



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:55 am GMT

PDB ID : 1LBG  
Title : LACTOSE OPERON REPRESSOR BOUND TO 21-BASE PAIR SYMMETRIC OPERATOR DNA, ALPHA CARBONS ONLY  
Authors : Lewis, M.; Chang, G.; Horton, N.C.; Kercher, M.A.; Pace, H.C.; Lu, P.  
Deposited on : 1996-01-03  
Resolution : 4.80 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

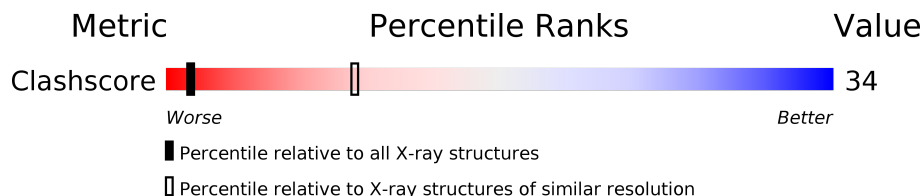
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.80 Å.




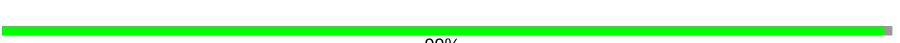
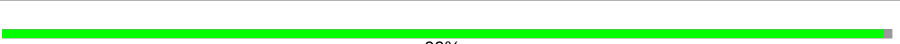
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric     | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|------------|-----------------------------|---|
| Clashscore | 112137                      | 1067 (5.90-3.70)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | E     | 21     |  |
| 1   | F     | 21     |  |
| 1   | G     | 21     |  |
| 1   | H     | 21     |  |
| 2   | A     | 360    |  |
| 2   | B     | 360    |  |
| 2   | C     | 360    |  |
| 2   | D     | 360    |  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (5'-D(\*GP\*AP\*AP\*TP\*TP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*CP\*TP\*CP\*AP\*CP\*AP\*AP\*TP\*T)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 1   | E     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 429   | 206 | 79 | 124 | 20 |         |         |       |
| 1   | F     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 429   | 206 | 79 | 124 | 20 |         |         |       |
| 1   | G     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 429   | 206 | 79 | 124 | 20 |         |         |       |
| 1   | H     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 429   | 206 | 79 | 124 | 20 |         |         |       |

- Molecule 2 is a protein called PROTEIN (LACTOSE OPERON REPRESSOR).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 2   | A     | 357      | Total | C   | 0       | 0       | 357   |
|     |       |          | 357   | 357 |         |         |       |
| 2   | B     | 357      | Total | C   | 0       | 0       | 357   |
|     |       |          | 357   | 357 |         |         |       |
| 2   | C     | 357      | Total | C   | 0       | 0       | 357   |
|     |       |          | 357   | 357 |         |         |       |
| 2   | D     | 357      | Total | C   | 0       | 0       | 357   |
|     |       |          | 357   | 357 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 109     | THR      | ALA    | CONFLICT | UNP P03023 |
| B     | 109     | THR      | ALA    | CONFLICT | UNP P03023 |
| C     | 109     | THR      | ALA    | CONFLICT | UNP P03023 |
| D     | 109     | THR      | ALA    | CONFLICT | UNP P03023 |

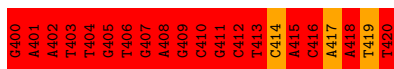
### 3 Residue-property plots [i](#)

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

Note EDS was not executed.

- Molecule 1: DNA (5'-D(\*GP\*AP\*AP\*TP\*TP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*CP\*TP\*CP\*AP\*CP\*AP\*AP\*TP\*T)-3')

Chain E: 



- Molecule 1: DNA (5'-D(\*GP\*AP\*AP\*TP\*TP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*CP\*TP\*CP\*AP\*CP\*AP\*AP\*TP\*T)-3')

Chain F: 



- Molecule 1: DNA (5'-D(\*GP\*AP\*AP\*TP\*TP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*CP\*TP\*CP\*AP\*CP\*AP\*AP\*TP\*T)-3')

Chain G: 



- Molecule 1: DNA (5'-D(\*GP\*AP\*AP\*TP\*TP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*CP\*TP\*CP\*AP\*CP\*AP\*AP\*TP\*T)-3')

Chain H: 



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain A: 



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain B:  99% .



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain C:  99% .



- Molecule 2: PROTEIN (LACTOSE OPERON REPRESSOR)

Chain D:  98% ..



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | C 1 2 1   | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 104.30Å 224.40Å 112.10Å<br>90.00° 95.70° 90.00° | Depositor |
| Resolution (Å)   | 15.00 – 4.80                                    | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (15.00-4.80)                    | Depositor |
| $R_{merge}$  | 0.06  | Depositor |
| $R_{sym}$  | (Not available)                                 | Depositor |
| Refinement program                                       | X-PLOR 3.1                                      | Depositor |
| R, $R_{free}$  | 0.260 , (Not available)                         | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 3144  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 15.0  | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$      | RMSZ        | $\# Z  > 5$      |
| 1   | E     | 3.40         | 68/481 (14.1%)   | 5.71        | 203/741 (27.4%)  |
| 1   | F     | 3.02         | 50/481 (10.4%)   | 5.29        | 200/741 (27.0%)  |
| 1   | G     | 3.59         | 49/481 (10.2%)   | 5.52        | 204/741 (27.5%)  |
| 1   | H     | 3.18         | 46/481 (9.6%)    | 5.51        | 203/741 (27.4%)  |
| All | All   | 3.31         | 213/1924 (11.1%) | 5.51        | 810/2964 (27.3%) |

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   | E     | 3                   | 18                  |
| 1   | F     | 1                   | 15                  |
| 1   | G     | 3                   | 16                  |
| 1   | H     | 3                   | 17                  |
| All | All   | 10                  | 66                  |

