidechain    |
| 3          | E            | 9          | G           | Sidechain    |
| 5          | F            | 12         | ARG         | Sidechain    |
| 5          | F            | 124        | VAL         | Peptide      |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | F     | 134 | ARG  | Sidechain |
| 5   | F     | 162 | ARG  | Sidechain |
| 5   | F     | 163 | TYR  | Sidechain |
| 5   | F     | 164 | ARG  | Sidechain |
| 5   | F     | 203 | GLN  | Peptide   |
| 5   | F     | 35  | THR  | Peptide   |
| 5   | F     | 7   | ARG  | Sidechain |
| 6   | G     | 124 | ARG  | Sidechain |
| 6   | G     | 149 | ARG  | Sidechain |
| 6   | G     | 177 | ARG  | Sidechain |
| 6   | G     | 6   | TYR  | Sidechain |
| 6   | G     | 76  | PHE  | Sidechain |
| 6   | G     | 91  | ARG  | Sidechain |
| 7   | H     | 20  | TYR  | Sidechain |
| 7   | H     | 27  | ARG  | Sidechain |
| 7   | H     | 48  | TYR  | Sidechain |
| 7   | H     | 5   | ARG  | Sidechain |
| 8   | I     | 101 | ARG  | Sidechain |
| 8   | I     | 4   | ARG  | Sidechain |
| 8   | I     | 52  | ARG  | Sidechain |
| 8   | I     | 69  | ARG  | Sidechain |
| 8   | I     | 78  | ARG  | Sidechain |
| 8   | I     | 95  | ARG  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 687   | 0        | 342      | 24      | 0            |
| 2   | A     | 3731  | 0        | 1828     | 67      | 0            |
| 3   | E     | 1640  | 0        | 827      | 29      | 0            |
| 4   | D     | 4393  | 0        | 4377     | 333     | 0            |
| 5   | F     | 1733  | 0        | 1824     | 152     | 0            |
| 6   | G     | 1420  | 0        | 1460     | 10      | 0            |
| 7   | H     | 410   | 0        | 440      | 1       | 0            |
| 8   | I     | 1182  | 0        | 1240     | 124     | 0            |
| All | All   | 15196 | 0        | 12338    | 421     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (421) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:1240:U:C4    | 8:I:31:VAL:HG12  | 1.20                     | 1.68              |
| 4:D:108:TYR:HA   | 5:F:118:PRO:CB   | 1.17                     | 1.59              |
| 4:D:108:TYR:CA   | 5:F:118:PRO:HB2  | 1.27                     | 1.57              |
| 4:D:108:TYR:CE2  | 5:F:121:MET:HB3  | 1.34                     | 1.57              |
| 4:D:523:PHE:CD1  | 8:I:130:LYS:HB2  | 1.37                     | 1.57              |
| 2:A:2169:A:C2    | 4:D:141:ASN:HB2  | 1.40                     | 1.55              |
| 4:D:111:TYR:CD1  | 5:F:147:PRO:HA   | 1.42                     | 1.53              |
| 4:D:536:ARG:NH1  | 8:I:137:ARG:NH2  | 1.65                     | 1.44              |
| 4:D:133:GLN:HG2  | 5:F:60:ARG:CD    | 1.44                     | 1.42              |
| 1:B:1240:U:C4    | 8:I:31:VAL:CG1   | 2.11                     | 1.34              |
| 4:D:536:ARG:NH1  | 8:I:137:ARG:HH22 | 0.83                     | 1.31              |
| 2:A:2113:U:C4'   | 4:D:147:ALA:HA   | 1.63                     | 1.29              |
| 4:D:108:TYR:CA   | 5:F:118:PRO:CB   | 1.94                     | 1.28              |
| 4:D:108:TYR:HB3  | 5:F:118:PRO:O    | 1.29                     | 1.28              |
| 4:D:322:LYS:CG   | 8:I:113:LYS:HZ3  | 1.45                     | 1.27              |
| 4:D:523:PHE:HD1  | 8:I:130:LYS:CB   | 1.45                     | 1.27              |
| 1:B:1240:U:C1'   | 8:I:37:THR:HG21  | 1.64                     | 1.27              |
| 4:D:129:GLU:OE1  | 5:F:143:GLY:HA3  | 1.18                     | 1.27              |
| 4:D:108:TYR:OH   | 5:F:121:MET:HG2  | 1.34                     | 1.26              |
| 4:D:533:TYR:HB2  | 8:I:129:ASN:O    | 1.08                     | 1.26              |
| 4:D:108:TYR:C    | 5:F:118:PRO:HB2  | 1.57                     | 1.25              |
| 2:A:2169:A:H2    | 4:D:141:ASN:CB   | 1.49                     | 1.23              |
| 4:D:322:LYS:HG3  | 8:I:113:LYS:NZ   | 1.51                     | 1.23              |
| 4:D:536:ARG:HH12 | 8:I:137:ARG:NH2  | 1.24                     | 1.22              |
| 4:D:108:TYR:CE2  | 5:F:121:MET:CB   | 2.22                     | 1.21              |
| 4:D:133:GLN:CG   | 5:F:60:ARG:HD2   | 1.70                     | 1.21              |
| 4:D:140:LEU:HD21 | 5:F:129:GLN:CG   | 1.69                     | 1.20              |
| 4:D:133:GLN:CG   | 5:F:60:ARG:CD    | 2.20                     | 1.19              |
| 4:D:111:TYR:CB   | 5:F:118:PRO:HG3  | 1.73                     | 1.18              |
| 4:D:125:GLN:NE2  | 5:F:144:THR:HG23 | 1.59                     | 1.18              |
| 4:D:108:TYR:CE1  | 5:F:145:VAL:HG11 | 1.79                     | 1.17              |
| 4:D:111:TYR:HB2  | 5:F:118:PRO:CG   | 1.74                     | 1.17              |
| 4:D:532:GLU:HG3  | 8:I:138:GLU:OE1  | 1.47                     | 1.14              |
| 2:A:2113:U:H1'   | 4:D:146:ARG:HG3  | 1.30                     | 1.14              |
| 4:D:536:ARG:HH22 | 8:I:137:ARG:NH1  | 1.43                     | 1.13              |
| 4:D:412:LEU:HD21 | 6:G:46:LYS:H     | 1.07                     | 1.13              |
| 2:A:2113:U:C5'   | 4:D:147:ALA:HA   | 1.80                     | 1.12              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:533:TYR:CB   | 8:I:129:ASN:O    | 1.96                     | 1.12              |
| 2:A:2169:A:C2    | 4:D:141:ASN:CB   | 2.25                     | 1.11              |
| 4:D:137:GLY:HA2  | 5:F:129:GLN:HE21 | 1.16                     | 1.11              |
| 4:D:130:GLU:HB3  | 5:F:55:SER:HB3   | 1.22                     | 1.10              |
| 4:D:523:PHE:HB2  | 8:I:130:LYS:HD2  | 1.31                     | 1.10              |
| 1:B:1240:U:C2    | 8:I:37:THR:CG2   | 2.35                     | 1.10              |
| 2:A:2113:U:C2    | 4:D:143:GLN:OE1  | 2.03                     | 1.10              |
| 4:D:111:TYR:CE1  | 5:F:147:PRO:HA   | 1.86                     | 1.09              |
| 4:D:111:TYR:CD1  | 5:F:147:PRO:CA   | 2.36                     | 1.08              |
| 2:A:2113:U:H1'   | 4:D:146:ARG:CG   | 1.84                     | 1.08              |
| 2:A:2113:U:C1'   | 4:D:146:ARG:HG3  | 1.81                     | 1.08              |
| 1:B:1240:U:O2    | 8:I:37:THR:CG2   | 2.03                     | 1.07              |
| 2:A:2113:U:C6    | 4:D:143:GLN:NE2  | 2.21                     | 1.07              |
| 4:D:108:TYR:HB3  | 5:F:118:PRO:C    | 1.74                     | 1.07              |
| 4:D:536:ARG:NH2  | 8:I:137:ARG:HH12 | 1.50                     | 1.06              |
| 3:E:3:C:H1'      | 4:D:277:ARG:NH2  | 1.72                     | 1.05              |
| 4:D:129:GLU:OE1  | 5:F:143:GLY:CA   | 2.03                     | 1.05              |
| 4:D:140:LEU:CD2  | 5:F:129:GLN:HG3  | 1.87                     | 1.04              |
| 1:B:1240:U:O4    | 8:I:31:VAL:HG12  | 1.58                     | 1.03              |
| 3:E:17:C:OP2     | 3:E:18:U:C5      | 2.11                     | 1.03              |
| 4:D:111:TYR:HE1  | 5:F:147:PRO:HB3  | 1.23                     | 1.02              |
| 1:B:1240:U:C5    | 8:I:31:VAL:CG1   | 2.43                     | 1.02              |
| 2:A:2113:U:C5    | 4:D:143:GLN:NE2  | 2.28                     | 1.02              |
| 4:D:111:TYR:CE1  | 5:F:147:PRO:CA   | 2.43                     | 1.01              |
| 4:D:133:GLN:OE1  | 5:F:141:LYS:HB3  | 1.60                     | 1.01              |
| 4:D:536:ARG:CZ   | 8:I:137:ARG:HH22 | 1.73                     | 1.01              |
| 1:B:1240:U:C5    | 8:I:31:VAL:HG12  | 1.96                     | 1.01              |
| 4:D:108:TYR:O    | 5:F:118:PRO:HB2  | 1.59                     | 1.00              |
| 4:D:111:TYR:CE2  | 5:F:145:VAL:HG23 | 1.96                     | 0.99              |
| 4:D:108:TYR:CG   | 5:F:118:PRO:HA   | 1.97                     | 0.99              |
| 4:D:108:TYR:HA   | 5:F:118:PRO:HB3  | 0.99                     | 0.98              |
| 4:D:523:PHE:CD1  | 8:I:130:LYS:CB   | 2.28                     | 0.98              |
| 3:E:3:C:C1'      | 4:D:277:ARG:HH21 | 1.77                     | 0.98              |
| 4:D:108:TYR:CB   | 5:F:118:PRO:O    | 2.10                     | 0.97              |
| 2:A:2113:U:H5'   | 4:D:147:ALA:HA   | 1.43                     | 0.97              |
| 4:D:412:LEU:HD21 | 6:G:46:LYS:N     | 1.80                     | 0.97              |
| 4:D:108:TYR:CE1  | 5:F:145:VAL:CG1  | 2.48                     | 0.97              |
| 4:D:140:LEU:HD21 | 5:F:129:GLN:HG3  | 0.99                     | 0.96              |
| 2:A:2169:A:N3    | 4:D:141:ASN:OD1  | 1.97                     | 0.96              |
| 4:D:141:ASN:OD1  | 5:F:127:LEU:HD13 | 1.65                     | 0.95              |
| 1:B:1240:U:C2    | 8:I:37:THR:HG23  | 2.00                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:111:TYR:HB2  | 5:F:118:PRO:HG3  | 0.95                     | 0.94              |
| 2:A:2113:U:C2'   | 4:D:146:ARG:HG3  | 1.97                     | 0.94              |
| 2:A:2113:U:O2'   | 4:D:146:ARG:HG3  | 1.67                     | 0.94              |
| 2:A:2113:U:H4'   | 4:D:147:ALA:HA   | 1.47                     | 0.93              |
| 4:D:118:PHE:CE2  | 5:F:148:ASN:ND2  | 2.37                     | 0.93              |
| 1:B:1240:U:H1'   | 8:I:37:THR:HG21  | 1.49                     | 0.92              |
| 5:F:60:ARG:HH12  | 5:F:164:ARG:NE   | 1.67                     | 0.92              |
| 4:D:533:TYR:HD1  | 4:D:533:TYR:O    | 1.53                     | 0.91              |
| 2:A:2169:A:C2    | 4:D:141:ASN:OD1  | 2.23                     | 0.91              |
| 4:D:111:TYR:HE2  | 5:F:145:VAL:HG23 | 1.36                     | 0.90              |
| 4:D:108:TYR:CZ   | 5:F:121:MET:HB3  | 2.07                     | 0.90              |
| 4:D:322:LYS:CG   | 8:I:113:LYS:NZ   | 2.21                     | 0.90              |
| 4:D:108:TYR:HE2  | 5:F:121:MET:HB3  | 1.32                     | 0.89              |
| 4:D:130:GLU:HB3  | 5:F:55:SER:CB    | 2.03                     | 0.89              |
| 4:D:130:GLU:O    | 5:F:55:SER:OG    | 1.90                     | 0.89              |
| 4:D:111:TYR:HD1  | 5:F:147:PRO:HA   | 1.21                     | 0.89              |
| 4:D:118:PHE:HD1  | 4:D:118:PHE:H    | 1.21                     | 0.89              |
| 3:E:72:C:O2'     | 4:D:278:GLN:O    | 1.89                     | 0.88              |
| 4:D:529:GLU:CD   | 8:I:135:LYS:HD2  | 1.93                     | 0.88              |
| 2:A:2113:U:C4'   | 4:D:147:ALA:CA   | 2.51                     | 0.87              |
| 8:I:125:ASP:OD1  | 8:I:130:LYS:HE2  | 1.75                     | 0.87              |
| 2:A:2113:U:O2    | 4:D:146:ARG:NE   | 2.08                     | 0.87              |
| 4:D:524:GLU:CB   | 8:I:110:ARG:NE   | 2.37                     | 0.87              |
| 4:D:111:TYR:HB3  | 5:F:83:ASN:ND2   | 1.90                     | 0.86              |
| 1:B:1240:U:O4'   | 8:I:37:THR:HG21  | 1.75                     | 0.86              |
| 4:D:133:GLN:OE1  | 5:F:141:LYS:CB   | 2.23                     | 0.86              |
| 4:D:524:GLU:OE1  | 8:I:110:ARG:HG3  | 1.75                     | 0.86              |
| 1:B:1240:U:O2    | 8:I:37:THR:HG22  | 1.75                     | 0.86              |
| 2:A:1907:G:N2    | 3:E:12:G:O3'     | 2.08                     | 0.86              |
| 4:D:108:TYR:CD1  | 5:F:118:PRO:HA   | 2.10                     | 0.85              |
| 4:D:108:TYR:CD1  | 5:F:145:VAL:HG21 | 2.11                     | 0.85              |
| 4:D:523:PHE:CE1  | 8:I:130:LYS:HB2  | 2.11                     | 0.85              |
| 4:D:111:TYR:CE1  | 5:F:147:PRO:HB3  | 2.12                     | 0.85              |
| 4:D:524:GLU:CG   | 8:I:110:ARG:NE   | 2.41                     | 0.84              |
| 4:D:118:PHE:HE2  | 5:F:148:ASN:ND2  | 1.74                     | 0.84              |
| 5:F:60:ARG:NH1   | 5:F:164:ARG:CD   | 2.41                     | 0.84              |
| 4:D:140:LEU:HD21 | 5:F:129:GLN:CB   | 2.08                     | 0.83              |
| 4:D:528:THR:HB   | 8:I:142:ARG:CZ   | 2.08                     | 0.83              |
| 4:D:524:GLU:CG   | 8:I:110:ARG:HE   | 1.92                     | 0.83              |
| 4:D:125:GLN:CD   | 5:F:144:THR:HA   | 1.99                     | 0.83              |
| 3:E:72:C:C5'     | 4:D:278:GLN:HE21 | 1.92                     | 0.82              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:D:533:TYR:HD2 | 8:I:130:LYS:HB3  | 1.43                     | 0.82              |
| 4:D:526:ASN:HB2 | 4:D:529:GLU:OE2  | 1.79                     | 0.82              |
| 4:D:322:LYS:CB  | 8:I:113:LYS:NZ   | 2.42                     | 0.82              |
| 4:D:108:TYR:CZ  | 5:F:121:MET:HG2  | 2.14                     | 0.82              |
| 3:E:17:C:OP2    | 3:E:18:U:C6      | 2.33                     | 0.82              |
| 4:D:528:THR:HB  | 8:I:142:ARG:NH2  | 1.94                     | 0.82              |
| 2:A:2113:U:H5'  | 4:D:147:ALA:CA   | 2.10                     | 0.81              |
| 4:D:108:TYR:O   | 5:F:118:PRO:CB   | 2.29                     | 0.81              |
| 4:D:533:TYR:CE2 | 8:I:130:LYS:HD3  | 2.16                     | 0.81              |
| 4:D:111:TYR:HE1 | 5:F:147:PRO:CB   | 1.94                     | 0.81              |
| 4:D:133:GLN:HG2 | 5:F:60:ARG:HD3   | 1.62                     | 0.81              |
| 4:D:524:GLU:HG2 | 8:I:110:ARG:CD   | 2.09                     | 0.81              |
| 4:D:526:ASN:N   | 4:D:529:GLU:OE2  | 2.13                     | 0.80              |
| 4:D:533:TYR:HD1 | 4:D:533:TYR:C    | 1.86                     | 0.80              |
| 4:D:533:TYR:CD1 | 4:D:533:TYR:C    | 2.51                     | 0.80              |
| 4:D:108:TYR:CB  | 5:F:118:PRO:CB   | 2.59                     | 0.80              |
| 4:D:108:TYR:CB  | 5:F:118:PRO:HB2  | 2.11                     | 0.80              |
| 4:D:108:TYR:HH  | 5:F:121:MET:HG2  | 1.43                     | 0.80              |
| 4:D:111:TYR:CE1 | 5:F:147:PRO:CB   | 2.66                     | 0.79              |
| 4:D:529:GLU:CG  | 8:I:135:LYS:HG3  | 2.13                     | 0.79              |
| 5:F:60:ARG:HH12 | 5:F:164:ARG:CZ   | 1.96                     | 0.78              |
| 1:B:1240:U:N1   | 8:I:37:THR:HG21  | 1.97                     | 0.78              |
| 4:D:108:TYR:CG  | 5:F:118:PRO:CA   | 2.65                     | 0.78              |
| 4:D:532:GLU:CG  | 8:I:138:GLU:OE1  | 2.29                     | 0.78              |
| 3:E:3:C:C2'     | 4:D:277:ARG:HH21 | 1.95                     | 0.78              |
| 4:D:322:LYS:HG3 | 8:I:113:LYS:HZ3  | 0.66                     | 0.78              |
| 4:D:129:GLU:CD  | 5:F:143:GLY:HA3  | 2.03                     | 0.77              |
| 4:D:108:TYR:CD2 | 5:F:121:MET:HB3  | 2.17                     | 0.77              |
| 2:A:1907:G:H21  | 3:E:13:C:P       | 2.07                     | 0.77              |
| 4:D:111:TYR:HB3 | 5:F:83:ASN:HD21  | 1.47                     | 0.77              |
| 4:D:529:GLU:CD  | 8:I:135:LYS:CD   | 2.53                     | 0.77              |
| 4:D:108:TYR:CE2 | 5:F:121:MET:CG   | 2.68                     | 0.77              |
| 4:D:529:GLU:CD  | 8:I:135:LYS:CG   | 2.53                     | 0.77              |
| 4:D:533:TYR:HE2 | 8:I:130:LYS:HD3  | 1.50                     | 0.77              |
| 4:D:412:LEU:CD2 | 6:G:46:LYS:H     | 1.94                     | 0.76              |
| 4:D:105:ASP:OD2 | 5:F:122:ARG:HB3  | 1.86                     | 0.76              |
| 4:D:108:TYR:CZ  | 5:F:121:MET:CB   | 2.66                     | 0.76              |
| 4:D:133:GLN:HG2 | 5:F:60:ARG:HD2   | 0.77                     | 0.75              |
| 4:D:529:GLU:OE1 | 8:I:135:LYS:HD2  | 1.87                     | 0.75              |
| 4:D:524:GLU:HB3 | 8:I:110:ARG:CZ   | 2.16                     | 0.74              |
| 4:D:108:TYR:CB  | 5:F:118:PRO:CA   | 2.64                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:524:GLU:CB   | 8:I:110:ARG:CZ   | 2.64                     | 0.74              |
| 4:D:108:TYR:CZ   | 5:F:145:VAL:HG11 | 2.20                     | 0.74              |
| 4:D:133:GLN:CG   | 5:F:60:ARG:HD3   | 2.16                     | 0.73              |
| 4:D:529:GLU:OE1  | 8:I:135:LYS:HB2  | 1.88                     | 0.73              |
| 4:D:524:GLU:HG2  | 8:I:110:ARG:HG3  | 1.71                     | 0.73              |
| 4:D:133:GLN:CD   | 5:F:60:ARG:HD3   | 2.09                     | 0.73              |
| 4:D:138:HIS:CE1  | 4:D:140:LEU:HD23 | 2.24                     | 0.73              |
| 4:D:412:LEU:HD21 | 6:G:46:LYS:HB2   | 1.71                     | 0.73              |
| 4:D:524:GLU:CD   | 8:I:110:ARG:HG3  | 2.09                     | 0.73              |
| 4:D:529:GLU:HG2  | 8:I:135:LYS:HG3  | 1.71                     | 0.73              |
| 4:D:529:GLU:OE2  | 8:I:135:LYS:NZ   | 2.18                     | 0.72              |
| 4:D:322:LYS:HB3  | 8:I:113:LYS:HZ1  | 1.55                     | 0.72              |
| 4:D:141:ASN:OD1  | 5:F:127:LEU:CD1  | 2.38                     | 0.72              |
| 4:D:536:ARG:HH12 | 8:I:137:ARG:CZ   | 2.01                     | 0.72              |
| 4:D:529:GLU:CD   | 8:I:135:LYS:HG3  | 2.10                     | 0.72              |
| 4:D:137:GLY:HA2  | 5:F:129:GLN:NE2  | 1.98                     | 0.72              |
| 5:F:60:ARG:NH1   | 5:F:164:ARG:NE   | 2.36                     | 0.72              |
| 4:D:322:LYS:CB   | 8:I:113:LYS:HZ1  | 2.00                     | 0.72              |
| 2:A:2169:A:C2    | 4:D:141:ASN:CG   | 2.64                     | 0.71              |
| 4:D:108:TYR:OH   | 5:F:121:MET:CG   | 2.28                     | 0.71              |
| 4:D:111:TYR:CD2  | 5:F:118:PRO:HG3  | 2.25                     | 0.71              |
| 4:D:533:TYR:HB2  | 8:I:129:ASN:C    | 2.08                     | 0.71              |
| 4:D:125:GLN:HE22 | 5:F:144:THR:HG23 | 1.51                     | 0.70              |
| 4:D:108:TYR:CD2  | 5:F:118:PRO:O    | 2.45                     | 0.70              |
| 4:D:111:TYR:CG   | 5:F:118:PRO:HG3  | 2.26                     | 0.70              |
| 2:A:2113:U:O2'   | 4:D:146:ARG:CG   | 2.40                     | 0.70              |
| 1:B:1240:U:C2    | 8:I:37:THR:HG21  | 2.16                     | 0.69              |
| 2:A:2113:U:H5''  | 4:D:150:ALA:HB3  | 1.74                     | 0.69              |
| 4:D:524:GLU:HG2  | 8:I:110:ARG:CG   | 2.23                     | 0.69              |
| 4:D:536:ARG:HH12 | 8:I:137:ARG:HH22 | 0.79                     | 0.69              |
| 4:D:108:TYR:O    | 5:F:118:PRO:CG   | 2.40                     | 0.69              |
| 3:E:3:C:O2       | 4:D:277:ARG:NH2  | 2.27                     | 0.68              |
| 4:D:532:GLU:HB3  | 8:I:138:GLU:CD   | 2.13                     | 0.68              |
| 3:E:3:C:C1'      | 4:D:277:ARG:NH2  | 2.40                     | 0.68              |
| 3:E:17:C:OP2     | 3:E:18:U:H5      | 1.70                     | 0.68              |
| 4:D:105:ASP:OD2  | 5:F:122:ARG:CB   | 2.42                     | 0.68              |
| 4:D:524:GLU:HG2  | 8:I:110:ARG:NE   | 2.07                     | 0.68              |
| 4:D:510:HIS:NE2  | 4:D:524:GLU:CD   | 2.48                     | 0.67              |
| 1:B:1240:U:N1    | 8:I:37:THR:CG2   | 2.55                     | 0.67              |
| 4:D:108:TYR:CZ   | 5:F:121:MET:CG   | 2.78                     | 0.67              |
| 4:D:524:GLU:CG   | 8:I:110:ARG:HG3  | 2.24                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:1240:U:O2    | 8:I:34:LYS:HB2   | 1.95                     | 0.66              |