All (213) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 620 | DT   | P-O5'   | 22.13 | 1.81        | 1.59     |
| 1   | G     | 620 | DT   | C5'-C4' | 20.02 | 1.73        | 1.51     |
| 1   | G     | 602 | DA   | P-O5'   | 19.05 | 1.78        | 1.59     |
| 1   | H     | 720 | DT   | P-O5'   | 17.03 | 1.76        | 1.59     |
| 1   | G     | 601 | DA   | O3'-P   | 16.98 | 1.81        | 1.61     |
| 1   | G     | 602 | DA   | C5'-C4' | 15.75 | 1.68        | 1.51     |
| 1   | F     | 518 | DA   | P-O5'   | 15.07 | 1.74        | 1.59     |
| 1   | G     | 620 | DT   | C4'-C3' | 14.12 | 1.67        | 1.53     |
| 1   | G     | 601 | DA   | C2'-C1' | 12.78 | 1.65        | 1.52     |
| 1   | H     | 719 | DT   | C5'-C4' | 12.57 | 1.65        | 1.51     |
| 1   | G     | 601 | DA   | C3'-C2' | 12.46 | 1.67        | 1.52     |
| 1   | H     | 718 | DA   | C4'-C3' | 12.36 | 1.65        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 601 | DA   | C3'-O3' | 12.16 | 1.59        | 1.44     |
| 1   | E     | 401 | DA   | O3'-P   | 12.02 | 1.75        | 1.61     |
| 1   | E     | 401 | DA   | C5'-C4' | 11.95 | 1.64        | 1.51     |
| 1   | G     | 602 | DA   | O3'-P   | 11.71 | 1.75        | 1.61     |
| 1   | E     | 406 | DT   | P-O5'   | 11.62 | 1.71        | 1.59     |
| 1   | E     | 404 | DT   | C4'-C3' | 11.57 | 1.65        | 1.53     |
| 1   | E     | 418 | DA   | C5'-C4' | 11.52 | 1.64        | 1.51     |
| 1   | H     | 719 | DT   | P-O5'   | 11.48 | 1.71        | 1.59     |
| 1   | F     | 518 | DA   | C5'-C4' | 11.10 | 1.63        | 1.51     |
| 1   | F     | 501 | DA   | O3'-P   | 11.07 | 1.74        | 1.61     |
| 1   | G     | 602 | DA   | C4'-C3' | 11.07 | 1.64        | 1.53     |
| 1   | H     | 701 | DA   | C1'-N9  | 10.90 | 1.63        | 1.49     |
| 1   | H     | 701 | DA   | N9-C4   | 10.72 | 1.44        | 1.37     |
| 1   | G     | 601 | DA   | N9-C4   | 10.72 | 1.44        | 1.37     |
| 1   | F     | 518 | DA   | C4'-C3' | 10.65 | 1.64        | 1.53     |
| 1   | E     | 406 | DT   | C5'-C4' | 10.64 | 1.63        | 1.51     |
| 1   | G     | 600 | DG   | C1'-N9  | 10.49 | 1.62        | 1.49     |
| 1   | H     | 719 | DT   | C4'-C3' | 10.47 | 1.63        | 1.53     |
| 1   | H     | 718 | DA   | C5'-C4' | 10.46 | 1.62        | 1.51     |
| 1   | E     | 416 | DC   | C5'-C4' | 10.28 | 1.62        | 1.51     |
| 1   | E     | 406 | DT   | C4'-C3' | 10.13 | 1.63        | 1.53     |
| 1   | E     | 418 | DA   | P-O5'   | 10.11 | 1.69        | 1.59     |
| 1   | H     | 717 | DA   | P-O5'   | 10.08 | 1.69        | 1.59     |
| 1   | E     | 401 | DA   | N9-C4   | 10.07 | 1.43        | 1.37     |
| 1   | H     | 701 | DA   | O3'-P   | 10.02 | 1.73        | 1.61     |
| 1   | E     | 401 | DA   | P-O5'   | 9.85  | 1.69        | 1.59     |
| 1   | G     | 600 | DG   | O3'-P   | 9.57  | 1.72        | 1.61     |
| 1   | E     | 404 | DT   | P-O5'   | 9.46  | 1.69        | 1.59     |
| 1   | F     | 500 | DG   | C3'-C2' | 9.40  | 1.63        | 1.52     |
| 1   | H     | 718 | DA   | P-O5'   | 9.28  | 1.69        | 1.59     |
| 1   | H     | 718 | DA   | O3'-P   | 9.10  | 1.72        | 1.61     |
| 1   | F     | 504 | DT   | C4'-C3' | 9.09  | 1.62        | 1.53     |
| 1   | F     | 500 | DG   | O3'-P   | 9.08  | 1.72        | 1.61     |
| 1   | H     | 716 | DC   | C5'-C4' | 9.04  | 1.61        | 1.51     |
| 1   | F     | 500 | DG   | C1'-N9  | 8.85  | 1.60        | 1.49     |
| 1   | F     | 518 | DA   | O3'-P   | 8.80  | 1.71        | 1.61     |
| 1   | E     | 401 | DA   | C4'-C3' | 8.78  | 1.62        | 1.53     |
| 1   | E     | 406 | DT   | O3'-P   | 8.74  | 1.71        | 1.61     |
| 1   | E     | 420 | DT   | C1'-N1  | 8.73  | 1.60        | 1.49     |
| 1   | H     | 701 | DA   | C2'-C1' | 8.71  | 1.61        | 1.52     |
| 1   | G     | 605 | DG   | C2'-C1' | 8.63  | 1.60        | 1.52     |
| 1   | H     | 717 | DA   | C2'-C1' | 8.39  | 1.60        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | H     | 702 | DA   | C2'-C1' | 8.30  | 1.60        | 1.52     |
| 1   | H     | 719 | DT   | O3'-P   | 8.25  | 1.71        | 1.61     |
| 1   | H     | 701 | DA   | C6-N1   | -8.12 | 1.29        | 1.35     |
| 1   | G     | 608 | DA   | O3'-P   | 8.08  | 1.70        | 1.61     |
| 1   | G     | 601 | DA   | C1'-N9  | 8.05  | 1.59        | 1.49     |
| 1   | E     | 403 | DT   | O3'-P   | 8.01  | 1.70        | 1.61     |
| 1   | E     | 419 | DT   | C5'-C4' | 7.93  | 1.60        | 1.51     |
| 1   | F     | 515 | DA   | C5'-C4' | 7.91  | 1.60        | 1.51     |
| 1   | F     | 515 | DA   | P-O5'   | 7.90  | 1.67        | 1.59     |
| 1   | F     | 504 | DT   | P-O5'   | 7.86  | 1.67        | 1.59     |
| 1   | H     | 701 | DA   | C3'-C2' | 7.85  | 1.61        | 1.52     |
| 1   | F     | 502 | DA   | P-O5'   | 7.85  | 1.67        | 1.59     |
| 1   | H     | 703 | DT   | C5-C7   | 7.83  | 1.54        | 1.50     |
| 1   | H     | 719 | DT   | C2'-C1' | 7.81  | 1.60        | 1.52     |
| 1   | E     | 401 | DA   | C3'-O3' | 7.81  | 1.54        | 1.44     |
| 1   | G     | 619 | DT   | C5-C7   | 7.63  | 1.54        | 1.50     |
| 1   | E     | 418 | DA   | C6-N1   | -7.60 | 1.30        | 1.35     |
| 1   | F     | 503 | DT   | C2'-C1' | 7.59  | 1.59        | 1.52     |
| 1   | F     | 509 | DG   | C2-N3   | -7.57 | 1.26        | 1.32     |
| 1   | E     | 419 | DT   | C5-C7   | -7.51 | 1.45        | 1.50     |
| 1   | E     | 420 | DT   | N1-C2   | 7.48  | 1.44        | 1.38     |
| 1   | G     | 620 | DT   | O5'-C5' | 7.27  | 1.60        | 1.42     |
| 1   | F     | 500 | DG   | C3'-O3' | 7.26  | 1.53        | 1.44     |
| 1   | F     | 518 | DA   | N9-C4   | 7.25  | 1.42        | 1.37     |
| 1   | E     | 402 | DA   | C2'-C1' | -7.24 | 1.45        | 1.52     |
| 1   | E     | 416 | DC   | O3'-P   | 7.21  | 1.69        | 1.61     |
| 1   | F     | 518 | DA   | C3'-O3' | 7.14  | 1.53        | 1.44     |
| 1   | H     | 720 | DT   | C5'-C4' | 7.12  | 1.59        | 1.51     |
| 1   | E     | 419 | DT   | N1-C2   | 7.12  | 1.43        | 1.38     |
| 1   | E     | 407 | DG   | C2'-C1' | 7.11  | 1.59        | 1.52     |
| 1   | G     | 602 | DA   | N9-C8   | -7.08 | 1.32        | 1.37     |
| 1   | H     | 704 | DT   | O3'-P   | 7.07  | 1.69        | 1.61     |
| 1   | H     | 718 | DA   | C3'-O3' | 7.06  | 1.53        | 1.44     |
| 1   | E     | 408 | DA   | P-O5'   | 7.06  | 1.66        | 1.59     |
| 1   | E     | 419 | DT   | P-O5'   | 7.04  | 1.66        | 1.59     |
| 1   | F     | 503 | DT   | P-O5'   | 7.02  | 1.66        | 1.59     |
| 1   | G     | 606 | DT   | P-O5'   | 6.98  | 1.66        | 1.59     |
| 1   | E     | 407 | DG   | O3'-P   | 6.97  | 1.69        | 1.61     |
| 1   | E     | 402 | DA   | N9-C8   | -6.95 | 1.32        | 1.37     |
| 1   | E     | 402 | DA   | C4'-C3' | -6.95 | 1.45        | 1.52     |
| 1   | E     | 404 | DT   | O3'-P   | 6.94  | 1.69        | 1.61     |
| 1   | H     | 717 | DA   | O3'-P   | 6.92  | 1.69        | 1.61     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 405 | DG   | O3'-P   | 6.91  | 1.69        | 1.61     |
| 1   | E     | 415 | DA   | C2'-C1' | 6.90  | 1.59        | 1.52     |
| 1   | G     | 602 | DA   | C3'-O3' | 6.89  | 1.52        | 1.44     |
| 1   | F     | 500 | DG   | C2'-C1' | 6.88  | 1.59        | 1.52     |
| 1   | G     | 617 | DA   | O3'-P   | 6.86  | 1.69        | 1.61     |
| 1   | F     | 510 | DC   | P-O5'   | 6.85  | 1.66        | 1.59     |
| 1   | F     | 510 | DC   | C2'-C1' | 6.84  | 1.59        | 1.52     |
| 1   | E     | 401 | DA   | C2'-C1' | 6.83  | 1.59        | 1.52     |
| 1   | E     | 407 | DG   | P-O5'   | 6.81  | 1.66        | 1.59     |
| 1   | E     | 418 | DA   | C3'-O3' | 6.79  | 1.52        | 1.44     |
| 1   | G     | 615 | DA   | P-O5'   | 6.75  | 1.66        | 1.59     |
| 1   | H     | 701 | DA   | O4'-C1' | 6.73  | 1.50        | 1.42     |
| 1   | H     | 700 | DG   | C5'-C4' | 6.73  | 1.58        | 1.51     |
| 1   | F     | 520 | DT   | C2'-C1' | 6.73  | 1.59        | 1.52     |
| 1   | F     | 504 | DT   | O3'-P   | 6.72  | 1.69        | 1.61     |
| 1   | F     | 505 | DG   | P-O5'   | 6.68  | 1.66        | 1.59     |
| 1   | G     | 613 | DT   | C5-C7   | 6.63  | 1.54        | 1.50     |
| 1   | G     | 605 | DG   | O3'-P   | 6.60  | 1.69        | 1.61     |
| 1   | G     | 620 | DT   | N3-C4   | -6.58 | 1.33        | 1.38     |
| 1   | E     | 403 | DT   | C4'-C3' | 6.58  | 1.59        | 1.53     |
| 1   | H     | 701 | DA   | C4'-O4' | 6.57  | 1.51        | 1.45     |
| 1   | H     | 710 | DC   | C2'-C1' | 6.56  | 1.58        | 1.52     |
| 1   | H     | 713 | DT   | C5-C7   | 6.56  | 1.53        | 1.50     |
| 1   | E     | 406 | DT   | C3'-O3' | 6.53  | 1.52        | 1.44     |
| 1   | E     | 420 | DT   | O4'-C1' | 6.53  | 1.50        | 1.42     |
| 1   | F     | 505 | DG   | C5'-C4' | 6.53  | 1.58        | 1.51     |
| 1   | G     | 602 | DA   | C5-C6   | -6.52 | 1.35        | 1.41     |
| 1   | E     | 405 | DG   | P-O5'   | 6.50  | 1.66        | 1.59     |
| 1   | F     | 509 | DG   | P-O5'   | 6.48  | 1.66        | 1.59     |
| 1   | G     | 600 | DG   | C3'-O3' | 6.45  | 1.52        | 1.44     |
| 1   | G     | 617 | DA   | P-O5'   | 6.30  | 1.66        | 1.59     |
| 1   | F     | 503 | DT   | C1'-N1  | 6.28  | 1.57        | 1.49     |
| 1   | G     | 619 | DT   | O3'-P   | 6.27  | 1.68        | 1.61     |
| 1   | E     | 403 | DT   | C5'-C4' | 6.25  | 1.58        | 1.51     |
| 1   | H     | 702 | DA   | C4'-C3' | -6.23 | 1.46        | 1.52     |
| 1   | E     | 418 | DA   | C4'-C3' | 6.18  | 1.59        | 1.53     |
| 1   | H     | 702 | DA   | P-O5'   | 6.17  | 1.66        | 1.59     |
| 1   | H     | 706 | DT   | P-O5'   | 6.14  | 1.65        | 1.59     |
| 1   | E     | 419 | DT   | N3-C4   | -6.13 | 1.33        | 1.38     |
| 1   | H     | 716 | DC   | P-O5'   | 6.12  | 1.65        | 1.59     |
| 1   | G     | 603 | DT   | P-O5'   | 6.12  | 1.65        | 1.59     |
| 1   | G     | 602 | DA   | C3'-C2' | -6.12 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 407 | DG   | N9-C4   | 6.11  | 1.42        | 1.38     |
| 1   | G     | 619 | DT   | C5'-C4' | -6.11 | 1.44        | 1.51     |
| 1   | H     | 720 | DT   | N1-C6   | -6.08 | 1.33        | 1.38     |
| 1   | G     | 616 | DC   | P-O5'   | 6.06  | 1.65        | 1.59     |
| 1   | E     | 417 | DA   | C6-N1   | -6.04 | 1.31        | 1.35     |
| 1   | F     | 509 | DG   | O3'-P   | 5.98  | 1.68        | 1.61     |
| 1   | H     | 720 | DT   | N1-C2   | 5.98  | 1.42        | 1.38     |
| 1   | E     | 420 | DT   | C5'-C4' | 5.97  | 1.57        | 1.51     |
| 1   | G     | 613 | DT   | O3'-P   | 5.95  | 1.68        | 1.61     |
| 1   | H     | 717 | DA   | C6-N1   | -5.95 | 1.31        | 1.35     |
| 1   | E     | 401 | DA   | N9-C8   | -5.94 | 1.32        | 1.37     |
| 1   | E     | 410 | DC   | C2'-C1' | 5.94  | 1.58        | 1.52     |
| 1   | G     | 610 | DC   | P-O5'   | 5.91  | 1.65        | 1.59     |
| 1   | E     | 404 | DT   | C3'-O3' | 5.90  | 1.51        | 1.44     |
| 1   | G     | 600 | DG   | C5'-C4' | 5.86  | 1.57        | 1.51     |
| 1   | H     | 701 | DA   | C5'-C4' | 5.85  | 1.57        | 1.51     |
| 1   | G     | 602 | DA   | C8-N7   | -5.82 | 1.27        | 1.31     |
| 1   | E     | 413 | DT   | C5'-C4' | 5.80  | 1.57        | 1.51     |
| 1   | G     | 618 | DA   | P-O5'   | 5.79  | 1.65        | 1.59     |
| 1   | H     | 702 | DA   | C6-N1   | -5.78 | 1.31        | 1.35     |
| 1   | F     | 519 | DT   | C5-C7   | 5.73  | 1.53        | 1.50     |
| 1   | E     | 404 | DT   | C5'-C4' | 5.72  | 1.57        | 1.51     |
| 1   | F     | 515 | DA   | C2'-C1' | 5.71  | 1.58        | 1.52     |
| 1   | F     | 502 | DA   | C5-C6   | -5.70 | 1.35        | 1.41     |
| 1   | G     | 606 | DT   | C2'-C1' | 5.70  | 1.58        | 1.52     |
| 1   | E     | 405 | DG   | C5-C4   | -5.67 | 1.34        | 1.38     |
| 1   | F     | 502 | DA   | O3'-P   | 5.65  | 1.68        | 1.61     |
| 1   | H     | 718 | DA   | N9-C4   | 5.64  | 1.41        | 1.37     |
| 1   | E     | 410 | DC   | P-O5'   | 5.62  | 1.65        | 1.59     |
| 1   | E     | 420 | DT   | C4'-O4' | 5.61  | 1.50        | 1.45     |
| 1   | E     | 410 | DC   | O3'-P   | 5.61  | 1.67        | 1.61     |
| 1   | G     | 615 | DA   | C5'-C4' | 5.60  | 1.57        | 1.51     |
| 1   | H     | 701 | DA   | C3'-O3' | 5.57  | 1.51        | 1.44     |
| 1   | F     | 505 | DG   | N9-C4   | -5.57 | 1.33        | 1.38     |
| 1   | F     | 520 | DT   | C5-C7   | -5.57 | 1.46        | 1.50     |
| 1   | F     | 518 | DA   | C2'-C1' | 5.56  | 1.57        | 1.52     |
| 1   | F     | 517 | DA   | C5'-C4' | 5.55  | 1.57        | 1.51     |
| 1   | F     | 519 | DT   | N1-C2   | 5.53  | 1.42        | 1.38     |
| 1   | G     | 620 | DT   | C3'-C2' | 5.53  | 1.58        | 1.52     |
| 1   | E     | 402 | DA   | O3'-P   | 5.47  | 1.67        | 1.61     |
| 1   | G     | 618 | DA   | O3'-P   | 5.46  | 1.67        | 1.61     |
| 1   | G     | 600 | DG   | C4'-C3' | 5.43  | 1.58        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 508 | DA   | C6-N1   | -5.41 | 1.31        | 1.35     |
| 1   | F     | 513 | DT   | C5-C7   | 5.40  | 1.53        | 1.50     |
| 1   | E     | 407 | DG   | C1'-N9  | 5.40  | 1.56        | 1.49     |
| 1   | F     | 508 | DA   | C5'-C4' | 5.38  | 1.57        | 1.51     |
| 1   | E     | 415 | DA   | C1'-N9  | 5.38  | 1.56        | 1.49     |
| 1   | F     | 507 | DG   | P-O5'   | 5.37  | 1.65        | 1.59     |
| 1   | H     | 720 | DT   | C4'-C3' | 5.37  | 1.58        | 1.53     |
| 1   | F     | 515 | DA   | O3'-P   | 5.35  | 1.67        | 1.61     |
| 1   | E     | 413 | DT   | O3'-P   | 5.35  | 1.67        | 1.61     |
| 1   | H     | 713 | DT   | C5'-C4' | 5.34  | 1.57        | 1.51     |
| 1   | G     | 620 | DT   | C5-C7   | -5.34 | 1.46        | 1.50     |
| 1   | F     | 509 | DG   | N3-C4   | -5.34 | 1.31        | 1.35     |
| 1   | G     | 614 | DC   | P-O5'   | 5.32  | 1.65        | 1.59     |
| 1   | E     | 419 | DT   | O3'-P   | 5.31  | 1.67        | 1.61     |
| 1   | F     | 509 | DG   | C5'-C4' | 5.26  | 1.57        | 1.51     |
| 1   | F     | 519 | DT   | P-O5'   | 5.26  | 1.65        | 1.59     |
| 1   | F     | 509 | DG   | N9-C4   | -5.24 | 1.33        | 1.38     |
| 1   | E     | 405 | DG   | C6-O6   | -5.19 | 1.19        | 1.24     |
| 1   | H     | 705 | DG   | C4'-O4' | -5.18 | 1.39        | 1.45     |
| 1   | E     | 416 | DC   | C2-N3   | 5.18  | 1.39        | 1.35     |
| 1   | E     | 409 | DG   | O3'-P   | 5.14  | 1.67        | 1.61     |
| 1   | F     | 506 | DT   | C5'-C4' | 5.11  | 1.56        | 1.51     |
| 1   | H     | 717 | DA   | C3'-C2' | 5.11  | 1.58        | 1.52     |
| 1   | E     | 417 | DA   | P-O5'   | 5.10  | 1.64        | 1.59     |
| 1   | G     | 608 | DA   | C5'-C4' | 5.10  | 1.56        | 1.51     |
| 1   | E     | 415 | DA   | N9-C4   | 5.09  | 1.41        | 1.37     |
| 1   | G     | 618 | DA   | C5'-C4' | 5.09  | 1.56        | 1.51     |
| 1   | H     | 719 | DT   | C3'-O3' | 5.08  | 1.50        | 1.44     |
| 1   | E     | 418 | DA   | O3'-P   | 5.07  | 1.67        | 1.61     |
| 1   | E     | 414 | DC   | P-O5'   | 5.05  | 1.64        | 1.59     |
| 1   | F     | 517 | DA   | C4'-C3' | 5.04  | 1.58        | 1.53     |
| 1   | E     | 403 | DT   | C3'-O3' | 5.03  | 1.50        | 1.44     |
| 1   | F     | 520 | DT   | N3-C4   | -5.01 | 1.34        | 1.38     |

All (810) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | E     | 420 | DT   | O4'-C1'-N1  | 41.82  | 137.27      | 108.00   |
| 1   | F     | 520 | DT   | O4'-C1'-N1  | 32.28  | 130.60      | 108.00   |
| 1   | H     | 702 | DA   | O4'-C4'-C3' | -30.45 | 87.73       | 106.00   |
| 1   | G     | 600 | DG   | O4'-C1'-N9  | 29.83  | 128.88      | 108.00   |
| 1   | E     | 401 | DA   | P-O3'-C3'   | 28.34  | 153.71      | 119.70   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | G     | 620 | DT   | O4'-C4'-C3' | -27.34 | 89.60       | 106.00   |
| 1   | E     | 405 | DG   | O4'-C1'-N9  | 25.42  | 125.80      | 108.00   |
| 1   | F     | 515 | DA   | O4'-C1'-N9  | 24.80  | 125.36      | 108.00   |
| 1   | E     | 402 | DA   | P-O3'-C3'   | 24.69  | 149.33      | 119.70   |
| 1   | E     | 403 | DT   | O4'-C1'-N1  | 24.48  | 125.14      | 108.00   |
| 1   | G     | 601 | DA   | C4'-C3'-C2' | -22.86 | 82.53       | 103.10   |
| 1   | E     | 416 | DC   | O4'-C1'-C2' | -22.63 | 87.80       | 105.90   |
| 1   | G     | 600 | DG   | P-O3'-C3'   | 22.50  | 146.69      | 119.70   |
| 1   | E     | 420 | DT   | O4'-C1'-C2' | -22.41 | 87.97       | 105.90   |
| 1   | G     | 601 | DA   | C8-N9-C4    | -21.71 | 97.12       | 105.80   |
| 1   | H     | 717 | DA   | C4'-C3'-C2' | -20.80 | 84.38       | 103.10   |
| 1   | G     | 620 | DT   | C1'-O4'-C4' | -20.66 | 89.44       | 110.10   |
| 1   | H     | 704 | DT   | O4'-C1'-N1  | 20.62  | 122.44      | 108.00   |
| 1   | E     | 404 | DT   | O4'-C1'-N1  | 20.61  | 122.43      | 108.00   |
| 1   | H     | 709 | DG   | O4'-C1'-N9  | 19.81  | 121.87      | 108.00   |
| 1   | H     | 707 | DG   | O4'-C4'-C3' | -19.70 | 94.18       | 106.00   |
| 1   | H     | 717 | DA   | C1'-O4'-C4' | -19.66 | 90.44       | 110.10   |
| 1   | G     | 616 | DC   | O4'-C1'-N1  | 19.53  | 121.67      | 108.00   |
| 1   | G     | 605 | DG   | C4'-C3'-C2' | -19.48 | 85.57       | 103.10   |
| 1   | F     | 500 | DG   | C8-N9-C4    | -19.22 | 98.71       | 106.40   |
| 1   | E     | 416 | DC   | O4'-C1'-N1  | 19.16  | 121.41      | 108.00   |
| 1   | G     | 604 | DT   | O4'-C1'-N1  | 19.11  | 121.38      | 108.00   |
| 1   | G     | 620 | DT   | O4'-C1'-N1  | 19.02  | 121.31      | 108.00   |
| 1   | H     | 701 | DA   | O4'-C1'-N9  | 18.77  | 121.14      | 108.00   |
| 1   | F     | 506 | DT   | P-O3'-C3'   | 18.48  | 141.87      | 119.70   |
| 1   | H     | 701 | DA   | C8-N9-C4    | -18.28 | 98.49       | 105.80   |
| 1   | E     | 415 | DA   | P-O3'-C3'   | 18.27  | 141.63      | 119.70   |
| 1   | F     | 518 | DA   | P-O3'-C3'   | 18.19  | 141.53      | 119.70   |
| 1   | E     | 409 | DG   | O4'-C1'-N9  | 18.00  | 120.60      | 108.00   |
| 1   | H     | 719 | DT   | C1'-O4'-C4' | -17.89 | 92.21       | 110.10   |
| 1   | F     | 509 | DG   | O4'-C1'-N9  | 17.71  | 120.40      | 108.00   |
| 1   | H     | 715 | DA   | O4'-C1'-N9  | 17.68  | 120.38      | 108.00   |
| 1   | G     | 601 | DA   | N9-C1'-C2'  | 17.67  | 146.17      | 112.60   |
| 1   | G     | 602 | DA   | C5-N7-C8    | -17.41 | 95.19       | 103.90   |
| 1   | H     | 712 | DC   | O4'-C1'-N1  | 17.33  | 120.13      | 108.00   |
| 1   | G     | 606 | DT   | O4'-C1'-N1  | 16.85  | 119.79      | 108.00   |
| 1   | H     | 718 | DA   | C4'-C3'-O3' | 16.80  | 151.69      | 109.70   |
| 1   | G     | 606 | DT   | P-O3'-C3'   | 16.79  | 139.84      | 119.70   |
| 1   | E     | 402 | DA   | N7-C8-N9    | 16.68  | 122.14      | 113.80   |
| 1   | F     | 519 | DT   | O4'-C1'-N1  | 16.66  | 119.67      | 108.00   |
| 1   | H     | 716 | DC   | P-O3'-C3'   | 16.53  | 139.54      | 119.70   |
| 1   | F     | 502 | DA   | C4'-C3'-C2' | -16.48 | 88.27       | 103.10   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | H     | 703 | DT   | O4'-C1'-N1  | 16.47  | 119.53      | 108.00   |
| 1   | H     | 710 | DC   | O4'-C1'-N1  | 16.34  | 119.44      | 108.00   |
| 1   | F     | 500 | DG   | O4'-C1'-N9  | 16.22  | 119.36      | 108.00   |
| 1   | F     | 515 | DA   | P-O3'-C3'   | 16.18  | 139.11      | 119.70   |
| 1   | G     | 601 | DA   | O4'-C1'-C2' | -16.13 | 93.00       | 105.90   |
| 1   | H     | 700 | DG   | P-O3'-C3'   | 16.06  | 138.98      | 119.70   |
| 1   | G     | 601 | DA   | P-O3'-C3'   | 15.99  | 138.89      | 119.70   |
| 1   | H     | 719 | DT   | C4'-C3'-C2' | -15.98 | 88.72       | 103.10   |
| 1   | H     | 702 | DA   | N9-C1'-C2'  | 15.98  | 142.96      | 112.60   |
| 1   | H     | 718 | DA   | C5'-C4'-C3' | 15.90  | 142.72      | 114.10   |
| 1   | H     | 705 | DG   | O4'-C4'-C3' | -15.84 | 96.50       | 106.00   |
| 1   | E     | 403 | DT   | O4'-C1'-C2' | -15.83 | 93.23       | 105.90   |
| 1   | H     | 701 | DA   | O4'-C4'-C3' | -15.79 | 96.53       | 106.00   |
| 1   | F     | 512 | DC   | O4'-C4'-C3' | -15.53 | 96.68       | 106.00   |
| 1   | G     | 617 | DA   | O4'-C1'-N9  | 15.48  | 118.83      | 108.00   |
| 1   | F     | 512 | DC   | O4'-C1'-N1  | 15.46  | 118.82      | 108.00   |
| 1   | G     | 608 | DA   | O4'-C4'-C3' | 15.45  | 115.27      | 106.00   |
| 1   | H     | 718 | DA   | C4'-C3'-C2' | -15.21 | 89.42       | 103.10   |
| 1   | G     | 612 | DC   | O4'-C1'-N1  | 15.20  | 118.64      | 108.00   |
| 1   | F     | 509 | DG   | N3-C2-N2    | -15.19 | 109.27      | 119.90   |
| 1   | H     | 719 | DT   | C5'-C4'-C3' | 15.19  | 141.44      | 114.10   |
| 1   | H     | 702 | DA   | O4'-C1'-C2' | -14.99 | 93.91       | 105.90   |
| 1   | H     | 701 | DA   | O4'-C1'-C2' | -14.94 | 93.95       | 105.90   |
| 1   | E     | 419 | DT   | P-O3'-C3'   | 14.85  | 137.51      | 119.70   |
| 1   | G     | 611 | DG   | O4'-C1'-N9  | 14.81  | 118.36      | 108.00   |
| 1   | F     | 500 | DG   | C2-N3-C4    | -14.68 | 104.56      | 111.90   |
| 1   | F     | 510 | DC   | O4'-C1'-N1  | 14.56  | 118.19      | 108.00   |
| 1   | E     | 417 | DA   | C4'-C3'-C2' | -14.55 | 90.00       | 103.10   |
| 1   | G     | 616 | DC   | O4'-C1'-C2' | -14.36 | 94.41       | 105.90   |
| 1   | H     | 719 | DT   | O4'-C4'-C3' | -14.34 | 97.39       | 106.00   |
| 1   | G     | 602 | DA   | P-O5'-C5'   | 14.29  | 143.77      | 120.90   |
| 1   | E     | 411 | DG   | O4'-C1'-N9  | 14.23  | 117.96      | 108.00   |
| 1   | E     | 402 | DA   | O4'-C1'-C2' | -14.19 | 94.55       | 105.90   |
| 1   | F     | 508 | DA   | P-O3'-C3'   | 14.17  | 136.71      | 119.70   |
| 1   | F     | 519 | DT   | O4'-C4'-C3' | -14.15 | 97.51       | 106.00   |
| 1   | E     | 402 | DA   | C8-N9-C4    | -14.14 | 100.14      | 105.80   |
| 1   | H     | 702 | DA   | C8-N9-C4    | -14.13 | 100.15      | 105.80   |
| 1   | G     | 618 | DA   | O4'-C1'-N9  | 14.00  | 117.80      | 108.00   |
| 1   | E     | 418 | DA   | O4'-C1'-N9  | 13.96  | 117.77      | 108.00   |
| 1   | E     | 406 | DT   | C4'-C3'-C2' | -13.92 | 90.57       | 103.10   |
| 1   | H     | 709 | DG   | N3-C2-N2    | -13.90 | 110.17      | 119.90   |
| 1   | F     | 514 | DC   | C4'-C3'-C2' | -13.81 | 90.67       | 103.10   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | E     | 420 | DT   | C6-N1-C2    | -13.77 | 114.41      | 121.30   |
| 1   | H     | 708 | DA   | P-O5'-C5'   | 13.64  | 142.72      | 120.90   |
| 1   | F     | 517 | DA   | O4'-C1'-N9  | 13.63  | 117.54      | 108.00   |
| 1   | H     | 702 | DA   | N1-C2-N3    | 13.60  | 136.10      | 129.30   |
| 1   | F     | 514 | DC   | O4'-C1'-N1  | 13.50  | 117.45      | 108.00   |
| 1   | F     | 501 | DA   | C4'-C3'-C2' | -13.43 | 91.01       | 103.10   |
| 1   | H     | 717 | DA   | C2-N3-C4    | -13.43 | 103.89      | 110.60   |
| 1   | G     | 608 | DA   | O4'-C1'-N9  | 13.33  | 117.33      | 108.00   |
| 1   | E     | 407 | DG   | O4'-C4'-C3' | -13.29 | 98.03       | 106.00   |
| 1   | G     | 620 | DT   | C4-C5-C7    | -13.24 | 111.06      | 119.00   |
| 1   | E     | 402 | DA   | O4'-C1'-N9  | 13.20  | 117.24      | 108.00   |
| 1   | G     | 610 | DC   | O4'-C1'-N1  | 13.20  | 117.24      | 108.00   |
| 1   | G     | 601 | DA   | N7-C8-N9    | 13.19  | 120.39      | 113.80   |
| 1   | F     | 506 | DT   | O4'-C1'-C2' | -13.17 | 95.36       | 105.90   |
| 1   | F     | 507 | DG   | O4'-C1'-C2' | -13.15 | 95.38       | 105.90   |
| 1   | F     | 507 | DG   | O4'-C1'-N9  | 13.05  | 117.14      | 108.00   |
| 1   | H     | 701 | DA   | P-O3'-C3'   | 13.00  | 135.30      | 119.70   |
| 1   | H     | 718 | DA   | O4'-C4'-C3' | -12.99 | 98.21       | 106.00   |
| 1   | G     | 618 | DA   | P-O3'-C3'   | 12.88  | 135.15      | 119.70   |
| 1   | H     | 700 | DG   | O4'-C1'-N9  | 12.81  | 116.97      | 108.00   |
| 1   | E     | 407 | DG   | C8-N9-C4    | -12.79 | 101.28      | 106.40   |
| 1   | G     | 618 | DA   | C8-N9-C4    | -12.77 | 100.69      | 105.80   |
| 1   | E     | 401 | DA   | C8-N9-C4    | -12.68 | 100.73      | 105.80   |
| 1   | E     | 415 | DA   | O4'-C1'-N9  | 12.67  | 116.87      | 108.00   |
| 1   | H     | 703 | DT   | O4'-C1'-C2' | -12.65 | 95.78       | 105.90   |
| 1   | F     | 501 | DA   | O4'-C1'-C2' | -12.60 | 95.82       | 105.90   |
| 1   | E     | 403 | DT   | C4'-C3'-C2' | -12.57 | 91.79       | 103.10   |
| 1   | F     | 500 | DG   | P-O3'-C3'   | 12.44  | 134.62      | 119.70   |
| 1   | G     | 608 | DA   | C4'-C3'-C2' | -12.42 | 91.92       | 103.10   |
| 1   | F     | 501 | DA   | O4'-C1'-N9  | 12.39  | 116.67      | 108.00   |
| 1   | F     | 520 | DT   | C4-C5-C6    | 12.38  | 125.43      | 118.00   |
| 1   | H     | 715 | DA   | P-O5'-C5'   | 12.37  | 140.69      | 120.90   |
| 1   | G     | 620 | DT   | C5'-C4'-C3' | 12.32  | 136.28      | 114.10   |
| 1   | H     | 700 | DG   | O4'-C4'-C3' | -12.25 | 98.65       | 106.00   |
| 1   | E     | 401 | DA   | C5'-C4'-C3' | 12.24  | 136.14      | 114.10   |
| 1   | H     | 717 | DA   | O4'-C1'-N9  | 12.20  | 116.54      | 108.00   |
| 1   | H     | 720 | DT   | O4'-C1'-N1  | 12.11  | 116.47      | 108.00   |
| 1   | E     | 404 | DT   | C4'-C3'-C2' | -12.10 | 92.21       | 103.10   |
| 1   | F     | 519 | DT   | P-O3'-C3'   | -12.10 | 105.19      | 119.70   |
| 1   | H     | 702 | DA   | C4'-C3'-C2' | -12.08 | 92.23       | 103.10   |
| 1   | F     | 510 | DC   | P-O3'-C3'   | 12.08  | 134.19      | 119.70   |
| 1   | E     | 417 | DA   | P-O5'-C5'   | 12.07  | 140.22      | 120.90   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | G     | 620 | DT   | C4-C5-C6    | 12.07  | 125.24      | 118.00   |
| 1   | G     | 614 | DC   | O4'-C1'-N1  | 12.06  | 116.44      | 108.00   |
| 1   | E     | 417 | DA   | O4'-C4'-C3' | 12.05  | 113.23      | 106.00   |
| 1   | E     | 416 | DC   | N3-C4-N4    | 12.01  | 126.41      | 118.00   |
| 1   | E     | 409 | DG   | C4-N9-C1'   | -11.94 | 110.98      | 126.50   |
| 1   | E     | 401 | DA   | O4'-C1'-N9  | 11.93  | 116.35      | 108.00   |
| 1   | F     | 504 | DT   | P-O3'-C3'   | 11.88  | 133.96      | 119.70   |
| 1   | E     | 407 | DG   | P-O5'-C5'   | 11.84  | 139.84      | 120.90   |
| 1   | E     | 415 | DA   | O4'-C1'-C2' | -11.83 | 96.44       | 105.90   |
| 1   | G     | 602 | DA   | C4'-C3'-C2' | -11.80 | 92.48       | 103.10   |
| 1   | E     | 408 | DA   | C8-N9-C4    | -11.79 | 101.09      | 105.80   |
| 1   | G     | 602 | DA   | C8-N9-C4    | -11.77 | 101.09      | 105.80   |
| 1   | F     | 500 | DG   | O4'-C1'-C2' | -11.74 | 96.50       | 105.90   |
| 1   | G     | 609 | DG   | P-O5'-C5'   | 11.73  | 139.67      | 120.90   |
| 1   | H     | 714 | DC   | O4'-C1'-N1  | 11.69  | 116.18      | 108.00   |
| 1   | H     | 718 | DA   | P-O5'-C5'   | 11.64  | 139.52      | 120.90   |
| 1   | F     | 500 | DG   | N9-C1'-C2'  | 11.60  | 134.64      | 112.60   |
| 1   | F     | 500 | DG   | N7-C8-N9    | 11.54  | 118.87      | 113.10   |
| 1   | H     | 710 | DC   | P-O3'-C3'   | 11.50  | 133.50      | 119.70   |
| 1   | F     | 507 | DG   | P-O3'-C3'   | 11.40  | 133.38      | 119.70   |
| 1   | G     | 607 | DG   | O4'-C1'-N9  | 11.40  | 115.98      | 108.00   |
| 1   | E     | 417 | DA   | C2-N3-C4    | -11.37 | 104.91      | 110.60   |
| 1   | E     | 415 | DA   | C8-N9-C4    | -11.31 | 101.28      | 105.80   |
| 1   | E     | 412 | DC   | C4'-C3'-C2' | -11.30 | 92.93       | 103.10   |
| 1   | H     | 701 | DA   | N1-C2-N3    | 11.24  | 134.92      | 129.30   |
| 1   | H     | 709 | DG   | C8-N9-C4    | -11.23 | 101.91      | 106.40   |
| 1   | E     | 419 | DT   | C4-C5-C6    | 11.14  | 124.69      | 118.00   |
| 1   | E     | 403 | DT   | N3-C2-O2    | -11.10 | 115.64      | 122.30   |
| 1   | G     | 600 | DG   | N3-C4-C5    | -10.99 | 123.11      | 128.60   |
| 1   | F     | 509 | DG   | N9-C4-C5    | 10.99  | 109.80      | 105.40   |
| 1   | F     | 514 | DC   | P-O5'-C5'   | 10.98  | 138.46      | 120.90   |
| 1   | F     | 502 | DA   | O4'-C4'-C3' | -10.96 | 99.42       | 106.00   |
| 1   | H     | 718 | DA   | O3'-P-O5'   | 10.89  | 124.70      | 104.00   |
| 1   | H     | 719 | DT   | C4'-C3'-O3' | 10.89  | 136.93      | 109.70   |
| 1   | H     | 720 | DT   | C4-C5-C6    | 10.88  | 124.53      | 118.00   |
| 1   | E     | 419 | DT   | N3-C2-O2    | -10.78 | 115.83      | 122.30   |
| 1   | E     | 406 | DT   | O4'-C1'-N1  | 10.76  | 115.53      | 108.00   |
| 1   | E     | 417 | DA   | N1-C2-N3    | 10.75  | 134.68      | 129.30   |
| 1   | G     | 608 | DA   | P-O5'-C5'   | 10.73  | 138.07      | 120.90   |
| 1   | H     | 717 | DA   | N1-C2-N3    | 10.65  | 134.63      | 129.30   |
| 1   | H     | 715 | DA   | O4'-C4'-C3' | 10.63  | 112.38      | 106.00   |
| 1   | F     | 509 | DG   | N1-C2-N2    | 10.63  | 125.76      | 116.20   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | E     | 413 | DT   | O4'-C1'-C2' | -10.59 | 97.43       | 105.90   |
| 1   | E     | 407 | DG   | N9-C1'-C2'  | 10.57  | 132.69      | 112.60   |
| 1   | G     | 615 | DA   | O4'-C1'-N9  | 10.54  | 115.38      | 108.00   |
| 1   | E     | 409 | DG   | N3-C2-N2    | -10.54 | 112.52      | 119.90   |
| 1   | F     | 520 | DT   | C5'-C4'-C3' | 10.53  | 133.06      | 114.10   |
| 1   | F     | 520 | DT   | C4-C5-C7    | -10.48 | 112.71      | 119.00   |
| 1   | F     | 509 | DG   | C8-N9-C4    | -10.43 | 102.23      | 106.40   |
| 1   | H     | 719 | DT   | P-O3'-C3'   | 10.41  | 132.19      | 119.70   |
| 1   | F     | 503 | DT   | O4'-C1'-C2' | -10.40 | 97.58       | 105.90   |
| 1   | H     | 701 | DA   | N9-C1'-C2'  | 10.38  | 132.33      | 112.60   |
| 1   | E     | 417 | DA   | O4'-C1'-C2' | -10.38 | 97.60       | 105.90   |
| 1   | F     | 518 | DA   | C4'-C3'-C2' | -10.37 | 93.77       | 103.10   |
| 1   | E     | 418 | DA   | O3'-P-O5'   | 10.36  | 123.69      | 104.00   |
| 1   | H     | 710 | DC   | P-O5'-C5'   | 10.35  | 137.46      | 120.90   |
| 1   | G     | 600 | DG   | C8-N9-C4    | -10.30 | 102.28      | 106.40   |
| 1   | F     | 500 | DG   | C5-C6-N1    | -10.26 | 106.37      | 111.50   |
| 1   | H     | 718 | DA   | C1'-O4'-C4' | -10.26 | 99.84       | 110.10   |
| 1   | G     | 617 | DA   | C4'-C3'-C2' | -10.25 | 93.88       | 103.10   |
| 1   | E     | 417 | DA   | O4'-C1'-N9  | 10.24  | 115.17      | 108.00   |
| 1   | G     | 601 | DA   | N1-C2-N3    | 10.21  | 134.41      | 129.30   |
| 1   | H     | 705 | DG   | O4'-C1'-N9  | -10.20 | 100.86      | 108.00   |
| 1   | E     | 402 | DA   | C5-N7-C8    | -10.19 | 98.80       | 103.90   |
| 1   | G     | 620 | DT   | P-O5'-C5'   | 10.11  | 137.08      | 120.90   |
| 1   | E     | 416 | DC   | C5-C4-N4    | -10.10 | 113.13      | 120.20   |
| 1   | E     | 401 | DA   | C3'-C2'-C1' | 10.08  | 114.60      | 102.50   |
| 1   | F     | 509 | DG   | N3-C4-N9    | -10.08 | 119.95      | 126.00   |
| 1   | H     | 701 | DA   | N7-C8-N9    | 10.02  | 118.81      | 113.80   |