| 2:A:2113:U:O4'   | 4:D:147:ALA:CA   | 2.44                     | 0.66              |
| 4:D:108:TYR:CB   | 5:F:118:PRO:C    | 2.57                     | 0.66              |
| 4:D:526:ASN:CB   | 4:D:529:GLU:OE2  | 2.44                     | 0.66              |
| 1:B:1240:U:N3    | 8:I:31:VAL:HG12  | 2.00                     | 0.66              |
| 3:E:3:C:H1'      | 4:D:277:ARG:HH22 | 1.58                     | 0.66              |
| 4:D:133:GLN:HE22 | 5:F:141:LYS:HD3  | 1.61                     | 0.65              |
| 5:F:60:ARG:NH1   | 5:F:164:ARG:CG   | 2.59                     | 0.65              |
| 4:D:133:GLN:HE22 | 5:F:141:LYS:CD   | 2.09                     | 0.65              |
| 4:D:524:GLU:HB2  | 8:I:110:ARG:NH2  | 2.12                     | 0.65              |
| 4:D:108:TYR:HD1  | 5:F:145:VAL:HG21 | 1.57                     | 0.65              |
| 4:D:322:LYS:HD2  | 8:I:113:LYS:HE2  | 1.79                     | 0.65              |
| 2:A:1907:G:N2    | 3:E:13:C:OP1     | 2.27                     | 0.65              |
| 3:E:54:G:H2'     | 3:E:55:U:C6      | 2.32                     | 0.65              |
| 4:D:524:GLU:CB   | 8:I:110:ARG:HE   | 2.06                     | 0.64              |
| 2:A:2113:U:O4'   | 4:D:147:ALA:HB2  | 1.97                     | 0.64              |
| 3:E:17:C:P       | 3:E:18:U:H5      | 2.21                     | 0.64              |
| 4:D:322:LYS:HG3  | 8:I:113:LYS:CE   | 2.28                     | 0.64              |
| 1:B:1240:U:C1'   | 8:I:37:THR:CG2   | 2.58                     | 0.63              |
| 4:D:108:TYR:HB3  | 5:F:118:PRO:CA   | 2.28                     | 0.63              |
| 2:A:2113:U:H1'   | 4:D:146:ARG:HG2  | 1.78                     | 0.63              |
| 4:D:130:GLU:CB   | 5:F:55:SER:HB3   | 2.13                     | 0.63              |
| 2:A:2113:U:O4'   | 4:D:147:ALA:HA   | 1.98                     | 0.62              |
| 4:D:108:TYR:CG   | 5:F:118:PRO:O    | 2.52                     | 0.62              |
| 4:D:108:TYR:O    | 5:F:118:PRO:HG2  | 1.99                     | 0.62              |
| 4:D:118:PHE:HD1  | 4:D:118:PHE:N    | 1.93                     | 0.62              |
| 4:D:510:HIS:HE2  | 4:D:524:GLU:CD   | 2.02                     | 0.62              |
| 4:D:536:ARG:CZ   | 8:I:138:GLU:OE2  | 2.47                     | 0.62              |
| 2:A:2113:U:O2    | 4:D:146:ARG:CZ   | 2.48                     | 0.62              |
| 2:A:2113:U:N3    | 4:D:143:GLN:OE1  | 2.32                     | 0.62              |
| 4:D:108:TYR:CA   | 5:F:118:PRO:HB3  | 1.94                     | 0.61              |
| 4:D:192:HIS:H    | 4:D:499:HIS:CE1  | 2.17                     | 0.61              |
| 4:D:108:TYR:CE1  | 5:F:145:VAL:HG21 | 2.35                     | 0.61              |
| 5:F:60:ARG:NH1   | 5:F:164:ARG:HD2  | 2.14                     | 0.61              |
| 3:E:72:C:H4'     | 4:D:278:GLN:HG3  | 1.82                     | 0.61              |
| 4:D:137:GLY:CA   | 5:F:129:GLN:HE21 | 2.02                     | 0.61              |
| 1:B:1240:U:O4'   | 8:I:37:THR:CG2   | 2.47                     | 0.61              |
| 4:D:101:LEU:HD22 | 5:F:126:GLN:HE21 | 1.66                     | 0.61              |
| 4:D:533:TYR:HD2  | 8:I:130:LYS:CB   | 2.13                     | 0.61              |
| 4:D:525:GLY:HA3  | 4:D:529:GLU:OE1  | 2.00                     | 0.60              |
| 4:D:322:LYS:HE3  | 8:I:112:ASP:C    | 2.22                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:524:GLU:CD   | 8:I:110:ARG:HE   | 2.03                     | 0.60              |
| 2:A:2169:A:H2    | 4:D:141:ASN:HB2  | 0.60                     | 0.60              |
| 4:D:111:TYR:CG   | 5:F:146:THR:O    | 2.55                     | 0.60              |
| 4:D:133:GLN:OE1  | 5:F:60:ARG:HD3   | 2.02                     | 0.60              |
| 5:F:60:ARG:NH1   | 5:F:164:ARG:HG2  | 2.17                     | 0.59              |
| 4:D:118:PHE:N    | 4:D:118:PHE:CD1  | 2.65                     | 0.59              |
| 4:D:532:GLU:CB   | 8:I:138:GLU:CD   | 2.71                     | 0.59              |
| 4:D:129:GLU:OE1  | 5:F:144:THR:N    | 2.35                     | 0.59              |
| 4:D:536:ARG:NH2  | 8:I:137:ARG:NH1  | 2.24                     | 0.59              |
| 1:B:1240:U:H3    | 8:I:31:VAL:H     | 1.49                     | 0.59              |
| 4:D:469:ASP:HA   | 4:D:497:ILE:HD12 | 1.85                     | 0.59              |
| 2:A:2113:U:C5'   | 4:D:150:ALA:HB3  | 2.33                     | 0.58              |
| 2:A:1907:G:N2    | 3:E:13:C:P       | 2.75                     | 0.58              |
| 4:D:510:HIS:CD2  | 4:D:524:GLU:OE2  | 2.57                     | 0.58              |
| 4:D:142:VAL:HG13 | 4:D:146:ARG:CZ   | 2.34                     | 0.57              |
| 4:D:311:LEU:HG   | 4:D:312:PHE:H    | 1.69                     | 0.57              |
| 5:F:60:ARG:HH12  | 5:F:164:ARG:CD   | 2.12                     | 0.57              |
| 2:A:2113:U:C2    | 4:D:143:GLN:CD   | 2.78                     | 0.57              |
| 2:A:1847:A:H62   | 2:A:1893:C:H41   | 1.52                     | 0.57              |
| 2:A:2113:U:N1    | 4:D:143:GLN:NE2  | 2.52                     | 0.57              |
| 4:D:111:TYR:HE2  | 5:F:145:VAL:CG2  | 2.14                     | 0.57              |
| 8:I:125:ASP:OD1  | 8:I:130:LYS:CE   | 2.49                     | 0.57              |
| 2:A:2113:U:H4'   | 4:D:147:ALA:CA   | 2.26                     | 0.57              |
| 4:D:536:ARG:HH22 | 8:I:137:ARG:HH12 | 0.68                     | 0.57              |
| 2:A:2113:U:O4'   | 4:D:147:ALA:CB   | 2.53                     | 0.56              |
| 4:D:133:GLN:CG   | 5:F:60:ARG:NE    | 2.68                     | 0.56              |
| 4:D:510:HIS:CD2  | 4:D:524:GLU:CD   | 2.78                     | 0.56              |
| 4:D:533:TYR:CD2  | 8:I:130:LYS:HB3  | 2.34                     | 0.56              |
| 4:D:524:GLU:HB2  | 8:I:110:ARG:CZ   | 2.35                     | 0.56              |
| 4:D:133:GLN:CD   | 5:F:60:ARG:CD    | 2.70                     | 0.56              |
| 4:D:412:LEU:CD2  | 6:G:46:LYS:HB2   | 2.36                     | 0.56              |
| 4:D:533:TYR:O    | 4:D:533:TYR:CD1  | 2.44                     | 0.56              |
| 4:D:108:TYR:HE1  | 5:F:145:VAL:CG1  | 2.14                     | 0.56              |
| 2:A:1843:C:H2'   | 2:A:1844:C:C6    | 2.41                     | 0.55              |
| 3:E:3:C:O2       | 4:D:277:ARG:NE   | 2.38                     | 0.55              |
| 3:E:3:C:O2       | 4:D:277:ARG:CZ   | 2.53                     | 0.55              |
| 1:B:1240:U:C5    | 8:I:31:VAL:HG11  | 2.36                     | 0.55              |
| 7:H:18:HIS:CE1   | 7:H:19:PHE:CZ    | 2.94                     | 0.55              |
| 1:B:1240:U:O4'   | 8:I:37:THR:OG1   | 2.23                     | 0.55              |
| 4:D:108:TYR:CE1  | 5:F:145:VAL:CG2  | 2.90                     | 0.55              |
| 4:D:533:TYR:CA   | 8:I:129:ASN:O    | 2.53                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:524:GLU:HB2  | 8:I:110:ARG:HH21 | 1.70                     | 0.54              |
| 4:D:529:GLU:HG2  | 8:I:135:LYS:CB   | 2.37                     | 0.54              |
| 4:D:529:GLU:HG2  | 8:I:135:LYS:CG   | 2.37                     | 0.54              |
| 4:D:108:TYR:HE2  | 5:F:121:MET:CB   | 1.94                     | 0.53              |
| 4:D:524:GLU:HB3  | 8:I:110:ARG:NE   | 2.13                     | 0.53              |
| 4:D:138:HIS:CD2  | 4:D:140:LEU:H    | 2.26                     | 0.53              |
| 4:D:529:GLU:OE2  | 8:I:135:LYS:HD2  | 2.09                     | 0.53              |
| 2:A:2113:U:H5'   | 4:D:150:ALA:CB   | 2.39                     | 0.53              |
| 4:D:140:LEU:CD2  | 5:F:129:GLN:CB   | 2.83                     | 0.53              |
| 4:D:526:ASN:H    | 4:D:529:GLU:CD   | 2.11                     | 0.52              |
| 3:E:72:C:H5'     | 4:D:278:GLN:HE21 | 1.69                     | 0.52              |
| 4:D:108:TYR:CE2  | 5:F:121:MET:HG2  | 2.43                     | 0.52              |
| 1:B:1240:U:O2    | 8:I:37:THR:HG21  | 1.98                     | 0.52              |
| 4:D:125:GLN:CG   | 5:F:144:THR:HA   | 2.39                     | 0.51              |
| 4:D:510:HIS:NE2  | 4:D:524:GLU:OE1  | 2.36                     | 0.51              |
| 2:A:2113:U:O2    | 4:D:143:GLN:OE1  | 2.28                     | 0.51              |
| 4:D:108:TYR:CD1  | 5:F:118:PRO:CA   | 2.88                     | 0.51              |
| 4:D:130:GLU:C    | 5:F:55:SER:HG    | 2.07                     | 0.51              |
| 4:D:118:PHE:CD2  | 5:F:148:ASN:ND2  | 2.78                     | 0.51              |
| 3:E:3:C:C2'      | 4:D:277:ARG:NH2  | 2.69                     | 0.51              |
| 4:D:118:PHE:CD2  | 5:F:147:PRO:HB2  | 2.46                     | 0.51              |
| 4:D:125:GLN:CD   | 5:F:144:THR:HG23 | 2.27                     | 0.51              |
| 4:D:125:GLN:HG2  | 4:D:126:GLY:N    | 2.26                     | 0.50              |
| 4:D:368:MET:HB3  | 4:D:380:ILE:HD12 | 1.92                     | 0.50              |
| 5:F:170:ILE:HG23 | 5:F:172:HIS:CE1  | 2.47                     | 0.50              |
| 6:G:39:VAL:HG22  | 6:G:39:VAL:O     | 2.11                     | 0.50              |
| 8:I:119:LEU:HD13 | 8:I:123:LEU:HG   | 1.94                     | 0.50              |
| 3:E:72:C:O5'     | 4:D:278:GLN:NE2  | 2.45                     | 0.50              |
| 2:A:2166:U:C5    | 2:A:2167:U:C4    | 3.00                     | 0.49              |
| 4:D:111:TYR:HD2  | 5:F:118:PRO:HB3  | 1.78                     | 0.49              |
| 4:D:97:VAL:HG21  | 4:D:135:HIS:CD2  | 2.47                     | 0.49              |
| 4:D:322:LYS:CE   | 8:I:112:ASP:O    | 2.60                     | 0.49              |
| 4:D:532:GLU:HB3  | 8:I:138:GLU:OE2  | 2.11                     | 0.49              |
| 8:I:28:ILE:HG21  | 8:I:101:ARG:HA   | 1.93                     | 0.49              |
| 4:D:111:TYR:HD2  | 5:F:118:PRO:CG   | 2.26                     | 0.49              |
| 4:D:108:TYR:HE2  | 5:F:121:MET:CG   | 2.16                     | 0.49              |
| 2:A:1843:C:H2'   | 2:A:1844:C:H6    | 1.79                     | 0.48              |
| 2:A:2113:U:C5'   | 4:D:147:ALA:CA   | 2.69                     | 0.48              |
| 2:A:2164:C:C2    | 2:A:2172:U:C5    | 3.02                     | 0.48              |
| 3:E:72:C:H4'     | 4:D:278:GLN:CG   | 2.43                     | 0.48              |
| 5:F:104:ILE:HD13 | 5:F:104:ILE:H    | 1.79                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 5:F:166:ASP:CG  | 5:F:170:ILE:HG22 | 2.34                     | 0.48              |
| 4:D:414:ILE:HB  | 6:G:44:ALA:HA    | 1.96                     | 0.48              |
| 8:I:137:ARG:O   | 8:I:141:HIS:CD2  | 2.67                     | 0.48              |
| 4:D:111:TYR:CD2 | 5:F:118:PRO:CG   | 2.96                     | 0.47              |
| 4:D:129:GLU:OE1 | 5:F:143:GLY:C    | 2.50                     | 0.47              |
| 4:D:111:TYR:CD1 | 5:F:146:THR:O    | 2.67                     | 0.47              |
| 2:A:1878:G:C6   | 2:A:1879:C:C4    | 3.02                     | 0.47              |
| 2:A:2169:A:N3   | 4:D:141:ASN:CG   | 2.65                     | 0.47              |
| 3:E:17:C:P      | 3:E:18:U:C5      | 3.01                     | 0.47              |
| 3:E:72:C:H6     | 3:E:72:C:H5'     | 1.78                     | 0.47              |
| 5:F:60:ARG:HH11 | 5:F:164:ARG:HD2  | 1.80                     | 0.47              |
| 4:D:105:ASP:OD2 | 5:F:122:ARG:HD3  | 2.15                     | 0.47              |
| 4:D:529:GLU:CG  | 8:I:135:LYS:CG   | 2.86                     | 0.47              |
| 2:A:2107:G:C6   | 2:A:2183:A:C2    | 3.03                     | 0.47              |
| 2:A:2115:G:H3'  | 2:A:2116:G:C5'   | 2.45                     | 0.47              |
| 4:D:111:TYR:CD2 | 5:F:146:THR:O    | 2.68                     | 0.47              |
| 5:F:151:GLU:HA  | 5:F:154:LYS:HE3  | 1.97                     | 0.47              |
| 4:D:125:GLN:HG3 | 5:F:144:THR:HA   | 1.96                     | 0.47              |
| 1:B:1242:G:C6   | 1:B:1243:C:C4    | 3.03                     | 0.46              |
| 4:D:412:LEU:CD2 | 6:G:46:LYS:N     | 2.63                     | 0.46              |
| 4:D:523:PHE:HB2 | 8:I:130:LYS:CD   | 2.22                     | 0.46              |
| 6:G:102:LEU:HA  | 6:G:106:ALA:HB3  | 1.97                     | 0.46              |
| 2:A:2183:A:H2'  | 2:A:2184:A:C8    | 2.50                     | 0.46              |
| 4:D:533:TYR:HE1 | 4:D:537:THR:HG1  | 1.63                     | 0.46              |
| 2:A:2107:G:C5   | 2:A:2183:A:C2    | 3.04                     | 0.46              |
| 2:A:2155:U:C5   | 2:A:2156:G:C5    | 3.04                     | 0.46              |
| 4:D:118:PHE:HB3 | 5:F:147:PRO:HB2  | 1.98                     | 0.46              |
| 4:D:523:PHE:CE2 | 4:D:525:GLY:O    | 2.69                     | 0.46              |
| 3:E:72:C:C4'    | 4:D:278:GLN:HE21 | 2.28                     | 0.45              |
| 8:I:125:ASP:HB3 | 8:I:131:GLY:CA   | 2.45                     | 0.45              |
| 3:E:72:C:C5'    | 4:D:278:GLN:NE2  | 2.72                     | 0.45              |
| 4:D:322:LYS:HE2 | 8:I:112:ASP:O    | 2.16                     | 0.45              |
| 4:D:125:GLN:OE1 | 5:F:144:THR:HA   | 2.15                     | 0.45              |
| 4:D:524:GLU:CB  | 8:I:110:ARG:NH2  | 2.76                     | 0.45              |
| 4:D:301:GLU:OE1 | 4:D:305:ARG:NH2  | 2.50                     | 0.45              |
| 4:D:526:ASN:HB2 | 8:I:135:LYS:HZ3  | 1.81                     | 0.45              |
| 4:D:311:LEU:HB2 | 4:D:482:ALA:HB1  | 1.98                     | 0.45              |
| 5:F:60:ARG:NH2  | 5:F:165:ASN:O    | 2.50                     | 0.45              |
| 4:D:511:ILE:HB  | 4:D:523:PHE:CD2  | 2.52                     | 0.44              |
| 4:D:529:GLU:OE2 | 8:I:135:LYS:CD   | 2.65                     | 0.44              |
| 4:D:533:TYR:CD2 | 8:I:130:LYS:HD3  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:325:GLU:OE1  | 8:I:113:LYS:HE3  | 2.17                     | 0.44              |
| 4:D:368:MET:CB   | 4:D:380:ILE:HD12 | 2.48                     | 0.44              |
| 4:D:510:HIS:HD2  | 4:D:524:GLU:OE2  | 1.99                     | 0.44              |
| 4:D:415:MET:HG3  | 4:D:424:SER:HB3  | 1.99                     | 0.43              |
| 2:A:2113:U:C4    | 4:D:143:GLN:NE2  | 2.79                     | 0.43              |
| 8:I:129:ASN:HA   | 8:I:134:VAL:HG21 | 1.99                     | 0.43              |
| 4:D:536:ARG:NH1  | 8:I:137:ARG:CZ   | 2.66                     | 0.43              |
| 4:D:529:GLU:HG2  | 8:I:135:LYS:HA   | 2.00                     | 0.43              |
| 2:A:2167:U:C4    | 2:A:2168:G:C5    | 3.07                     | 0.43              |
| 4:D:524:GLU:HB2  | 8:I:110:ARG:NE   | 2.27                     | 0.43              |
| 4:D:322:LYS:HE3  | 8:I:112:ASP:CA   | 2.49                     | 0.43              |
| 8:I:125:ASP:HB3  | 8:I:131:GLY:HA2  | 2.00                     | 0.43              |
| 4:D:511:ILE:HB   | 4:D:523:PHE:HD2  | 1.84                     | 0.43              |
| 2:A:2113:U:C2    | 4:D:143:GLN:NE2  | 2.87                     | 0.42              |
| 4:D:528:THR:CB   | 8:I:142:ARG:NH2  | 2.77                     | 0.42              |
| 5:F:104:ILE:H    | 5:F:104:ILE:CD1  | 2.32                     | 0.42              |
| 5:F:76:ALA:HB2   | 5:F:111:PHE:CE2  | 2.53                     | 0.42              |
| 3:E:17:C:O5'     | 3:E:18:U:H5      | 2.03                     | 0.42              |
| 2:A:2113:U:H4'   | 4:D:146:ARG:O    | 2.20                     | 0.42              |
| 4:D:111:TYR:HB2  | 5:F:118:PRO:HG2  | 1.88                     | 0.42              |
| 4:D:133:GLN:CD   | 5:F:60:ARG:HH11  | 2.23                     | 0.42              |
| 2:A:1885:A:O4'   | 4:D:4:PHE:HZ     | 2.03                     | 0.42              |
| 2:A:2108:A:C2    | 2:A:2109:U:C5    | 3.08                     | 0.42              |
| 4:D:523:PHE:CB   | 8:I:130:LYS:HD2  | 2.23                     | 0.42              |
| 4:D:533:TYR:HE1  | 4:D:537:THR:OG1  | 2.03                     | 0.42              |
| 5:F:104:ILE:HD13 | 5:F:104:ILE:N    | 2.35                     | 0.42              |
| 4:D:105:ASP:OD2  | 5:F:122:ARG:CD   | 2.67                     | 0.42              |
| 4:D:523:PHE:CZ   | 4:D:530:TYR:HB2  | 2.54                     | 0.42              |
| 4:D:532:GLU:CB   | 8:I:138:GLU:OE1  | 2.67                     | 0.42              |
| 2:A:2096:C:H2'   | 2:A:2097:A:C8    | 2.55                     | 0.41              |
| 2:A:2168:G:N2    | 2:A:2171:A:C8    | 2.88                     | 0.41              |
| 4:D:133:GLN:OE1  | 5:F:141:LYS:CG   | 2.68                     | 0.41              |
| 8:I:45:ALA:HA    | 8:I:120:ALA:HB2  | 2.01                     | 0.41              |
| 2:A:2115:G:H3'   | 2:A:2116:G:H5''  | 2.01                     | 0.41              |
| 4:D:322:LYS:HB3  | 8:I:113:LYS:NZ   | 2.22                     | 0.41              |
| 4:D:108:TYR:CE1  | 5:F:145:VAL:HG13 | 2.48                     | 0.41              |
| 4:D:330:ARG:HB3  | 4:D:377:SER:HB3  | 2.03                     | 0.41              |
| 2:A:1846:G:H3'   | 2:A:1847:A:H5''  | 2.02                     | 0.41              |
| 2:A:1878:G:C5    | 2:A:1879:C:C5    | 3.08                     | 0.41              |
| 4:D:133:GLN:OE1  | 5:F:141:LYS:CA   | 2.69                     | 0.41              |
| 4:D:111:TYR:CE2  | 5:F:145:VAL:CG2  | 2.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:138:HIS:HE1  | 5:F:129:GLN:HB2  | 1.86                     | 0.41              |
| 5:F:5:THR:O      | 5:F:9:ARG:HG3    | 2.20                     | 0.41              |
| 5:F:47:ASN:HB2   | 5:F:211:LYS:O    | 2.21                     | 0.41              |
| 8:I:68:VAL:HG11  | 8:I:103:ILE:HG13 | 2.02                     | 0.41              |
| 2:A:1846:G:C6    | 2:A:1847:A:C6    | 3.09                     | 0.41              |
| 4:D:73:TYR:HA    | 4:D:185:LEU:O    | 2.20                     | 0.40              |
| 4:D:111:TYR:CE1  | 5:F:147:PRO:N    | 2.88                     | 0.40              |
| 2:A:2113:U:H5'   | 4:D:147:ALA:O    | 2.21                     | 0.40              |
| 5:F:60:ARG:CZ    | 5:F:164:ARG:HG2  | 2.51                     | 0.40              |
| 4:D:108:TYR:CZ   | 5:F:145:VAL:CG1  | 2.95                     | 0.40              |
| 4:D:322:LYS:HE3  | 8:I:112:ASP:O    | 2.21                     | 0.40              |
| 4:D:533:TYR:CD2  | 8:I:130:LYS:CG   | 3.04                     | 0.40              |
| 4:D:412:LEU:HD21 | 6:G:46:LYS:CB    | 2.44                     | 0.40              |
| 4:D:222:LEU:HD23 | 4:D:222:LEU:HA   | 1.87                     | 0.40              |
| 4:D:354:ILE:HB   | 4:D:497:ILE:HG12 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 4   | D     | 552/561 (98%)   | 508 (92%)  | 27 (5%)  | 17 (3%)  | 4           | 27 |
| 5   | F     | 232/234 (99%)   | 199 (86%)  | 23 (10%) | 10 (4%)  | 2           | 22 |
| 6   | G     | 176/178 (99%)   | 138 (78%)  | 26 (15%) | 12 (7%)  | 1           | 15 |
| 7   | H     | 48/50 (96%)     | 38 (79%)   | 9 (19%)  | 1 (2%)   | 7           | 36 |
| 8   | I     | 149/151 (99%)   | 119 (80%)  | 23 (15%) | 7 (5%)   | 2           | 21 |
| All | All   | 1157/1174 (99%) | 1002 (87%) | 108 (9%) | 47 (4%)  | 5           | 22 |