| 1   | E     | 420 | DT   | P-O5'-C5'   | 9.98   | 136.87      | 120.90   |
| 1   | G     | 609 | DG   | P-O3'-C3'   | 9.95   | 131.64      | 119.70   |
| 1   | H     | 709 | DG   | N9-C4-C5    | 9.94   | 109.38      | 105.40   |
| 1   | F     | 512 | DC   | N1-C2-O2    | 9.88   | 124.83      | 118.90   |
| 1   | E     | 408 | DA   | N1-C2-N3    | 9.86   | 134.23      | 129.30   |
| 1   | E     | 409 | DG   | N1-C2-N2    | 9.86   | 125.07      | 116.20   |
| 1   | E     | 409 | DG   | N9-C1'-C2'  | 9.85   | 131.32      | 112.60   |
| 1   | G     | 605 | DG   | C1'-O4'-C4' | -9.85  | 100.25      | 110.10   |
| 1   | E     | 405 | DG   | P-O5'-C5'   | 9.84   | 136.64      | 120.90   |
| 1   | G     | 619 | DT   | O3'-P-O5'   | 9.84   | 122.69      | 104.00   |
| 1   | H     | 702 | DA   | C5-N7-C8    | -9.82  | 98.99       | 103.90   |
| 1   | F     | 518 | DA   | O4'-C1'-N9  | 9.81   | 114.86      | 108.00   |
| 1   | E     | 411 | DG   | P-O5'-C5'   | 9.78   | 136.55      | 120.90   |
| 1   | F     | 506 | DT   | C4-C5-C6    | 9.77   | 123.86      | 118.00   |
| 1   | F     | 514 | DC   | P-O3'-C3'   | 9.74   | 131.39      | 119.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 603 | DT   | N3-C2-O2    | -9.74 | 116.45      | 122.30   |
| 1   | G     | 620 | DT   | N1-C1'-C2'  | 9.73  | 131.09      | 112.60   |
| 1   | G     | 618 | DA   | N7-C8-N9    | 9.72  | 118.66      | 113.80   |
| 1   | G     | 601 | DA   | O3'-P-O5'   | 9.72  | 122.47      | 104.00   |
| 1   | G     | 607 | DG   | C4'-C3'-C2' | -9.70 | 94.37       | 103.10   |
| 1   | G     | 620 | DT   | C5-C6-N1    | -9.64 | 117.92      | 123.70   |
| 1   | G     | 602 | DA   | O4'-C1'-N9  | 9.59  | 114.72      | 108.00   |
| 1   | G     | 602 | DA   | C5-C6-N6    | -9.57 | 116.04      | 123.70   |
| 1   | G     | 606 | DT   | C4-C5-C6    | 9.57  | 123.74      | 118.00   |
| 1   | H     | 712 | DC   | N1-C2-O2    | 9.57  | 124.64      | 118.90   |
| 1   | E     | 420 | DT   | C4-C5-C6    | 9.54  | 123.72      | 118.00   |
| 1   | G     | 619 | DT   | C3'-C2'-C1' | -9.53 | 91.07       | 102.50   |
| 1   | E     | 406 | DT   | P-O3'-C3'   | 9.53  | 131.13      | 119.70   |
| 1   | H     | 712 | DC   | O4'-C4'-C3' | -9.51 | 100.30      | 106.00   |
| 1   | E     | 420 | DT   | C5'-C4'-O4' | 9.49  | 127.33      | 109.30   |
| 1   | E     | 404 | DT   | C4-C5-C7    | -9.48 | 113.31      | 119.00   |
| 1   | E     | 403 | DT   | C6-N1-C2    | -9.48 | 116.56      | 121.30   |
| 1   | F     | 518 | DA   | C8-N9-C4    | -9.48 | 102.01      | 105.80   |
| 1   | F     | 507 | DG   | C8-N9-C4    | -9.47 | 102.61      | 106.40   |
| 1   | G     | 602 | DA   | N1-C6-N6    | 9.43  | 124.26      | 118.60   |
| 1   | E     | 420 | DT   | C3'-C2'-C1' | 9.43  | 113.81      | 102.50   |
| 1   | G     | 607 | DG   | C8-N9-C4    | -9.40 | 102.64      | 106.40   |
| 1   | H     | 717 | DA   | C5-C6-N1    | -9.39 | 113.00      | 117.70   |
| 1   | E     | 416 | DC   | C4'-C3'-C2' | -9.38 | 94.66       | 103.10   |
| 1   | F     | 502 | DA   | P-O5'-C5'   | 9.37  | 135.90      | 120.90   |
| 1   | F     | 501 | DA   | N1-C2-N3    | 9.37  | 133.99      | 129.30   |
| 1   | H     | 717 | DA   | C8-N9-C4    | -9.37 | 102.05      | 105.80   |
| 1   | F     | 501 | DA   | N7-C8-N9    | 9.36  | 118.48      | 113.80   |
| 1   | F     | 503 | DT   | N1-C1'-C2'  | 9.36  | 130.38      | 112.60   |
| 1   | F     | 513 | DT   | O4'-C1'-C2' | -9.36 | 98.41       | 105.90   |
| 1   | F     | 504 | DT   | O4'-C1'-N1  | 9.33  | 114.53      | 108.00   |
| 1   | F     | 519 | DT   | N3-C2-O2    | -9.32 | 116.71      | 122.30   |
| 1   | E     | 408 | DA   | N7-C8-N9    | 9.30  | 118.45      | 113.80   |
| 1   | F     | 503 | DT   | O4'-C4'-C3' | -9.30 | 100.42      | 106.00   |
| 1   | E     | 401 | DA   | C4'-C3'-O3' | 9.29  | 132.92      | 109.70   |
| 1   | G     | 603 | DT   | O4'-C1'-C2' | -9.24 | 98.51       | 105.90   |
| 1   | H     | 707 | DG   | C8-N9-C4    | -9.20 | 102.72      | 106.40   |
| 1   | F     | 516 | DC   | O4'-C4'-C3' | -9.19 | 100.48      | 106.00   |
| 1   | H     | 713 | DT   | O4'-C1'-C2' | -9.15 | 98.58       | 105.90   |
| 1   | E     | 420 | DT   | O5'-C5'-C4' | 9.15  | 133.87      | 111.00   |
| 1   | H     | 720 | DT   | N3-C2-O2    | -9.11 | 116.83      | 122.30   |
| 1   | G     | 617 | DA   | N1-C2-N3    | 9.10  | 133.85      | 129.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | F     | 516 | DC   | P-O5'-C5'   | 9.09  | 135.45      | 120.90   |
| 1   | E     | 410 | DC   | N1-C2-O2    | 9.09  | 124.36      | 118.90   |
| 1   | G     | 606 | DT   | C4-C5-C7    | -9.07 | 113.56      | 119.00   |
| 1   | E     | 417 | DA   | C8-N9-C4    | -9.06 | 102.18      | 105.80   |
| 1   | H     | 709 | DG   | N1-C2-N2    | 9.04  | 124.34      | 116.20   |
| 1   | E     | 401 | DA   | N7-C8-N9    | 9.03  | 118.31      | 113.80   |
| 1   | H     | 717 | DA   | N9-C1'-C2'  | 9.01  | 129.73      | 112.60   |
| 1   | H     | 719 | DT   | O4'-C1'-N1  | 8.99  | 114.30      | 108.00   |
| 1   | F     | 517 | DA   | N1-C2-N3    | 8.99  | 133.79      | 129.30   |
| 1   | E     | 420 | DT   | N3-C2-O2    | -8.97 | 116.92      | 122.30   |
| 1   | H     | 707 | DG   | N9-C1'-C2'  | 8.97  | 129.64      | 112.60   |
| 1   | H     | 717 | DA   | C5-C6-N6    | 8.96  | 130.87      | 123.70   |
| 1   | F     | 501 | DA   | C8-N9-C4    | -8.96 | 102.22      | 105.80   |
| 1   | F     | 510 | DC   | P-O5'-C5'   | 8.95  | 135.21      | 120.90   |
| 1   | E     | 401 | DA   | O4'-C1'-C2' | -8.94 | 98.75       | 105.90   |
| 1   | G     | 600 | DG   | C6-N1-C2    | -8.92 | 119.75      | 125.10   |
| 1   | G     | 611 | DG   | C4'-C3'-C2' | -8.92 | 95.07       | 103.10   |
| 1   | G     | 609 | DG   | O4'-C1'-N9  | 8.90  | 114.23      | 108.00   |
| 1   | G     | 600 | DG   | N9-C4-C5    | 8.90  | 108.96      | 105.40   |
| 1   | E     | 417 | DA   | N9-C4-C5    | 8.88  | 109.35      | 105.80   |
| 1   | G     | 602 | DA   | N9-C1'-C2'  | -8.87 | 95.75       | 112.60   |
| 1   | F     | 500 | DG   | C3'-C2'-C1' | 8.87  | 113.14      | 102.50   |
| 1   | F     | 517 | DA   | C2-N3-C4    | -8.85 | 106.17      | 110.60   |
| 1   | H     | 712 | DC   | C4'-C3'-C2' | -8.84 | 95.15       | 103.10   |
| 1   | F     | 502 | DA   | C2-N3-C4    | -8.81 | 106.20      | 110.60   |
| 1   | E     | 405 | DG   | N1-C2-N2    | 8.78  | 124.10      | 116.20   |
| 1   | G     | 607 | DG   | O4'-C1'-C2' | -8.76 | 98.89       | 105.90   |
| 1   | E     | 416 | DC   | P-O3'-C3'   | 8.74  | 130.19      | 119.70   |
| 1   | H     | 717 | DA   | O4'-C1'-C2' | -8.73 | 98.92       | 105.90   |
| 1   | F     | 519 | DT   | O5'-P-OP1   | -8.68 | 97.89       | 105.70   |
| 1   | H     | 715 | DA   | C4'-C3'-C2' | -8.66 | 95.31       | 103.10   |
| 1   | E     | 404 | DT   | C4-C5-C6    | 8.65  | 123.19      | 118.00   |
| 1   | H     | 702 | DA   | C2-N3-C4    | -8.65 | 106.28      | 110.60   |
| 1   | F     | 516 | DC   | N3-C4-N4    | 8.64  | 124.05      | 118.00   |
| 1   | H     | 704 | DT   | P-O3'-C3'   | 8.64  | 130.07      | 119.70   |
| 1   | E     | 407 | DG   | N7-C8-N9    | 8.64  | 117.42      | 113.10   |
| 1   | G     | 605 | DG   | C5'-C4'-C3' | 8.64  | 129.65      | 114.10   |
| 1   | E     | 406 | DT   | O4'-C1'-C2' | -8.62 | 99.00       | 105.90   |
| 1   | G     | 613 | DT   | P-O3'-C3'   | 8.62  | 130.05      | 119.70   |
| 1   | E     | 404 | DT   | O4'-C4'-C3' | 8.61  | 111.16      | 106.00   |
| 1   | G     | 618 | DA   | N1-C6-N6    | -8.60 | 113.44      | 118.60   |
| 1   | G     | 612 | DC   | C4'-C3'-C2' | -8.59 | 95.37       | 103.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | F     | 515 | DA   | O4'-C4'-C3' | 8.58  | 111.15      | 106.00   |
| 1   | G     | 600 | DG   | N3-C2-N2    | -8.54 | 113.92      | 119.90   |
| 1   | F     | 504 | DT   | C4-C5-C6    | 8.54  | 123.12      | 118.00   |
| 1   | H     | 717 | DA   | N9-C4-C5    | 8.53  | 109.21      | 105.80   |
| 1   | F     | 508 | DA   | O4'-C1'-C2' | -8.51 | 99.09       | 105.90   |
| 1   | G     | 601 | DA   | O5'-P-OP2   | -8.51 | 98.04       | 105.70   |
| 1   | F     | 504 | DT   | C4'-C3'-C2' | -8.51 | 95.44       | 103.10   |
| 1   | F     | 520 | DT   | C5-C6-N1    | -8.50 | 118.60      | 123.70   |
| 1   | H     | 707 | DG   | N7-C8-N9    | 8.44  | 117.32      | 113.10   |
| 1   | H     | 701 | DA   | N9-C4-C5    | 8.42  | 109.17      | 105.80   |
| 1   | G     | 606 | DT   | O4'-C1'-C2' | -8.41 | 99.17       | 105.90   |
| 1   | F     | 514 | DC   | C6-N1-C2    | -8.40 | 116.94      | 120.30   |
| 1   | H     | 720 | DT   | O4'-C1'-C2' | -8.39 | 99.18       | 105.90   |
| 1   | F     | 515 | DA   | C4'-C3'-C2' | -8.38 | 95.56       | 103.10   |
| 1   | E     | 417 | DA   | C5-C6-N6    | 8.37  | 130.40      | 123.70   |
| 1   | F     | 519 | DT   | N1-C1'-C2'  | 8.35  | 128.46      | 112.60   |
| 1   | H     | 703 | DT   | P-O3'-C3'   | 8.35  | 129.71      | 119.70   |
| 1   | G     | 618 | DA   | N9-C4-C5    | 8.34  | 109.14      | 105.80   |
| 1   | E     | 420 | DT   | C4-C5-C7    | -8.34 | 114.00      | 119.00   |
| 1   | E     | 404 | DT   | P-O3'-C3'   | 8.32  | 129.69      | 119.70   |
| 1   | F     | 515 | DA   | P-O5'-C5'   | 8.31  | 134.19      | 120.90   |
| 1   | E     | 402 | DA   | C4'-C3'-O3' | 8.29  | 130.44      | 109.70   |
| 1   | E     | 400 | DG   | O4'-C1'-N9  | 8.29  | 113.80      | 108.00   |
| 1   | H     | 704 | DT   | O4'-C1'-C2' | -8.28 | 99.28       | 105.90   |
| 1   | H     | 702 | DA   | P-O3'-C3'   | -8.27 | 109.77      | 119.70   |
| 1   | G     | 607 | DG   | O4'-C4'-C3' | 8.27  | 110.96      | 106.00   |
| 1   | H     | 715 | DA   | N1-C6-N6    | 8.27  | 123.56      | 118.60   |
| 1   | F     | 503 | DT   | C6-N1-C2    | -8.26 | 117.17      | 121.30   |
| 1   | E     | 407 | DG   | O4'-C1'-C2' | -8.26 | 99.29       | 105.90   |
| 1   | F     | 502 | DA   | N1-C6-N6    | 8.25  | 123.55      | 118.60   |
| 1   | G     | 603 | DT   | O4'-C1'-N1  | 8.23  | 113.76      | 108.00   |
| 1   | H     | 712 | DC   | C1'-O4'-C4' | -8.21 | 101.89      | 110.10   |
| 1   | G     | 604 | DT   | N3-C4-O4    | 8.20  | 124.82      | 119.90   |
| 1   | G     | 601 | DA   | N9-C4-C5    | 8.18  | 109.07      | 105.80   |
| 1   | G     | 608 | DA   | O5'-C5'-C4' | 8.17  | 131.43      | 111.00   |
| 1   | G     | 602 | DA   | C4'-C3'-O3' | 8.16  | 130.11      | 109.70   |
| 1   | E     | 400 | DG   | C2-N3-C4    | -8.16 | 107.82      | 111.90   |
| 1   | F     | 500 | DG   | C1'-O4'-C4' | 8.16  | 118.26      | 110.10   |
| 1   | H     | 713 | DT   | C5-C4-O4    | -8.15 | 119.20      | 124.90   |
| 1   | F     | 514 | DC   | N3-C2-O2    | -8.14 | 116.20      | 121.90   |
| 1   | G     | 616 | DC   | C4'-C3'-C2' | -8.14 | 95.78       | 103.10   |
| 1   | F     | 520 | DT   | O4'-C4'-C3' | -8.10 | 101.14      | 106.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 601 | DA   | C3'-C2'-C1' | 8.08  | 112.19      | 102.50   |
| 1   | G     | 602 | DA   | O4'-C1'-C2' | -8.07 | 99.44       | 105.90   |
| 1   | H     | 713 | DT   | N3-C4-O4    | 8.07  | 124.74      | 119.90   |
| 1   | E     | 416 | DC   | C6-N1-C2    | -8.06 | 117.08      | 120.30   |
| 1   | G     | 615 | DA   | N9-C4-C5    | 8.05  | 109.02      | 105.80   |
| 1   | G     | 618 | DA   | C5-C6-N6    | 8.05  | 130.14      | 123.70   |
| 1   | G     | 608 | DA   | C8-N9-C4    | -8.04 | 102.59      | 105.80   |
| 1   | H     | 711 | DG   | O4'-C1'-C2' | -8.03 | 99.47       | 105.90   |
| 1   | F     | 500 | DG   | N9-C4-C5    | 8.03  | 108.61      | 105.40   |
| 1   | E     | 415 | DA   | C4'-C3'-O3' | 8.02  | 129.76      | 109.70   |
| 1   | G     | 601 | DA   | C5-C6-N6    | 8.02  | 130.12      | 123.70   |
| 1   | H     | 700 | DG   | O4'-C1'-C2' | -8.01 | 99.49       | 105.90   |
| 1   | H     | 718 | DA   | P-O3'-C3'   | 8.01  | 129.31      | 119.70   |
| 1   | G     | 618 | DA   | O4'-C1'-C2' | -8.00 | 99.50       | 105.90   |
| 1   | G     | 604 | DT   | O4'-C4'-C3' | 7.98  | 110.79      | 106.00   |
| 1   | H     | 707 | DG   | O4'-C1'-C2' | -7.97 | 99.52       | 105.90   |
| 1   | E     | 410 | DC   | N3-C2-O2    | -7.97 | 116.32      | 121.90   |
| 1   | H     | 700 | DG   | C8-N9-C4    | -7.96 | 103.21      | 106.40   |
| 1   | E     | 407 | DG   | N3-C4-C5    | -7.95 | 124.62      | 128.60   |
| 1   | H     | 719 | DT   | N1-C1'-C2'  | 7.93  | 127.66      | 112.60   |
| 1   | E     | 406 | DT   | C4-C5-C6    | 7.92  | 122.75      | 118.00   |
| 1   | F     | 504 | DT   | N3-C4-O4    | 7.90  | 124.64      | 119.90   |
| 1   | H     | 702 | DA   | C1'-O4'-C4' | -7.87 | 102.23      | 110.10   |
| 1   | G     | 619 | DT   | O4'-C4'-C3' | -7.85 | 101.29      | 106.00   |
| 1   | F     | 511 | DG   | P-O3'-C3'   | 7.84  | 129.11      | 119.70   |
| 1   | F     | 503 | DT   | C4'-C3'-C2' | -7.84 | 96.05       | 103.10   |
| 1   | H     | 710 | DC   | N3-C2-O2    | -7.80 | 116.44      | 121.90   |
| 1   | H     | 714 | DC   | O4'-C1'-C2' | -7.79 | 99.67       | 105.90   |
| 1   | F     | 515 | DA   | N1-C2-N3    | 7.79  | 133.19      | 129.30   |
| 1   | G     | 613 | DT   | C4'-C3'-C2' | -7.78 | 96.10       | 103.10   |
| 1   | E     | 405 | DG   | C2-N3-C4    | 7.77  | 115.79      | 111.90   |
| 1   | E     | 409 | DG   | O4'-C4'-C3' | 7.77  | 110.66      | 106.00   |
| 1   | G     | 610 | DC   | N1-C2-O2    | 7.77  | 123.56      | 118.90   |
| 1   | E     | 417 | DA   | O5'-C5'-C4' | 7.75  | 130.38      | 111.00   |
| 1   | H     | 716 | DC   | O4'-C1'-C2' | -7.75 | 99.70       | 105.90   |
| 1   | G     | 611 | DG   | C5'-C4'-C3' | -7.73 | 100.18      | 114.10   |
| 1   | E     | 405 | DG   | C5-C6-O6    | -7.73 | 123.97      | 128.60   |
| 1   | E     | 420 | DT   | N1-C2-N3    | 7.71  | 119.23      | 114.60   |
| 1   | H     | 714 | DC   | O4'-C4'-C3' | -7.70 | 101.38      | 106.00   |
| 1   | E     | 405 | DG   | C5-C6-N1    | 7.67  | 115.34      | 111.50   |
| 1   | E     | 417 | DA   | C5-C6-N1    | -7.67 | 113.86      | 117.70   |
| 1   | F     | 508 | DA   | C2-N3-C4    | -7.67 | 106.77      | 110.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | F     | 515 | DA   | C2-N3-C4    | -7.65 | 106.77      | 110.60   |
| 1   | H     | 710 | DC   | N1-C2-O2    | 7.65  | 123.49      | 118.90   |
| 1   | E     | 415 | DA   | N1-C2-N3    | 7.64  | 133.12      | 129.30   |
| 1   | F     | 503 | DT   | O3'-P-O5'   | 7.63  | 118.50      | 104.00   |
| 1   | G     | 608 | DA   | O3'-P-O5'   | 7.63  | 118.49      | 104.00   |
| 1   | H     | 708 | DA   | O4'-C1'-N9  | 7.62  | 113.33      | 108.00   |
| 1   | F     | 508 | DA   | C4'-C3'-C2' | -7.61 | 96.25       | 103.10   |
| 1   | F     | 514 | DC   | O4'-C4'-C3' | 7.61  | 110.56      | 106.00   |
| 1   | E     | 408 | DA   | N9-C1'-C2'  | 7.59  | 127.02      | 112.60   |
| 1   | E     | 401 | DA   | P-O5'-C5'   | 7.59  | 133.04      | 120.90   |
| 1   | G     | 602 | DA   | C5'-C4'-C3' | 7.59  | 127.75      | 114.10   |
| 1   | E     | 410 | DC   | O4'-C1'-N1  | 7.56  | 113.30      | 108.00   |
| 1   | G     | 617 | DA   | C2-N3-C4    | -7.56 | 106.82      | 110.60   |
| 1   | E     | 414 | DC   | P-O5'-C5'   | 7.55  | 132.97      | 120.90   |
| 1   | F     | 517 | DA   | O5'-C5'-C4' | 7.54  | 129.86      | 111.00   |
| 1   | F     | 502 | DA   | C4'-C3'-O3' | 7.52  | 128.49      | 109.70   |
| 1   | F     | 503 | DT   | N1-C2-N3    | 7.49  | 119.10      | 114.60   |
| 1   | H     | 717 | DA   | N3-C4-N9    | -7.48 | 121.41      | 127.40   |
| 1   | G     | 601 | DA   | C2-N3-C4    | -7.48 | 106.86      | 110.60   |
| 1   | H     | 713 | DT   | O4'-C1'-N1  | 7.47  | 113.23      | 108.00   |
| 1   | E     | 414 | DC   | P-O3'-C3'   | 7.46  | 128.65      | 119.70   |
| 1   | H     | 701 | DA   | C5-C6-N6    | 7.44  | 129.65      | 123.70   |
| 1   | H     | 704 | DT   | C4-C5-C6    | 7.43  | 122.46      | 118.00   |
| 1   | F     | 516 | DC   | O5'-C5'-C4' | 7.42  | 129.54      | 111.00   |
| 1   | G     | 615 | DA   | C8-N9-C4    | -7.42 | 102.83      | 105.80   |
| 1   | G     | 619 | DT   | P-O3'-C3'   | 7.42  | 128.60      | 119.70   |
| 1   | G     | 602 | DA   | C3'-C2'-C1' | 7.38  | 111.36      | 102.50   |
| 1   | H     | 716 | DC   | N1-C2-O2    | 7.38  | 123.33      | 118.90   |
| 1   | E     | 406 | DT   | C4'-C3'-O3' | 7.36  | 128.11      | 109.70   |
| 1   | E     | 408 | DA   | O4'-C1'-C2' | -7.35 | 100.02      | 105.90   |
| 1   | F     | 508 | DA   | O5'-C5'-C4' | 7.35  | 129.37      | 111.00   |
| 1   | F     | 500 | DG   | C5-N7-C8    | -7.34 | 100.63      | 104.30   |
| 1   | F     | 501 | DA   | C4'-C3'-O3' | 7.34  | 128.06      | 109.70   |
| 1   | E     | 405 | DG   | C1'-O4'-C4' | -7.34 | 102.76      | 110.10   |
| 1   | E     | 415 | DA   | N7-C8-N9    | 7.33  | 117.47      | 113.80   |
| 1   | H     | 702 | DA   | C6-N1-C2    | -7.33 | 114.20      | 118.60   |
| 1   | E     | 415 | DA   | N1-C6-N6    | 7.33  | 123.00      | 118.60   |
| 1   | E     | 418 | DA   | C5'-C4'-C3' | 7.33  | 127.28      | 114.10   |
| 1   | H     | 709 | DG   | N7-C8-N9    | 7.32  | 116.76      | 113.10   |
| 1   | E     | 405 | DG   | C4-N9-C1'   | -7.32 | 116.99      | 126.50   |
| 1   | F     | 502 | DA   | C5'-C4'-O4' | -7.32 | 95.40       | 109.30   |
| 1   | G     | 612 | DC   | O4'-C4'-C3' | -7.31 | 101.58      | 104.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | F     | 506 | DT   | C6-C5-C7    | -7.31 | 118.51      | 122.90   |
| 1   | G     | 614 | DC   | N3-C4-C5    | -7.31 | 118.98      | 121.90   |
| 1   | G     | 614 | DC   | P-O5'-C5'   | 7.29  | 132.57      | 120.90   |
| 1   | F     | 506 | DT   | O4'-C1'-N1  | 7.28  | 113.09      | 108.00   |
| 1   | E     | 418 | DA   | C2-N3-C4    | -7.25 | 106.97      | 110.60   |
| 1   | H     | 704 | DT   | O4'-C4'-C3' | 7.25  | 110.35      | 106.00   |
| 1   | H     | 701 | DA   | C1'-O4'-C4' | 7.25  | 117.35      | 110.10   |
| 1   | H     | 715 | DA   | O4'-C1'-C2' | -7.25 | 100.10      | 105.90   |
| 1   | G     | 608 | DA   | C1'-O4'-C4' | -7.25 | 102.85      | 110.10   |
| 1   | G     | 607 | DG   | P-O3'-C3'   | 7.24  | 128.39      | 119.70   |
| 1   | H     | 719 | DT   | P-O5'-C5'   | 7.23  | 132.47      | 120.90   |
| 1   | E     | 416 | DC   | O5'-P-OP2   | -7.21 | 99.21       | 105.70   |
| 1   | E     | 405 | DG   | C8-N9-C1'   | 7.21  | 136.37      | 127.00   |
| 1   | G     | 606 | DT   | C6-N1-C2    | -7.21 | 117.70      | 121.30   |
| 1   | H     | 704 | DT   | C4'-C3'-C2' | -7.19 | 96.63       | 103.10   |
| 1   | F     | 520 | DT   | C4'-C3'-C2' | -7.17 | 96.65       | 103.10   |
| 1   | G     | 606 | DT   | O5'-P-OP2   | -7.14 | 99.28       | 105.70   |
| 1   | E     | 418 | DA   | C4'-C3'-C2' | -7.14 | 96.68       | 103.10   |
| 1   | E     | 414 | DC   | C6-N1-C2    | -7.13 | 117.45      | 120.30   |
| 1   | H     | 711 | DG   | N3-C4-N9    | 7.13  | 130.28      | 126.00   |
| 1   | F     | 519 | DT   | C4-C5-C6    | 7.13  | 122.28      | 118.00   |
| 1   | E     | 413 | DT   | P-O5'-C5'   | 7.12  | 132.29      | 120.90   |
| 1   | G     | 616 | DC   | N3-C2-O2    | -7.12 | 116.92      | 121.90   |
| 1   | F     | 520 | DT   | P-O5'-C5'   | 7.11  | 132.28      | 120.90   |
| 1   | F     | 505 | DG   | C4-N9-C1'   | -7.08 | 117.29      | 126.50   |
| 1   | F     | 501 | DA   | C2-N3-C4    | -7.08 | 107.06      | 110.60   |
| 1   | H     | 718 | DA   | C8-N9-C4    | -7.08 | 102.97      | 105.80   |
| 1   | G     | 609 | DG   | C5'-C4'-O4' | -7.06 | 95.89       | 109.30   |
| 1   | H     | 714 | DC   | N3-C4-C5    | -7.06 | 119.08      | 121.90   |
| 1   | H     | 706 | DT   | O4'-C4'-C3' | 7.05  | 110.23      | 106.00   |
| 1   | G     | 601 | DA   | C5-C6-N1    | -7.04 | 114.18      | 117.70   |
| 1   | G     | 611 | DG   | O4'-C1'-C2' | -7.03 | 100.28      | 105.90   |
| 1   | E     | 420 | DT   | C4'-C3'-C2' | -7.03 | 96.78       | 103.10   |
| 1   | E     | 418 | DA   | C8-N9-C4    | -7.02 | 102.99      | 105.80   |
| 1   | G     | 610 | DC   | N3-C2-O2    | -7.01 | 116.99      | 121.90   |
| 1   | E     | 404 | DT   | C5'-C4'-O4' | -7.00 | 96.00       | 109.30   |
| 1   | F     | 506 | DT   | C4'-C3'-O3' | 6.99  | 127.18      | 109.70   |
| 1   | H     | 719 | DT   | C4-C5-C6    | 6.98  | 122.19      | 118.00   |
| 1   | H     | 705 | DG   | O4'-C1'-C2' | -6.97 | 100.33      | 105.90   |
| 1   | G     | 600 | DG   | C2-N3-C4    | 6.96  | 115.38      | 111.90   |
| 1   | G     | 601 | DA   | C4'-C3'-O3' | 6.95  | 127.07      | 109.70   |
| 1   | E     | 409 | DG   | C5-C6-O6    | -6.93 | 124.44      | 128.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 607 | DG   | N7-C8-N9    | 6.92  | 116.56      | 113.10   |
| 1   | H     | 702 | DA   | N7-C8-N9    | 6.91  | 117.26      | 113.80   |
| 1   | F     | 516 | DC   | O4'-C1'-C2' | -6.90 | 100.38      | 105.90   |
| 1   | G     | 601 | DA   | C2'-C3'-O3' | 6.88  | 135.30      | 112.60   |
| 1   | G     | 620 | DT   | C4'-C3'-O3' | 6.88  | 126.89      | 109.70   |
| 1   | H     | 709 | DG   | N3-C4-N9    | -6.87 | 121.88      | 126.00   |
| 1   | H     | 705 | DG   | N9-C1'-C2'  | 6.85  | 125.61      | 112.60   |
| 1   | H     | 715 | DA   | C5-C6-N6    | -6.85 | 118.22      | 123.70   |
| 1   | F     | 512 | DC   | C1'-O4'-C4' | -6.83 | 103.27      | 110.10   |
| 1   | G     | 606 | DT   | P-O5'-C5'   | 6.82  | 131.82      | 120.90   |
| 1   | H     | 718 | DA   | O4'-C1'-N9  | 6.82  | 112.78      | 108.00   |
| 1   | G     | 606 | DT   | C4'-C3'-O3' | 6.80  | 126.71      | 109.70   |
| 1   | F     | 515 | DA   | C4'-C3'-O3' | 6.80  | 126.70      | 109.70   |
| 1   | H     | 719 | DT   | N1-C2-N3    | 6.80  | 118.68      | 114.60   |
| 1   | E     | 415 | DA   | C3'-C2'-C1' | 6.79  | 110.65      | 102.50   |
| 1   | F     | 508 | DA   | P-O5'-C5'   | 6.79  | 131.76      | 120.90   |
| 1   | E     | 412 | DC   | C2-N3-C4    | 6.78  | 123.29      | 119.90   |
| 1   | G     | 619 | DT   | P-O5'-C5'   | -6.78 | 110.05      | 120.90   |
| 1   | H     | 705 | DG   | N7-C8-N9    | 6.78  | 116.49      | 113.10   |
| 1   | F     | 506 | DT   | O5'-P-OP2   | -6.77 | 99.60       | 105.70   |
| 1   | E     | 415 | DA   | C2-N3-C4    | -6.77 | 107.21      | 110.60   |
| 1   | E     | 405 | DG   | O4'-C4'-C3' | 6.77  | 110.06      | 106.00   |
| 1   | G     | 604 | DT   | C4'-C3'-C2' | -6.77 | 97.01       | 103.10   |
| 1   | F     | 508 | DA   | O4'-C4'-C3' | 6.75  | 110.05      | 106.00   |
| 1   | E     | 407 | DG   | C4'-C3'-C2' | -6.74 | 97.03       | 103.10   |
| 1   | F     | 500 | DG   | C4'-C3'-C2' | -6.74 | 97.03       | 103.10   |
| 1   | G     | 605 | DG   | C8-N9-C4    | -6.72 | 103.71      | 106.40   |
| 1   | F     | 505 | DG   | C5-N7-C8    | -6.72 | 100.94      | 104.30   |
| 1   | H     | 707 | DG   | C8-N9-C1'   | -6.71 | 118.27      | 127.00   |
| 1   | F     | 507 | DG   | N3-C2-N2    | -6.71 | 115.20      | 119.90   |
| 1   | G     | 618 | DA   | C4'-C3'-O3' | 6.69  | 126.42      | 109.70   |
| 1   | G     | 602 | DA   | O5'-P-OP2   | -6.68 | 99.69       | 105.70   |
| 1   | F     | 516 | DC   | C4'-C3'-C2' | -6.67 | 97.10       | 103.10   |
| 1   | H     | 708 | DA   | C8-N9-C4    | -6.66 | 103.14      | 105.80   |
| 1   | H     | 707 | DG   | O3'-P-O5'   | 6.66  | 116.65      | 104.00   |
| 1   | E     | 405 | DG   | N3-C2-N2    | -6.66 | 115.24      | 119.90   |
| 1   | F     | 509 | DG   | C4-N9-C1'   | -6.61 | 117.90      | 126.50   |
| 1   | G     | 604 | DT   | O4'-C1'-C2' | -6.61 | 100.61      | 105.90   |
| 1   | E     | 404 | DT   | N3-C2-O2    | -6.61 | 118.34      | 122.30   |
| 1   | H     | 704 | DT   | C6-C5-C7    | -6.60 | 118.94      | 122.90   |
| 1   | H     | 702 | DA   | O4'-C1'-N9  | -6.60 | 103.38      | 108.00   |
| 1   | H     | 706 | DT   | P-O5'-C5'   | -6.60 | 110.34      | 120.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 612 | DC   | N1-C2-O2    | 6.59  | 122.86      | 118.90   |
| 1   | F     | 508 | DA   | N1-C2-N3    | 6.58  | 132.59      | 129.30   |
| 1   | G     | 606 | DT   | N3-C2-O2    | -6.58 | 118.35      | 122.30   |
| 1   | E     | 407 | DG   | C4-N9-C1'   | 6.58  | 135.06      | 126.50   |
| 1   | E     | 419 | DT   | C6-N1-C2    | -6.57 | 118.01      | 121.30   |
| 1   | E     | 419 | DT   | N1-C1'-C2'  | 6.55  | 125.06      | 112.60   |
| 1   | E     | 401 | DA   | C4-C5-C6    | 6.55  | 120.27      | 117.00   |
| 1   | E     | 418 | DA   | N1-C2-N3    | 6.55  | 132.57      | 129.30   |
| 1   | F     | 518 | DA   | C3'-C2'-C1' | 6.54  | 110.35      | 102.50   |
| 1   | F     | 507 | DG   | C4'-C3'-C2' | -6.54 | 97.22       | 103.10   |
| 1   | H     | 714 | DC   | C4'-C3'-O3' | 6.54  | 126.04      | 109.70   |
| 1   | H     | 709 | DG   | P-O3'-C3'   | 6.53  | 127.54      | 119.70   |
| 1   | G     | 616 | DC   | N3-C4-C5    | -6.53 | 119.29      | 121.90   |
| 1   | E     | 408 | DA   | C2-N3-C4    | -6.52 | 107.34      | 110.60   |
| 1   | F     | 512 | DC   | N1-C1'-C2'  | 6.52  | 124.98      | 112.60   |
| 1   | E     | 404 | DT   | N1-C2-N3    | 6.51  | 118.51      | 114.60   |
| 1   | G     | 605 | DG   | O3'-P-O5'   | 6.50  | 116.35      | 104.00   |
| 1   | F     | 509 | DG   | N7-C8-N9    | 6.49  | 116.35      | 113.10   |
| 1   | F     | 510 | DC   | N3-C2-O2    | -6.49 | 117.36      | 121.90   |
| 1   | G     | 610 | DC   | P-O3'-C3'   | 6.49  | 127.48      | 119.70   |
| 1   | E     | 418 | DA   | O4'-C1'-C2' | -6.49 | 100.71      | 105.90   |
| 1   | H     | 702 | DA   | C5'-C4'-C3' | 6.49  | 125.77      | 114.10   |
| 1   | G     | 618 | DA   | P-O5'-C5'   | 6.48  | 131.27      | 120.90   |
| 1   | H     | 703 | DT   | O5'-P-OP2   | -6.47 | 99.88       | 105.70   |
| 1   | G     | 603 | DT   | O3'-P-O5'   | 6.46  | 116.27      | 104.00   |
| 1   | H     | 720 | DT   | P-O5'-C5'   | 6.46  | 131.24      | 120.90   |
| 1   | H     | 706 | DT   | C6-C5-C7    | -6.44 | 119.04      | 122.90   |
| 1   | F     | 520 | DT   | O4'-C1'-C2' | -6.44 | 100.75      | 105.90   |
| 1   | H     | 705 | DG   | C8-N9-C4    | -6.43 | 103.83      | 106.40   |
| 1   | E     | 419 | DT   | P-O5'-C5'   | 6.40  | 131.14      | 120.90   |
| 1   | F     | 518 | DA   | C5'-C4'-C3' | 6.40  | 125.61      | 114.10   |
| 1   | G     | 615 | DA   | P-O3'-C3'   | -6.39 | 112.03      | 119.70   |
| 1   | H     | 716 | DC   | N3-C2-O2    | -6.39 | 117.43      | 121.90   |
| 1   | H     | 717 | DA   | N7-C8-N9    | 6.38  | 116.99      | 113.80   |
| 1   | E     | 411 | DG   | C8-N9-C4    | -6.37 | 103.85      | 106.40   |
| 1   | H     | 719 | DT   | O3'-P-O5'   | 6.37  | 116.11      | 104.00   |
| 1   | H     | 701 | DA   | C3'-C2'-C1' | 6.37  | 110.14      | 102.50   |
| 1   | F     | 504 | DT   | C5'-C4'-O4' | -6.34 | 97.24       | 109.30   |
| 1   | H     | 709 | DG   | C3'-C2'-C1' | 6.34  | 110.11      | 102.50   |
| 1   | F     | 506 | DT   | C3'-C2'-C1' | 6.33  | 110.09      | 102.50   |
| 1   | F     | 509 | DG   | C4'-C3'-C2' | -6.32 | 97.41       | 103.10   |
| 1   | F     | 519 | DT   | P-O5'-C5'   | 6.32  | 131.00      | 120.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 616 | DC   | P-O5'-C5'   | 6.31  | 131.00      | 120.90   |
| 1   | H     | 701 | DA   | C4-C5-C6    | 6.31  | 120.16      | 117.00   |
| 1   | G     | 620 | DT   | C3'-C2'-C1' | -6.31 | 94.93       | 102.50   |
| 1   | E     | 405 | DG   | O5'-P-OP1   | -6.30 | 100.03      | 105.70   |
| 1   | G     | 614 | DC   | O4'-C4'-C3' | -6.30 | 101.98      | 104.50   |
| 1   | H     | 706 | DT   | C4-C5-C6    | 6.30  | 121.78      | 118.00   |
| 1   | H     | 715 | DA   | C1'-O4'-C4' | -6.29 | 103.81      | 110.10   |
| 1   | F     | 520 | DT   | C5'-C4'-O4' | 6.29  | 121.25      | 109.30   |
| 1   | H     | 701 | DA   | C2-N3-C4    | -6.28 | 107.46      | 110.60   |
| 1   | G     | 607 | DG   | N3-C2-N2    | -6.28 | 115.51      | 119.90   |
| 1   | E     | 413 | DT   | N1-C1'-C2'  | 6.28  | 124.52      | 112.60   |
| 1   | E     | 419 | DT   | C4-C5-C7    | -6.27 | 115.24      | 119.00   |
| 1   | E     | 406 | DT   | O3'-P-O5'   | 6.27  | 115.91      | 104.00   |
| 1   | F     | 517 | DA   | C4'-C3'-O3' | 6.26  | 125.36      | 109.70   |
| 1   | F     | 510 | DC   | O4'-C1'-C2' | -6.26 | 100.89      | 105.90   |
| 1   | E     | 410 | DC   | O3'-P-O5'   | 6.25  | 115.88      | 104.00   |
| 1   | G     | 605 | DG   | O4'-C1'-C2' | -6.23 | 100.91      | 105.90   |
| 1   | H     | 708 | DA   | N1-C2-N3    | 6.23  | 132.42      | 129.30   |
| 1   | G     | 607 | DG   | N9-C4-C5    | 6.22  | 107.89      | 105.40   |
| 1   | H     | 713 | DT   | P-O5'-C5'   | 6.22  | 130.85      | 120.90   |
| 1   | F     | 506 | DT   | O3'-P-O5'   | 6.22  | 115.82      | 104.00   |
| 1   | E     | 403 | DT   | O3'-P-O5'   | 6.21  | 115.80      | 104.00   |
| 1   | H     | 712 | DC   | N3-C2-O2    | -6.21 | 117.55      | 121.90   |
| 1   | H     | 704 | DT   | C6-N1-C2    | -6.20 | 118.20      | 121.30   |
| 1   | H     | 713 | DT   | C4'-C3'-C2' | -6.20 | 97.52       | 103.10   |
| 1   | F     | 509 | DG   | C5-N7-C8    | -6.18 | 101.21      | 104.30   |
| 1   | H     | 700 | DG   | O3'-P-O5'   | 6.17  | 115.72      | 104.00   |
| 1   | F     | 506 | DT   | P-O5'-C5'   | 6.16  | 130.76      | 120.90   |
| 1   | F     | 504 | DT   | N3-C4-C5    | -6.15 | 111.51      | 115.20   |
| 1   | G     | 602 | DA   | O5'-C5'-C4' | 6.15  | 126.37      | 111.00   |
| 1   | H     | 717 | DA   | C5'-C4'-O4' | 6.14  | 120.96      | 109.30   |
| 1   | E     | 401 | DA   | C8-N9-C1'   | -6.13 | 116.66      | 127.70   |
| 1   | F     | 517 | DA   | O4'-C1'-C2' | -6.12 | 101.00      | 105.90   |
| 1   | F     | 514 | DC   | N1-C2-N3    | 6.11  | 123.48      | 119.20   |
| 1   | G     | 604 | DT   | O5'-P-OP1   | -6.11 | 100.20      | 105.70   |
| 1   | E     | 400 | DG   | P-O3'-C3'   | 6.10  | 127.02      | 119.70   |
| 1   | E     | 412 | DC   | C1'-O4'-C4' | -6.09 | 104.01      | 110.10   |
| 1   | E     | 404 | DT   | C1'-O4'-C4' | -6.09 | 104.01      | 110.10   |
| 1   | H     | 709 | DG   | C5-N7-C8    | -6.08 | 101.26      | 104.30   |
| 1   | H     | 705 | DG   | P-O5'-C5'   | 6.08  | 130.62      | 120.90   |
| 1   | F     | 512 | DC   | C2-N3-C4    | 6.06  | 122.93      | 119.90   |
| 1   | G     | 614 | DC   | C6-N1-C2    | -6.06 | 117.88      | 120.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 609 | DG   | C8-N9-C4    | -6.05 | 103.98      | 106.40   |
| 1   | H     | 707 | DG   | C4-N9-C1'   | 6.05  | 134.37      | 126.50   |
| 1   | F     | 518 | DA   | O4'-C4'-C3' | 6.05  | 109.63      | 106.00   |
| 1   | F     | 507 | DG   | N7-C8-N9    | 6.03  | 116.11      | 113.10   |
| 1   | H     | 709 | DG   | C4-N9-C1'   | -6.03 | 118.67      | 126.50   |
| 1   | F     | 505 | DG   | N3-C4-N9    | -6.02 | 122.39      | 126.00   |
| 1   | F     | 502 | DA   | C1'-O4'-C4' | -6.02 | 104.08      | 110.10   |
| 1   | E     | 403 | DT   | C4-C5-C6    | 6.02  | 121.61      | 118.00   |
| 1   | F     | 518 | DA   | N7-C8-N9    | 6.02  | 116.81      | 113.80   |
| 1   | F     | 510 | DC   | N1-C2-O2    | 6.01  | 122.51      | 118.90   |
| 1   | H     | 716 | DC   | O4'-C1'-N1  | 6.01  | 112.21      | 108.00   |
| 1   | E     | 403 | DT   | C4'-C3'-O3' | 6.01  | 124.73      | 109.70   |
| 1   | F     | 515 | DA   | C8-N9-C4    | -6.01 | 103.39      | 105.80   |