All (47) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 83  | GLU  |
| 4   | D     | 91  | GLU  |
| 4   | D     | 143 | GLN  |
| 4   | D     | 317 | PRO  |
| 6   | G     | 102 | LEU  |
| 4   | D     | 165 | GLY  |
| 4   | D     | 194 | ASP  |
| 4   | D     | 283 | ARG  |
| 4   | D     | 295 | GLU  |
| 5   | F     | 4   | LEU  |
| 5   | F     | 167 | LYS  |
| 5   | F     | 203 | GLN  |
| 6   | G     | 78  | ILE  |
| 6   | G     | 84  | ILE  |
| 6   | G     | 100 | GLU  |
| 6   | G     | 104 | THR  |
| 8   | I     | 13  | PRO  |
| 8   | I     | 126 | ALA  |
| 8   | I     | 139 | ASP  |
| 4   | D     | 155 | ASP  |
| 4   | D     | 208 | PHE  |
| 4   | D     | 243 | ASN  |
| 5   | F     | 100 | LEU  |
| 5   | F     | 159 | GLY  |
| 5   | F     | 204 | ALA  |
| 6   | G     | 2   | LYS  |
| 6   | G     | 96  | TRP  |
| 8   | I     | 112 | ASP  |
| 4   | D     | 93  | ALA  |
| 4   | D     | 299 | SER  |
| 5   | F     | 110 | ASN  |
| 6   | G     | 51  | ASN  |
| 6   | G     | 101 | ARG  |
| 7   | H     | 4   | ILE  |
| 8   | I     | 52  | ARG  |
| 4   | D     | 181 | PRO  |
| 6   | G     | 125 | GLY  |
| 8   | I     | 10  | LYS  |
| 6   | G     | 4   | HIS  |
| 6   | G     | 39  | VAL  |
| 4   | D     | 142 | VAL  |
| 4   | D     | 279 | GLY  |
| 8   | I     | 28  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 225 | VAL  |
| 5   | F     | 73  | VAL  |
| 5   | F     | 147 | PRO  |
| 5   | F     | 233 | VAL  |

### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4   | D     | 465/472 (98%)  | 436 (94%) | 29 (6%)  | 18          | 43 |
| 5   | F     | 181/181 (100%) | 170 (94%) | 11 (6%)  | 18          | 44 |
| 6   | G     | 149/149 (100%) | 143 (96%) | 6 (4%)   | 31          | 55 |
| 7   | H     | 45/45 (100%)   | 44 (98%)  | 1 (2%)   | 52          | 71 |
| 8   | I     | 124/124 (100%) | 119 (96%) | 5 (4%)   | 31          | 55 |
| All | All   | 964/971 (99%)  | 912 (95%) | 52 (5%)  | 26          | 47 |

All (52) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 17  | PRO  |
| 4   | D     | 40  | LEU  |
| 4   | D     | 41  | ASN  |
| 4   | D     | 48  | LEU  |
| 4   | D     | 97  | VAL  |
| 4   | D     | 118 | PHE  |
| 4   | D     | 125 | GLN  |
| 4   | D     | 127 | ARG  |
| 4   | D     | 152 | ARG  |
| 4   | D     | 169 | ARG  |
| 4   | D     | 188 | GLU  |
| 4   | D     | 190 | THR  |
| 4   | D     | 191 | ASN  |
| 4   | D     | 203 | ARG  |
| 4   | D     | 204 | PHE  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 4          | D            | 246        | SER         |
| 4          | D            | 266        | ARG         |
| 4          | D            | 276        | VAL         |
| 4          | D            | 277        | ARG         |
| 4          | D            | 305        | ARG         |
| 4          | D            | 318        | ARG         |
| 4          | D            | 363        | SER         |
| 4          | D            | 440        | LYS         |
| 4          | D            | 474        | ASP         |
| 4          | D            | 477        | ILE         |
| 4          | D            | 478        | GLU         |
| 4          | D            | 498        | SER         |
| 4          | D            | 523        | PHE         |
| 4          | D            | 533        | TYR         |
| 5          | F            | 1          | MET         |
| 5          | F            | 16         | ASP         |
| 5          | F            | 38         | PHE         |
| 5          | F            | 40         | GLU         |
| 5          | F            | 43         | ASP         |
| 5          | F            | 48         | LEU         |
| 5          | F            | 69         | THR         |
| 5          | F            | 104        | ILE         |
| 5          | F            | 113        | VAL         |
| 5          | F            | 162        | ARG         |
| 5          | F            | 224        | VAL         |
| 6          | G            | 64         | PRO         |
| 6          | G            | 84         | ILE         |
| 6          | G            | 99         | PHE         |
| 6          | G            | 114        | ARG         |
| 6          | G            | 142        | TYR         |
| 6          | G            | 147        | ARG         |
| 7          | H            | 46         | VAL         |
| 8          | I            | 8          | GLN         |
| 8          | I            | 39         | GLU         |
| 8          | I            | 49         | LEU         |
| 8          | I            | 72         | VAL         |
| 8          | I            | 93         | VAL         |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 4          | D            | 76         | GLN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 138 | HIS  |
| 4   | D     | 162 | ASN  |
| 4   | D     | 257 | GLN  |
| 4   | D     | 278 | GLN  |
| 5   | F     | 126 | GLN  |
| 5   | F     | 129 | GLN  |
| 5   | F     | 172 | HIS  |
| 7   | H     | 18  | HIS  |
| 8   | I     | 51  | GLN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 1   | B     | 30/101 (29%)  | 12 (40%)          | 3 (10%)         |
| 2   | A     | 172/360 (47%) | 53 (30%)          | 9 (5%)          |
| 3   | E     | 76/77 (98%)   | 19 (25%)          | 1 (1%)          |
| All | All   | 278/538 (51%) | 84 (30%)          | 13 (4%)         |