| 1   | G     | 605 | DG   | P-O5'-C5'   | 6.00  | 130.50      | 120.90   |
| 1   | F     | 516 | DC   | N1-C2-O2    | 6.00  | 122.50      | 118.90   |
| 1   | F     | 516 | DC   | C5-C4-N4    | -6.00 | 116.00      | 120.20   |
| 1   | G     | 620 | DT   | N3-C4-C5    | -5.99 | 111.60      | 115.20   |
| 1   | H     | 701 | DA   | C4'-C3'-O3' | 5.99  | 124.68      | 109.70   |
| 1   | F     | 517 | DA   | O4'-C4'-C3' | 5.99  | 109.59      | 106.00   |
| 1   | H     | 711 | DG   | N3-C4-C5    | -5.99 | 125.61      | 128.60   |
| 1   | E     | 415 | DA   | P-O5'-C5'   | 5.99  | 130.48      | 120.90   |
| 1   | G     | 601 | DA   | C4-N9-C1'   | 5.98  | 137.06      | 126.30   |
| 1   | E     | 419 | DT   | O5'-P-OP1   | -5.96 | 100.33      | 105.70   |
| 1   | H     | 714 | DC   | C6-N1-C2    | -5.96 | 117.92      | 120.30   |
| 1   | F     | 509 | DG   | P-O3'-C3'   | 5.94  | 126.83      | 119.70   |
| 1   | F     | 514 | DC   | N3-C4-C5    | -5.94 | 119.53      | 121.90   |
| 1   | H     | 710 | DC   | O4'-C1'-C2' | -5.92 | 101.17      | 105.90   |
| 1   | E     | 403 | DT   | C3'-C2'-C1' | 5.91  | 109.59      | 102.50   |
| 1   | F     | 517 | DA   | N7-C8-N9    | 5.91  | 116.75      | 113.80   |
| 1   | G     | 619 | DT   | C5'-C4'-C3' | -5.90 | 103.48      | 114.10   |
| 1   | F     | 505 | DG   | C4'-C3'-C2' | -5.89 | 97.80       | 103.10   |
| 1   | G     | 606 | DT   | C3'-C2'-C1' | 5.89  | 109.56      | 102.50   |
| 1   | E     | 412 | DC   | O4'-C4'-C3' | -5.88 | 102.15      | 104.50   |
| 1   | E     | 407 | DG   | C4'-C3'-O3' | 5.87  | 124.36      | 109.70   |
| 1   | E     | 417 | DA   | N3-C4-N9    | -5.87 | 122.71      | 127.40   |
| 1   | H     | 715 | DA   | O5'-C5'-C4' | 5.87  | 125.67      | 111.00   |
| 1   | E     | 416 | DC   | C5'-C4'-O4' | 5.86  | 120.42      | 109.30   |
| 1   | H     | 706 | DT   | C4'-C3'-C2' | -5.86 | 97.83       | 103.10   |
| 1   | E     | 403 | DT   | C6-C5-C7    | -5.85 | 119.39      | 122.90   |
| 1   | E     | 401 | DA   | C1'-O4'-C4' | 5.85  | 115.95      | 110.10   |
| 1   | F     | 509 | DG   | C4'-C3'-O3' | 5.84  | 124.29      | 109.70   |
| 1   | F     | 516 | DC   | P-O3'-C3'   | -5.83 | 112.71      | 119.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 604 | DT   | O5'-C5'-C4' | 5.82  | 125.55      | 111.00   |
| 1   | G     | 613 | DT   | N1-C1'-C2'  | 5.82  | 123.66      | 112.60   |
| 1   | F     | 519 | DT   | C6-N1-C2    | -5.81 | 118.39      | 121.30   |
| 1   | F     | 513 | DT   | N1-C1'-C2'  | 5.81  | 123.63      | 112.60   |
| 1   | E     | 407 | DG   | C5'-C4'-C3' | 5.80  | 124.54      | 114.10   |
| 1   | E     | 413 | DT   | C4-C5-C6    | 5.80  | 121.48      | 118.00   |
| 1   | F     | 505 | DG   | C1'-O4'-C4' | -5.79 | 104.31      | 110.10   |
| 1   | G     | 617 | DA   | O4'-C4'-C3' | 5.79  | 109.47      | 106.00   |
| 1   | G     | 608 | DA   | C2-N3-C4    | -5.78 | 107.71      | 110.60   |
| 1   | F     | 520 | DT   | N3-C4-C5    | -5.77 | 111.74      | 115.20   |
| 1   | H     | 700 | DG   | C4'-C3'-O3' | 5.75  | 124.09      | 109.70   |
| 1   | F     | 508 | DA   | O4'-C1'-N9  | 5.75  | 112.03      | 108.00   |
| 1   | H     | 719 | DT   | O5'-P-OP1   | -5.75 | 100.52      | 105.70   |
| 1   | E     | 406 | DT   | O4'-C4'-C3' | 5.75  | 109.45      | 106.00   |
| 1   | H     | 710 | DC   | C4'-C3'-C2' | -5.75 | 97.92       | 103.10   |
| 1   | G     | 617 | DA   | N7-C8-N9    | 5.75  | 116.67      | 113.80   |
| 1   | F     | 517 | DA   | C5'-C4'-C3' | 5.75  | 124.44      | 114.10   |
| 1   | E     | 413 | DT   | C6-C5-C7    | -5.74 | 119.45      | 122.90   |
| 1   | H     | 701 | DA   | N1-C6-N6    | -5.74 | 115.16      | 118.60   |
| 1   | H     | 704 | DT   | N3-C2-O2    | -5.74 | 118.86      | 122.30   |
| 1   | H     | 719 | DT   | C6-C5-C7    | -5.74 | 119.46      | 122.90   |
| 1   | E     | 406 | DT   | C4-C5-C7    | -5.73 | 115.56      | 119.00   |
| 1   | F     | 513 | DT   | N3-C4-O4    | 5.73  | 123.34      | 119.90   |
| 1   | H     | 707 | DG   | P-O3'-C3'   | 5.73  | 126.57      | 119.70   |
| 1   | H     | 720 | DT   | C3'-C2'-C1' | 5.72  | 109.36      | 102.50   |
| 1   | H     | 708 | DA   | P-O3'-C3'   | 5.72  | 126.56      | 119.70   |
| 1   | E     | 415 | DA   | C4-C5-C6    | 5.71  | 119.86      | 117.00   |
| 1   | F     | 502 | DA   | C5'-C4'-C3' | 5.69  | 124.33      | 114.10   |
| 1   | G     | 611 | DG   | N3-C4-C5    | -5.68 | 125.76      | 128.60   |
| 1   | E     | 412 | DC   | N1-C2-O2    | 5.68  | 122.31      | 118.90   |
| 1   | H     | 720 | DT   | C5-C6-N1    | -5.67 | 120.30      | 123.70   |
| 1   | G     | 619 | DT   | N3-C4-C5    | -5.67 | 111.80      | 115.20   |
| 1   | F     | 509 | DG   | C5'-C4'-O4' | -5.66 | 98.54       | 109.30   |
| 1   | F     | 503 | DT   | C4-C5-C6    | 5.66  | 121.40      | 118.00   |
| 1   | F     | 518 | DA   | O5'-C5'-C4' | 5.66  | 125.15      | 111.00   |
| 1   | E     | 411 | DG   | C4'-C3'-C2' | -5.66 | 98.01       | 103.10   |
| 1   | F     | 507 | DG   | C3'-C2'-C1' | 5.66  | 109.29      | 102.50   |
| 1   | F     | 508 | DA   | C4'-C3'-O3' | 5.65  | 123.83      | 109.70   |
| 1   | E     | 407 | DG   | O5'-P-OP2   | -5.65 | 100.62      | 105.70   |
| 1   | G     | 606 | DT   | N1-C2-N3    | 5.65  | 117.99      | 114.60   |
| 1   | H     | 705 | DG   | P-O3'-C3'   | -5.65 | 112.92      | 119.70   |
| 1   | H     | 705 | DG   | C4'-C3'-C2' | -5.65 | 98.02       | 103.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | F     | 520 | DT   | N1-C2-N3    | 5.64  | 117.99      | 114.60   |
| 1   | H     | 709 | DG   | P-O5'-C5'   | 5.64  | 129.93      | 120.90   |
| 1   | E     | 414 | DC   | O4'-C1'-N1  | 5.64  | 111.95      | 108.00   |
| 1   | E     | 419 | DT   | C2-N3-C4    | -5.64 | 123.82      | 127.20   |
| 1   | H     | 708 | DA   | N7-C8-N9    | 5.63  | 116.62      | 113.80   |
| 1   | F     | 505 | DG   | C8-N9-C1'   | 5.63  | 134.32      | 127.00   |
| 1   | H     | 718 | DA   | N9-C1'-C2'  | 5.63  | 123.29      | 112.60   |
| 1   | E     | 419 | DT   | O4'-C1'-C2' | -5.62 | 101.40      | 105.90   |
| 1   | E     | 403 | DT   | N1-C2-N3    | 5.62  | 117.97      | 114.60   |
| 1   | F     | 508 | DA   | N1-C6-N6    | 5.62  | 121.97      | 118.60   |
| 1   | G     | 618 | DA   | C3'-C2'-C1' | 5.62  | 109.24      | 102.50   |
| 1   | H     | 711 | DG   | C6-C5-N7    | -5.61 | 127.04      | 130.40   |
| 1   | E     | 404 | DT   | C5-C6-N1    | -5.60 | 120.34      | 123.70   |
| 1   | F     | 517 | DA   | C5-N7-C8    | -5.60 | 101.10      | 103.90   |
| 1   | F     | 503 | DT   | C3'-C2'-C1' | 5.60  | 109.22      | 102.50   |
| 1   | F     | 503 | DT   | O4'-C1'-N1  | 5.60  | 111.92      | 108.00   |
| 1   | H     | 720 | DT   | C4-C5-C7    | -5.60 | 115.64      | 119.00   |
| 1   | F     | 502 | DA   | C5-C6-N1    | -5.59 | 114.90      | 117.70   |
| 1   | E     | 419 | DT   | N1-C2-N3    | 5.57  | 117.94      | 114.60   |
| 1   | H     | 703 | DT   | C4-C5-C6    | 5.57  | 121.34      | 118.00   |
| 1   | G     | 603 | DT   | C6-N1-C2    | -5.57 | 118.52      | 121.30   |
| 1   | E     | 407 | DG   | C4-C5-C6    | 5.56  | 122.14      | 118.80   |
| 1   | G     | 604 | DT   | C4-C5-C6    | 5.56  | 121.33      | 118.00   |
| 1   | G     | 619 | DT   | O4'-C1'-N1  | 5.56  | 111.89      | 108.00   |
| 1   | G     | 604 | DT   | C2'-C3'-O3' | -5.55 | 94.27       | 112.60   |
| 1   | E     | 416 | DC   | C3'-C2'-C1' | 5.55  | 109.16      | 102.50   |
| 1   | G     | 604 | DT   | OP1-P-OP2   | 5.54  | 127.92      | 119.60   |
| 1   | G     | 611 | DG   | N3-C4-N9    | 5.54  | 129.33      | 126.00   |
| 1   | F     | 510 | DC   | C3'-C2'-C1' | 5.54  | 109.15      | 102.50   |
| 1   | E     | 405 | DG   | N1-C2-N3    | -5.54 | 120.58      | 123.90   |
| 1   | F     | 516 | DC   | O3'-P-O5'   | 5.53  | 114.51      | 104.00   |
| 1   | G     | 615 | DA   | C2-N3-C4    | -5.53 | 107.83      | 110.60   |
| 1   | H     | 720 | DT   | N1-C2-N3    | 5.53  | 117.92      | 114.60   |
| 1   | H     | 720 | DT   | C1'-O4'-C4' | 5.52  | 115.62      | 110.10   |
| 1   | G     | 610 | DC   | C4'-C3'-C2' | -5.52 | 98.13       | 103.10   |
| 1   | G     | 612 | DC   | N3-C2-O2    | -5.52 | 118.04      | 121.90   |
| 1   | G     | 615 | DA   | P-O5'-C5'   | 5.52  | 129.73      | 120.90   |
| 1   | F     | 511 | DG   | N3-C4-N9    | 5.50  | 129.30      | 126.00   |
| 1   | G     | 602 | DA   | P-O3'-C3'   | 5.50  | 126.30      | 119.70   |
| 1   | F     | 507 | DG   | C4'-C3'-O3' | 5.50  | 123.45      | 109.70   |
| 1   | G     | 615 | DA   | N3-C4-N9    | -5.50 | 123.00      | 127.40   |
| 1   | G     | 617 | DA   | C5-N7-C8    | -5.49 | 101.16      | 103.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 605 | DG   | N9-C1'-C2'  | 5.49  | 123.03      | 112.60   |
| 1   | H     | 708 | DA   | C2-N3-C4    | -5.49 | 107.86      | 110.60   |
| 1   | G     | 605 | DG   | C4'-C3'-O3' | 5.48  | 123.40      | 109.70   |
| 1   | H     | 701 | DA   | C4-N9-C1'   | 5.47  | 136.14      | 126.30   |
| 1   | G     | 612 | DC   | C2-N3-C4    | 5.45  | 122.63      | 119.90   |
| 1   | F     | 519 | DT   | C4'-C3'-O3' | 5.45  | 123.32      | 109.70   |
| 1   | G     | 601 | DA   | C4-C5-C6    | 5.45  | 119.72      | 117.00   |
| 1   | G     | 604 | DT   | C4-C5-C7    | -5.45 | 115.73      | 119.00   |
| 1   | G     | 620 | DT   | O5'-C5'-C4' | 5.44  | 124.61      | 111.00   |
| 1   | H     | 719 | DT   | N3-C4-C5    | -5.44 | 111.94      | 115.20   |
| 1   | F     | 512 | DC   | C6-N1-C1'   | -5.44 | 114.27      | 120.80   |
| 1   | G     | 602 | DA   | N9-C4-C5    | -5.43 | 103.63      | 105.80   |
| 1   | G     | 613 | DT   | C3'-C2'-C1' | 5.43  | 109.01      | 102.50   |
| 1   | G     | 612 | DC   | C1'-O4'-C4' | -5.42 | 104.68      | 110.10   |
| 1   | F     | 520 | DT   | N3-C2-O2    | -5.41 | 119.05      | 122.30   |
| 1   | F     | 501 | DA   | C5'-C4'-C3' | 5.41  | 123.84      | 114.10   |
| 1   | F     | 511 | DG   | N3-C4-C5    | -5.41 | 125.90      | 128.60   |
| 1   | E     | 418 | DA   | P-O3'-C3'   | 5.40  | 126.18      | 119.70   |
| 1   | H     | 710 | DC   | N3-C4-C5    | -5.40 | 119.74      | 121.90   |
| 1   | E     | 410 | DC   | O4'-C1'-C2' | -5.40 | 101.58      | 105.90   |
| 1   | G     | 616 | DC   | O5'-P-OP2   | -5.38 | 100.85      | 105.70   |
| 1   | E     | 406 | DT   | N3-C2-O2    | -5.38 | 119.07      | 122.30   |
| 1   | F     | 508 | DA   | C8-N9-C4    | -5.38 | 103.65      | 105.80   |
| 1   | E     | 401 | DA   | N3-C4-C5    | -5.37 | 123.04      | 126.80   |
| 1   | G     | 620 | DT   | N3-C2-O2    | -5.37 | 119.08      | 122.30   |
| 1   | E     | 404 | DT   | C4'-C3'-O3' | 5.35  | 123.08      | 109.70   |
| 1   | G     | 602 | DA   | C2'-C3'-O3' | -5.32 | 95.04       | 112.60   |
| 1   | H     | 710 | DC   | C3'-C2'-C1' | 5.32  | 108.88      | 102.50   |
| 1   | H     | 700 | DG   | C5-C6-N1    | 5.32  | 114.16      | 111.50   |
| 1   | G     | 608 | DA   | N9-C4-C5    | 5.30  | 107.92      | 105.80   |
| 1   | E     | 419 | DT   | C5-C6-N1    | -5.30 | 120.52      | 123.70   |
| 1   | E     | 407 | DG   | C8-N9-C1'   | -5.30 | 120.11      | 127.00   |
| 1   | F     | 514 | DC   | O5'-C5'-C4' | 5.30  | 124.25      | 111.00   |
| 1   | E     | 414 | DC   | N3-C2-O2    | -5.29 | 118.19      | 121.90   |
| 1   | G     | 617 | DA   | C8-N9-C4    | -5.27 | 103.69      | 105.80   |
| 1   | F     | 517 | DA   | C4'-C3'-C2' | -5.26 | 98.37       | 103.10   |
| 1   | F     | 518 | DA   | N3-C4-C5    | -5.23 | 123.14      | 126.80   |
| 1   | G     | 616 | DC   | C2-N1-C1'   | -5.23 | 113.05      | 118.80   |
| 1   | G     | 614 | DC   | P-O3'-C3'   | -5.23 | 113.42      | 119.70   |
| 1   | H     | 707 | DG   | C6-C5-N7    | -5.23 | 127.26      | 130.40   |
| 1   | G     | 616 | DC   | C4'-C3'-O3' | 5.21  | 122.74      | 109.70   |
| 1   | E     | 401 | DA   | N3-C4-N9    | 5.21  | 131.57      | 127.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | E     | 405 | DG   | C4'-C3'-O3' | 5.20  | 122.71      | 112.30   |
| 1   | F     | 516 | DC   | C5-C6-N1    | 5.20  | 123.60      | 121.00   |
| 1   | F     | 517 | DA   | O3'-P-O5'   | 5.20  | 113.88      | 104.00   |
| 1   | E     | 400 | DG   | C3'-C2'-C1' | 5.20  | 108.74      | 102.50   |
| 1   | G     | 615 | DA   | C5-C6-N1    | -5.20 | 115.10      | 117.70   |
| 1   | E     | 406 | DT   | C3'-C2'-C1' | 5.19  | 108.73      | 102.50   |
| 1   | H     | 700 | DG   | N3-C4-C5    | -5.19 | 126.00      | 128.60   |
| 1   | H     | 712 | DC   | N1-C1'-C2'  | 5.19  | 122.46      | 112.60   |
| 1   | F     | 500 | DG   | C5-C6-O6    | 5.19  | 131.71      | 128.60   |
| 1   | G     | 602 | DA   | N7-C8-N9    | 5.18  | 116.39      | 113.80   |
| 1   | G     | 608 | DA   | C5-C6-N1    | -5.18 | 115.11      | 117.70   |
| 1   | G     | 603 | DT   | N1-C2-N3    | 5.18  | 117.71      | 114.60   |
| 1   | E     | 409 | DG   | P-O5'-C5'   | 5.17  | 129.18      | 120.90   |
| 1   | H     | 710 | DC   | C6-N1-C2    | -5.17 | 118.23      | 120.30   |
| 1   | H     | 711 | DG   | O4'-C1'-N9  | 5.17  | 111.62      | 108.00   |
| 1   | G     | 600 | DG   | N9-C1'-C2'  | 5.17  | 122.42      | 112.60   |
| 1   | G     | 605 | DG   | N9-C4-C5    | 5.16  | 107.47      | 105.40   |
| 1   | F     | 520 | DT   | C2-N1-C1'   | -5.16 | 109.95      | 118.20   |
| 1   | G     | 608 | DA   | C4'-C3'-O3' | 5.15  | 122.60      | 112.30   |
| 1   | H     | 717 | DA   | C5'-C4'-C3' | 5.15  | 123.37      | 114.10   |
| 1   | E     | 402 | DA   | C4'-C3'-C2' | -5.15 | 98.47       | 103.10   |
| 1   | G     | 609 | DG   | N7-C8-N9    | 5.14  | 115.67      | 113.10   |
| 1   | H     | 701 | DA   | C5-C6-N1    | -5.14 | 115.13      | 117.70   |
| 1   | E     | 411 | DG   | N7-C8-N9    | 5.13  | 115.67      | 113.10   |
| 1   | H     | 701 | DA   | O5'-C5'-C4' | 5.12  | 123.81      | 111.00   |
| 1   | H     | 720 | DT   | C6-C5-C7    | -5.12 | 119.83      | 122.90   |
| 1   | F     | 505 | DG   | C5-C6-N1    | -5.09 | 108.95      | 111.50   |
| 1   | E     | 402 | DA   | C4-N9-C1'   | 5.09  | 135.46      | 126.30   |
| 1   | H     | 719 | DT   | N3-C2-O2    | -5.08 | 119.25      | 122.30   |
| 1   | G     | 608 | DA   | O4'-C1'-C2' | -5.08 | 101.84      | 105.90   |
| 1   | F     | 503 | DT   | C4'-C3'-O3' | 5.07  | 122.44      | 112.30   |
| 1   | F     | 505 | DG   | C6-N1-C2    | 5.07  | 128.14      | 125.10   |
| 1   | G     | 613 | DT   | O4'-C1'-N1  | 5.05  | 111.54      | 108.00   |
| 1   | E     | 416 | DC   | N3-C2-O2    | -5.05 | 118.37      | 121.90   |
| 1   | G     | 603 | DT   | C4-C5-C6    | 5.04  | 121.02      | 118.00   |
| 1   | G     | 620 | DT   | N1-C2-N3    | 5.04  | 117.62      | 114.60   |
| 1   | H     | 714 | DC   | C4'-C3'-C2' | -5.04 | 98.56       | 103.10   |
| 1   | G     | 612 | DC   | N3-C4-C5    | -5.04 | 119.89      | 121.90   |
| 1   | E     | 402 | DA   | C1'-O4'-C4' | 5.02  | 115.12      | 110.10   |
| 1   | F     | 513 | DT   | P-O3'-C3'   | 5.02  | 125.72      | 119.70   |
| 1   | E     | 414 | DC   | N3-C4-C5    | -5.02 | 119.89      | 121.90   |
| 1   | E     | 404 | DT   | N3-C4-C5    | -5.01 | 112.19      | 115.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 613 | DT   | O4'-C1'-C2' | -5.01 | 101.89      | 105.90   |
| 1   | H     | 707 | DG   | N3-C4-C5    | -5.01 | 126.09      | 128.60   |
| 1   | H     | 709 | DG   | C4'-C3'-O3' | 5.01  | 122.33      | 112.30   |
| 1   | E     | 410 | DC   | C4'-C3'-O3' | 5.01  | 122.33      | 112.30   |
| 1   | E     | 404 | DT   | C6-N1-C2    | -5.01 | 118.80      | 121.30   |
| 1   | G     | 617 | DA   | N9-C4-C5    | 5.00  | 107.80      | 105.80   |
| 1   | E     | 418 | DA   | P-O5'-C5'   | 5.00  | 128.90      | 120.90   |