All (84) RNA backbone outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1238 | A    |
| 1   | B     | 1240 | U    |
| 1   | B     | 1243 | C    |
| 1   | B     | 1292 | G    |
| 1   | B     | 1293 | C    |
| 1   | B     | 1299 | A    |
| 1   | B     | 1300 | G    |
| 1   | B     | 1302 | C    |
| 1   | B     | 1304 | G    |
| 1   | B     | 1305 | G    |
| 1   | B     | 1335 | U    |
| 1   | B     | 1336 | C    |
| 2   | A     | 1846 | G    |
| 2   | A     | 1847 | A    |
| 2   | A     | 1848 | A    |
| 2   | A     | 1858 | A    |
| 2   | A     | 1859 | U    |
| 2   | A     | 1869 | G    |
| 2   | A     | 1870 | C    |
| 2   | A     | 1871 | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | A            | 1872       | A           |
| 2          | A            | 1874       | C           |
| 2          | A            | 1884       | G           |
| 2          | A            | 1888       | G           |
| 2          | A            | 1903       | G           |
| 2          | A            | 1905       | C           |
| 2          | A            | 1906       | G           |
| 2          | A            | 1907       | G           |
| 2          | A            | 2102       | G           |
| 2          | A            | 2104       | C           |
| 2          | A            | 2110       | G           |
| 2          | A            | 2111       | U           |
| 2          | A            | 2112       | G           |
| 2          | A            | 2113       | U           |
| 2          | A            | 2117       | A           |
| 2          | A            | 2119       | A           |
| 2          | A            | 2127       | G           |
| 2          | A            | 2130       | U           |
| 2          | A            | 2131       | U           |
| 2          | A            | 2132       | U           |
| 2          | A            | 2133       | G           |
| 2          | A            | 2134       | A           |
| 2          | A            | 2135       | A           |
| 2          | A            | 2136       | G           |
| 2          | A            | 2137       | U           |
| 2          | A            | 2144       | G           |
| 2          | A            | 2146       | C           |
| 2          | A            | 2147       | A           |
| 2          | A            | 2148       | G           |
| 2          | A            | 2149       | U           |
| 2          | A            | 2152       | G           |
| 2          | A            | 2153       | C           |
| 2          | A            | 2155       | U           |
| 2          | A            | 2157       | G           |
| 2          | A            | 2158       | A           |
| 2          | A            | 2159       | G           |
| 2          | A            | 2162       | G           |
| 2          | A            | 2164       | C           |
| 2          | A            | 2165       | C           |
| 2          | A            | 2167       | U           |
| 2          | A            | 2176       | A           |
| 2          | A            | 2179       | C           |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | A     | 2181 | U    |
| 2   | A     | 2187 | U    |
| 2   | A     | 2192 | U    |
| 3   | E     | 5    | G    |
| 3   | E     | 8    | U    |
| 3   | E     | 9    | G    |
| 3   | E     | 13   | C    |
| 3   | E     | 17   | C    |
| 3   | E     | 18   | U    |
| 3   | E     | 19   | G    |
| 3   | E     | 20   | G    |
| 3   | E     | 21   | U    |
| 3   | E     | 22   | A    |
| 3   | E     | 48   | U    |
| 3   | E     | 49   | C    |
| 3   | E     | 50   | G    |
| 3   | E     | 54   | G    |
| 3   | E     | 72   | C    |
| 3   | E     | 74   | A    |
| 3   | E     | 75   | C    |
| 3   | E     | 76   | C    |
| 3   | E     | 77   | A    |