All (10) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | E     | 402 | DA   | C3'  |
| 1   | E     | 405 | DG   | C1'  |
| 1   | E     | 409 | DG   | C1'  |
| 1   | F     | 520 | DT   | C4'  |
| 1   | G     | 600 | DG   | C1'  |
| 1   | G     | 601 | DA   | C1'  |
| 1   | G     | 620 | DT   | C1'  |
| 1   | H     | 702 | DA   | C1'  |
| 1   | H     | 718 | DA   | C3'  |
| 1   | H     | 719 | DT   | C4'  |

All (66) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | E     | 400 | DG   | Sidechain |
| 1   | E     | 401 | DA   | Sidechain |
| 1   | E     | 402 | DA   | Sidechain |
| 1   | E     | 403 | DT   | Sidechain |
| 1   | E     | 404 | DT   | Sidechain |
| 1   | E     | 405 | DG   | Sidechain |
| 1   | E     | 406 | DT   | Sidechain |
| 1   | E     | 407 | DG   | Sidechain |
| 1   | E     | 408 | DA   | Sidechain |
| 1   | E     | 409 | DG   | Sidechain |
| 1   | E     | 410 | DC   | Sidechain |
| 1   | E     | 411 | DG   | Sidechain |
| 1   | E     | 412 | DC   | Sidechain |
| 1   | E     | 413 | DT   | Sidechain |
| 1   | E     | 415 | DA   | Sidechain |
| 1   | E     | 416 | DC   | Sidechain |
| 1   | E     | 418 | DA   | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | E     | 420 | DT   | Sidechain |
| 1   | F     | 500 | DG   | Sidechain |
| 1   | F     | 501 | DA   | Sidechain |
| 1   | F     | 503 | DT   | Sidechain |
| 1   | F     | 504 | DT   | Sidechain |
| 1   | F     | 505 | DG   | Sidechain |
| 1   | F     | 508 | DA   | Sidechain |
| 1   | F     | 509 | DG   | Sidechain |
| 1   | F     | 510 | DC   | Sidechain |
| 1   | F     | 512 | DC   | Sidechain |
| 1   | F     | 513 | DT   | Sidechain |
| 1   | F     | 515 | DA   | Sidechain |
| 1   | F     | 516 | DC   | Sidechain |
| 1   | F     | 517 | DA   | Sidechain |
| 1   | F     | 519 | DT   | Sidechain |
| 1   | F     | 520 | DT   | Sidechain |
| 1   | G     | 600 | DG   | Sidechain |
| 1   | G     | 601 | DA   | Sidechain |
| 1   | G     | 602 | DA   | Sidechain |
| 1   | G     | 604 | DT   | Sidechain |
| 1   | G     | 606 | DT   | Sidechain |
| 1   | G     | 608 | DA   | Sidechain |
| 1   | G     | 609 | DG   | Sidechain |
| 1   | G     | 610 | DC   | Sidechain |
| 1   | G     | 611 | DG   | Sidechain |
| 1   | G     | 612 | DC   | Sidechain |
| 1   | G     | 613 | DT   | Sidechain |
| 1   | G     | 614 | DC   | Sidechain |
| 1   | G     | 615 | DA   | Sidechain |
| 1   | G     | 616 | DC   | Sidechain |
| 1   | G     | 619 | DT   | Sidechain |
| 1   | G     | 620 | DT   | Sidechain |
| 1   | H     | 700 | DG   | Sidechain |
| 1   | H     | 701 | DA   | Sidechain |
| 1   | H     | 702 | DA   | Sidechain |
| 1   | H     | 704 | DT   | Sidechain |
| 1   | H     | 706 | DT   | Sidechain |
| 1   | H     | 707 | DG   | Sidechain |
| 1   | H     | 708 | DA   | Sidechain |
| 1   | H     | 709 | DG   | Sidechain |
| 1   | H     | 710 | DC   | Sidechain |
| 1   | H     | 712 | DC   | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | H     | 713 | DT   | Sidechain |
| 1   | H     | 714 | DC   | Sidechain |
| 1   | H     | 715 | DA   | Sidechain |
| 1   | H     | 716 | DC   | Sidechain |
| 1   | H     | 717 | DA   | Sidechain |
| 1   | H     | 718 | DA   | Sidechain |
| 1   | H     | 719 | DT   | Sidechain |