All (13) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1299 | A    |
| 1   | B     | 1332 | A    |
| 1   | B     | 1335 | U    |
| 2   | A     | 1871 | A    |
| 2   | A     | 2110 | G    |
| 2   | A     | 2126 | A    |
| 2   | A     | 2129 | C    |
| 2   | A     | 2152 | G    |
| 2   | A     | 2157 | G    |
| 2   | A     | 2158 | A    |
| 2   | A     | 2159 | G    |
| 2   | A     | 2172 | U    |
| 3   | E     | 9    | G    |

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

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

## 5.5 Carbohydrates [i](#)

There are no 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](#)

There are no chain breaks in this entry.



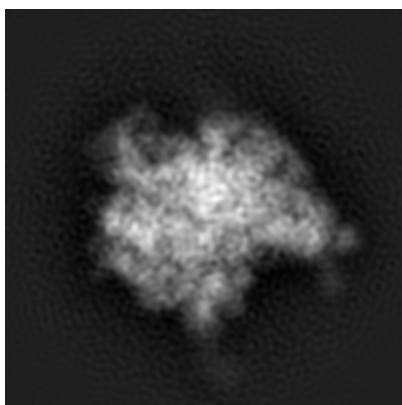
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5784. These allow visual inspection of the internal detail of the map and identification of artifacts.

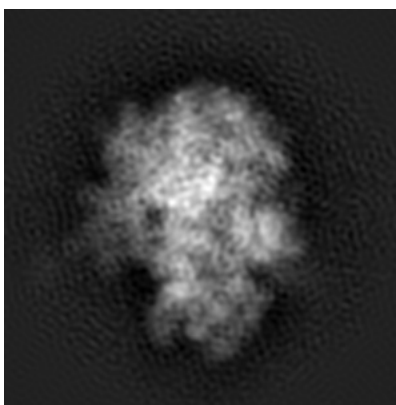
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

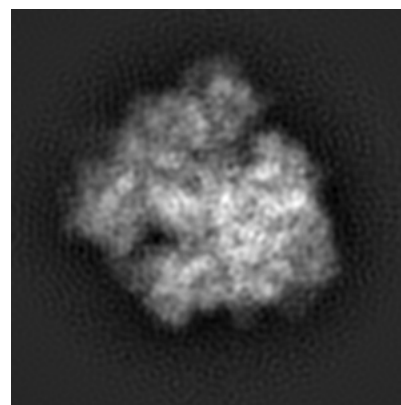
#### 6.1.1 Primary map



X



Y

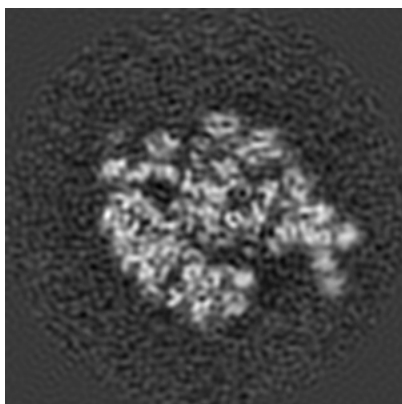


Z

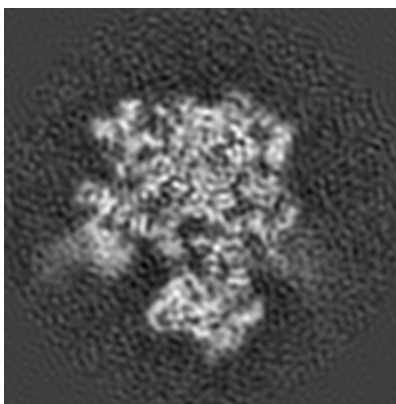
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

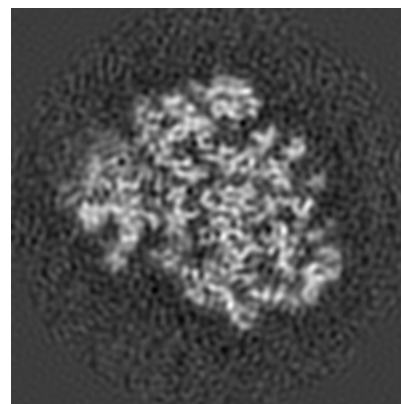
#### 6.2.1 Primary map



X Index: 67



Y Index: 67

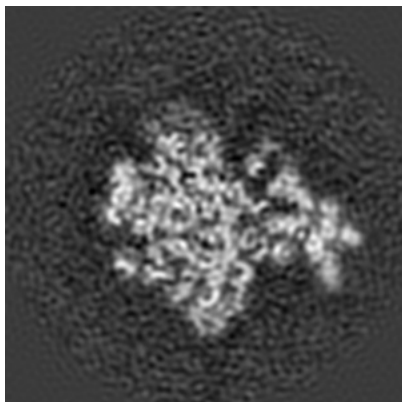


Z Index: 67

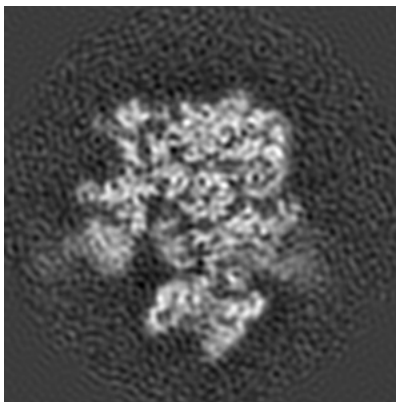
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

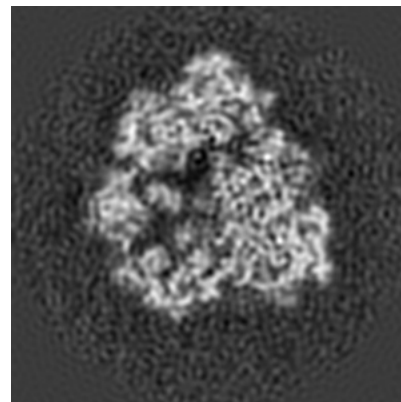
### 6.3.1 Primary map



X Index: 71



Y Index: 69

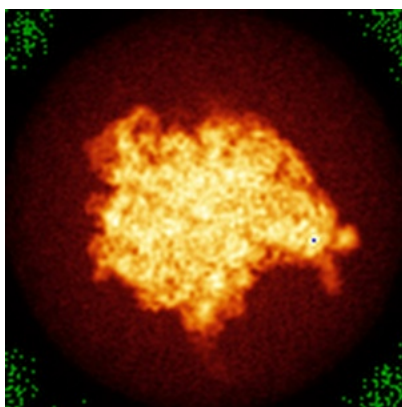


Z Index: 58

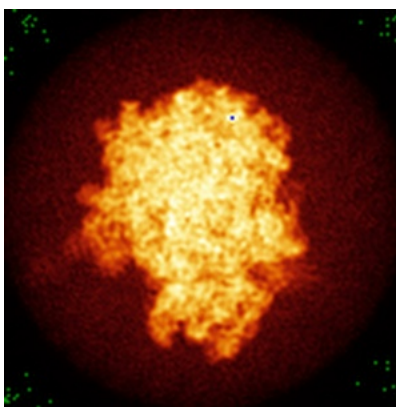
The images above show the largest variance slices of the map in three orthogonal directions.

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

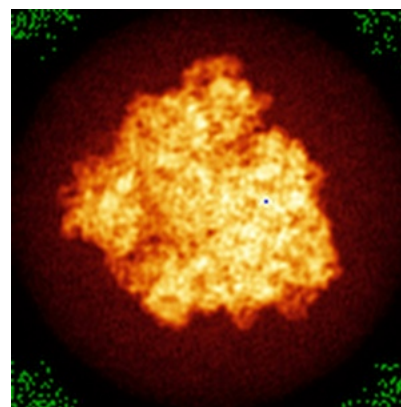
### 6.4.1 Primary map



X



Y

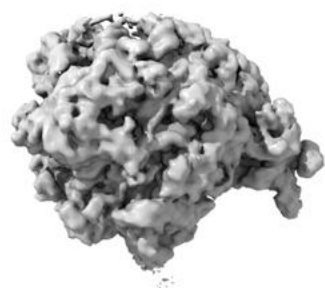


Z

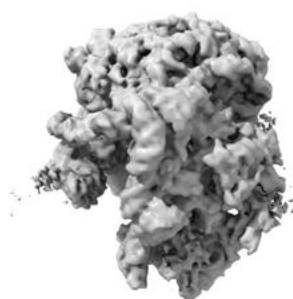
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

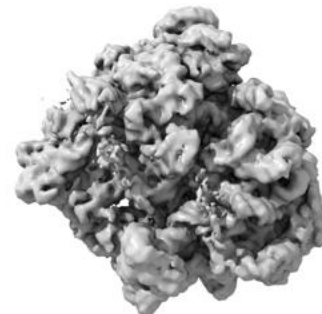
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 80.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

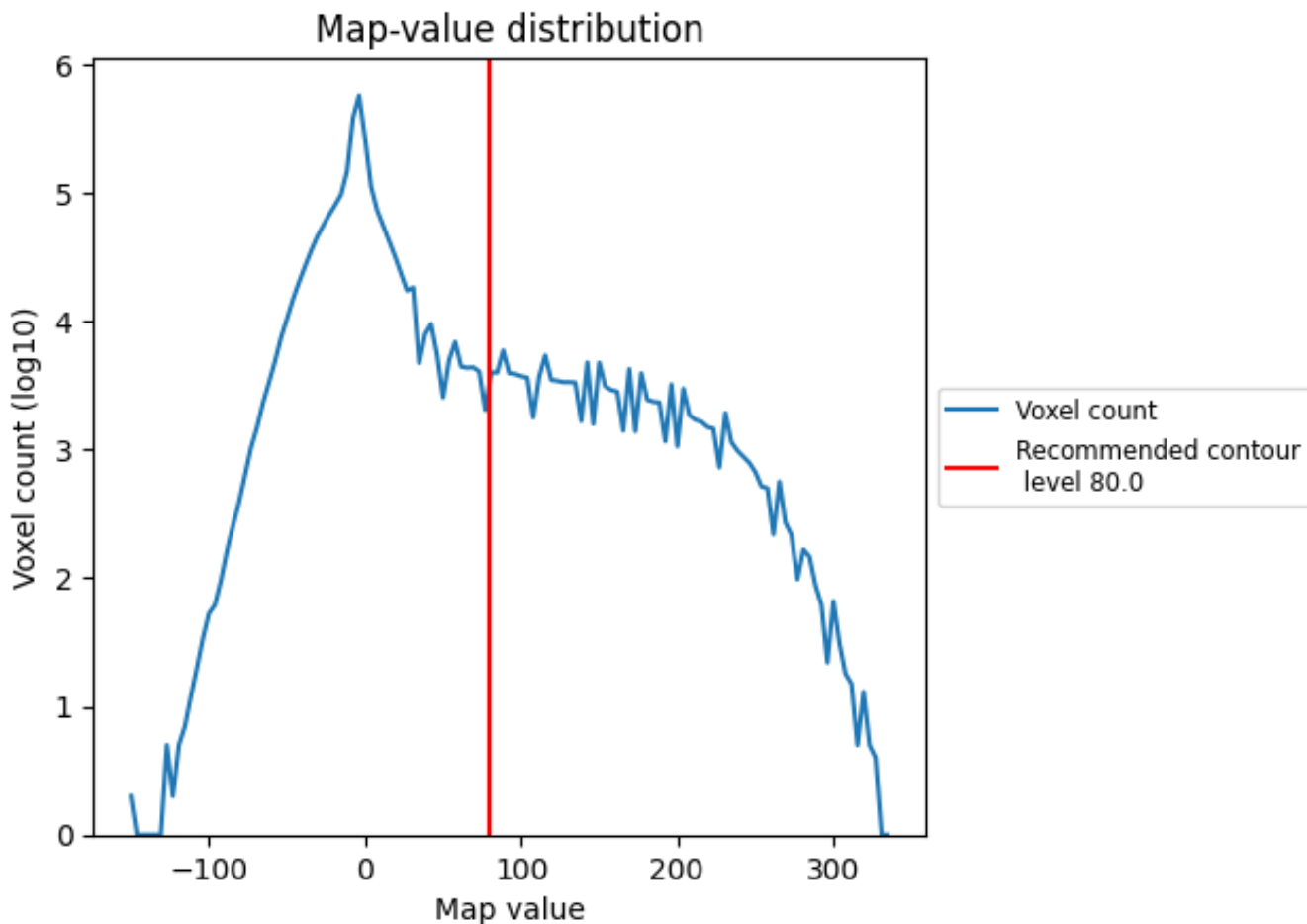
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

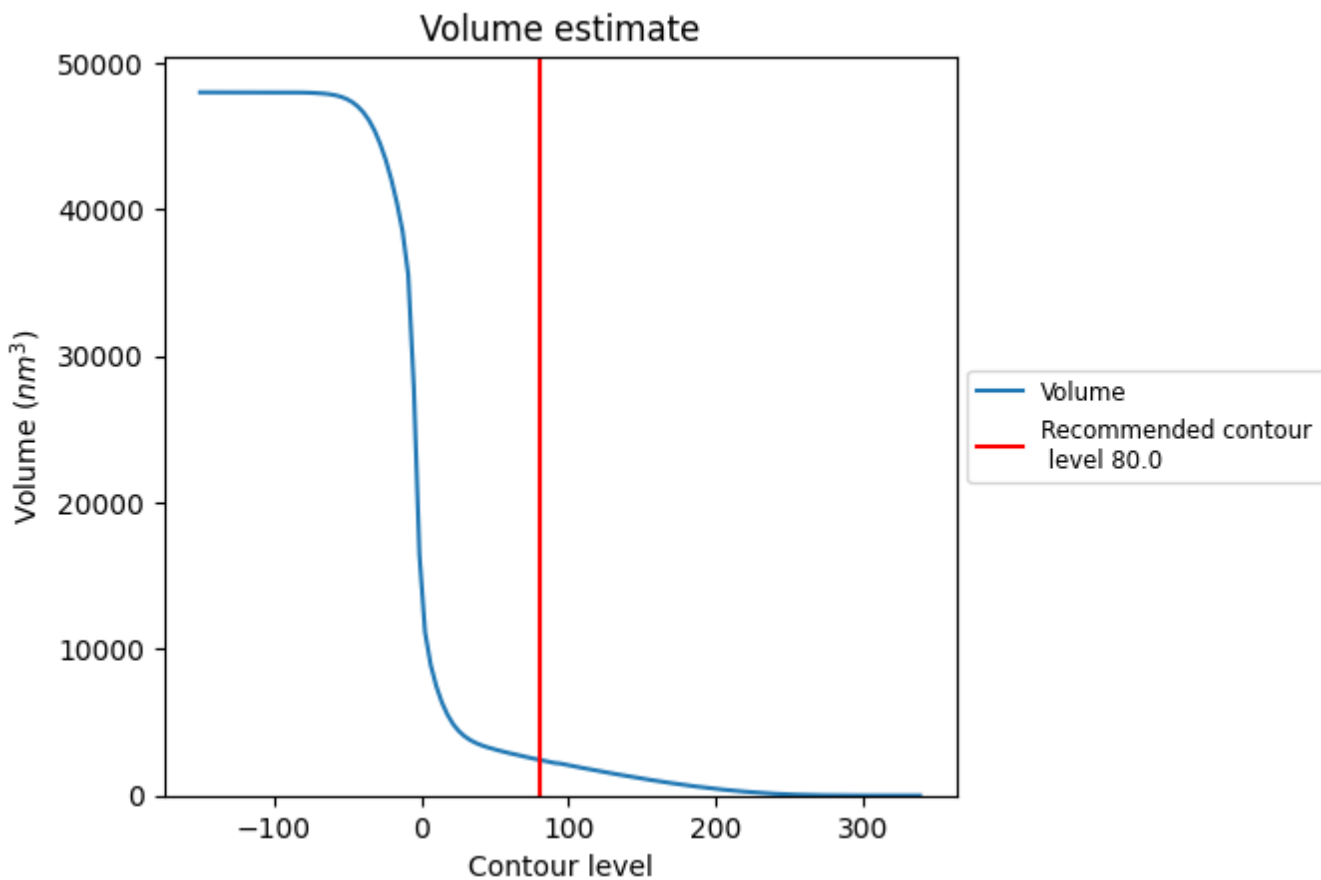
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

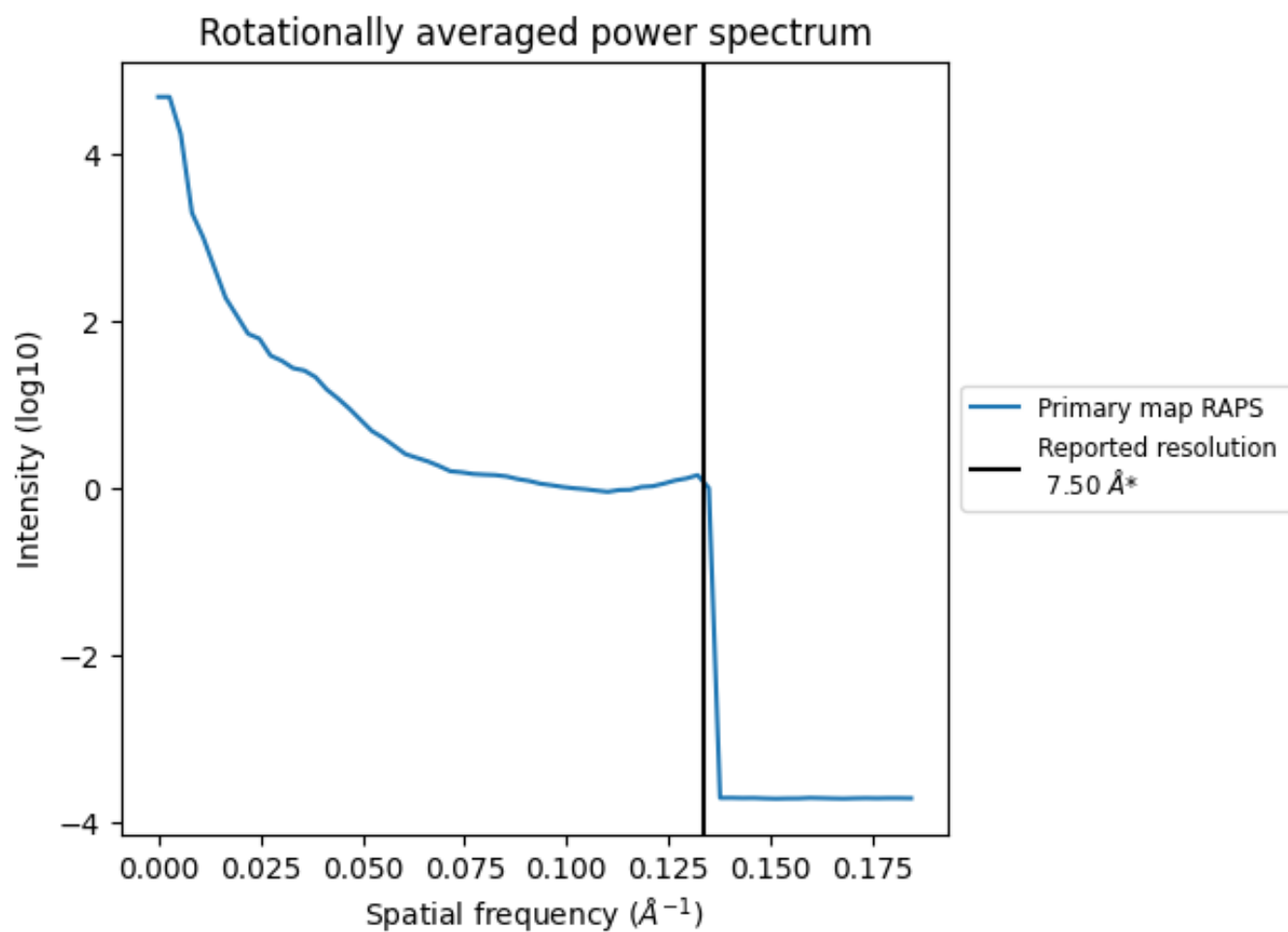
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2444 nm<sup>3</sup>; this corresponds to an approximate mass of 2208 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.133 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5784 and PDB model 3J5S. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 80.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



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



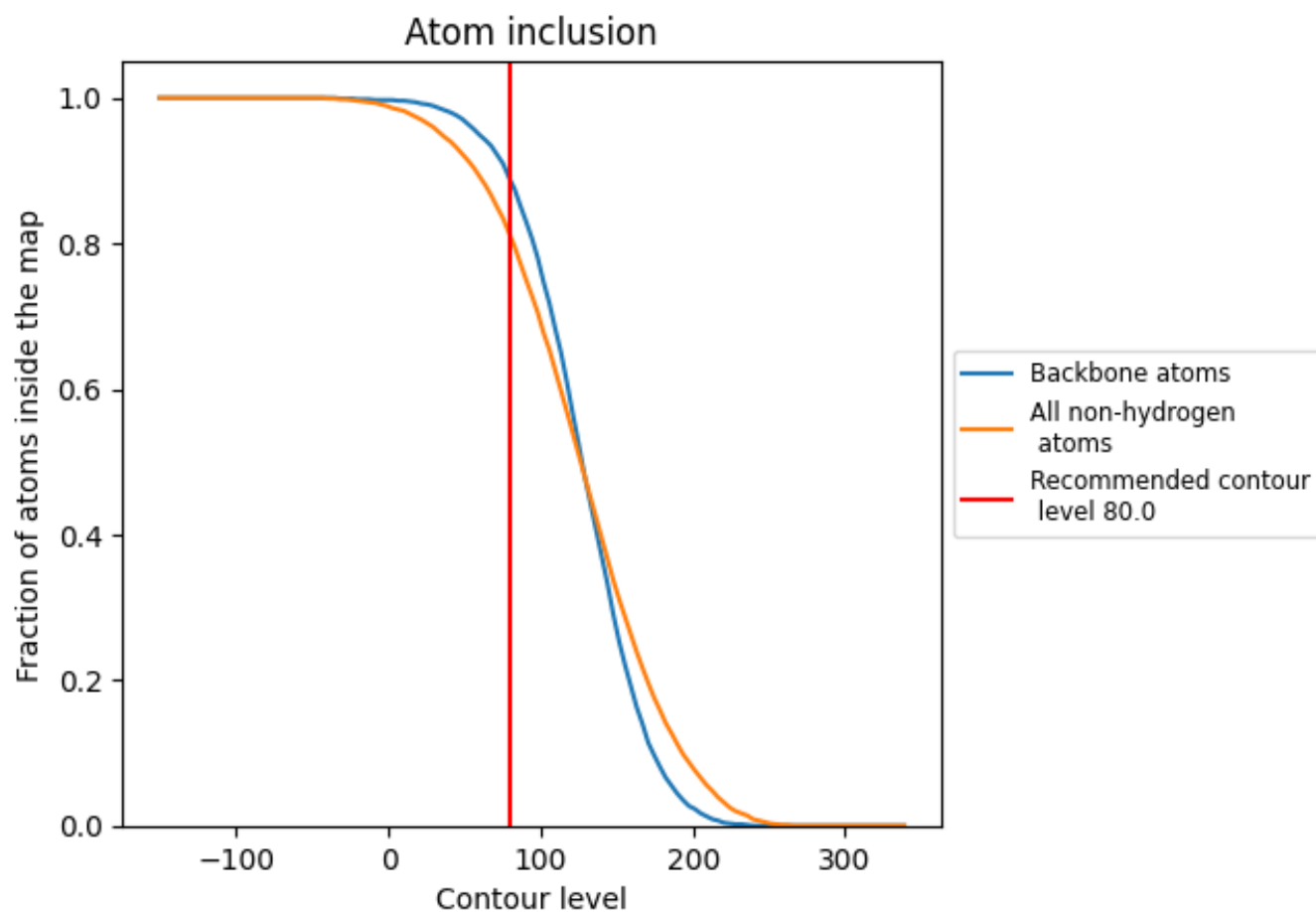
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (80.0).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (80.0) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8110 |  0.1220 |
| A     |  0.9550 |  0.1600 |
| B     |  0.9880 |  0.1690 |
| D     |  0.6450 |  0.1120 |
| E     |  0.8680 |  0.1700 |
| F     |  0.8670 |  0.0700 |
| G     |  0.8440 |  0.0980 |
| H     |  0.7710 |  0.0940 |
| I     |  0.6640 |  0.0650 |