## 5.2 Too-close contacts [i](#)

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   | E     | 429   | 0        | 239      | 40      | 0            |
| 1   | F     | 429   | 0        | 239      | 37      | 0            |
| 1   | G     | 429   | 0        | 239      | 42      | 6            |
| 1   | H     | 429   | 0        | 239      | 38      | 0            |
| 2   | A     | 357   | 0        | 0        | 0       | 0            |
| 2   | B     | 357   | 0        | 0        | 0       | 0            |
| 2   | C     | 357   | 0        | 0        | 0       | 0            |
| 2   | D     | 357   | 0        | 0        | 1       | 6            |
| All | All   | 3144  | 0        | 956      | 139     | 6            |

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 34.

All (139) 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:F:501:DA:H2'  | 1:F:502:DA:H1' | 1.40                     | 1.01              |
| 1:G:601:DA:H3'  | 1:G:602:DA:N7  | 1.94                     | 0.82              |
| 1:H:701:DA:H3'  | 1:H:702:DA:C8  | 2.16                     | 0.80              |
| 1:F:511:DG:N3   | 1:F:512:DC:H1' | 1.98                     | 0.78              |
| 1:E:405:DG:H2'' | 1:E:406:DT:H71 | 1.66                     | 0.77              |
| 1:E:416:DC:H42  | 1:F:505:DG:H1  | 1.33                     | 0.76              |
| 1:G:611:DG:H2'' | 1:G:612:DC:C6  | 2.22                     | 0.74              |
| 1:G:611:DG:N3   | 1:G:612:DC:H1' | 2.01                     | 0.74              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:712:DC:H2'  | 1:H:713:DT:C6   | 2.24                     | 0.73              |
| 1:H:711:DG:N3   | 1:H:712:DC:H1'  | 2.04                     | 0.72              |
| 1:G:617:DA:H2'' | 1:G:618:DA:N7   | 2.04                     | 0.72              |
| 1:F:512:DC:H2'  | 1:F:513:DT:C6   | 2.24                     | 0.72              |
| 1:H:709:DG:H2'' | 1:H:710:DC:C6   | 2.25                     | 0.71              |
| 1:G:619:DT:H3   | 1:H:702:DA:H2   | 1.40                     | 0.70              |
| 1:E:410:DC:H3'  | 1:E:411:DG:C8   | 2.27                     | 0.69              |
| 1:E:408:DA:H5'' | 1:E:408:DA:H8   | 1.57                     | 0.69              |
| 1:H:708:DA:H8   | 1:H:708:DA:H5'' | 1.57                     | 0.69              |
| 1:G:602:DA:H2'' | 1:G:603:DT:OP2  | 1.94                     | 0.68              |
| 1:F:518:DA:H2'' | 1:F:519:DT:H4'  | 1.75                     | 0.68              |
| 1:G:603:DT:H2'' | 1:G:604:DT:C6   | 2.28                     | 0.68              |
| 1:E:401:DA:H2'' | 1:E:402:DA:C8   | 2.27                     | 0.67              |
| 1:E:403:DT:OP2  | 1:E:403:DT:H6   | 1.77                     | 0.67              |
| 1:E:419:DT:H3'  | 1:E:420:DT:H3'  | 1.77                     | 0.67              |
| 1:E:402:DA:C8   | 1:E:402:DA:OP2  | 2.49                     | 0.66              |
| 1:E:414:DC:H2'  | 1:E:415:DA:C8   | 2.31                     | 0.66              |
| 1:G:604:DT:H2'  | 1:G:604:DT:OP1  | 1.96                     | 0.66              |
| 1:F:506:DT:H2'' | 1:F:507:DG:H5'  | 1.78                     | 0.66              |
| 1:H:701:DA:H2'  | 1:H:702:DA:H2'' | 1.76                     | 0.65              |
| 1:H:704:DT:H2'  | 1:H:704:DT:OP2  | 1.97                     | 0.65              |
| 1:F:519:DT:H2'  | 1:F:520:DT:H4'  | 1.79                     | 0.65              |
| 1:G:611:DG:H2'' | 1:G:612:DC:H6   | 1.62                     | 0.64              |
| 1:E:414:DC:H6   | 1:E:414:DC:O5'  | 1.82                     | 0.63              |
| 1:H:715:DA:H2'' | 1:H:716:DC:C5   | 2.34                     | 0.63              |
| 1:H:709:DG:H2'' | 1:H:710:DC:C5   | 2.34                     | 0.63              |
| 1:E:401:DA:H2'' | 1:E:402:DA:N9   | 2.13                     | 0.62              |
| 1:E:415:DA:H2'' | 1:E:416:DC:H6   | 1.64                     | 0.62              |
| 1:E:402:DA:H8   | 1:E:402:DA:OP2  | 1.83                     | 0.62              |
| 1:G:618:DA:C2   | 1:G:619:DT:H1'  | 2.35                     | 0.62              |
| 1:H:704:DT:H1'  | 1:H:705:DG:OP2  | 2.00                     | 0.62              |
| 1:H:718:DA:H2'  | 1:H:719:DT:OP2  | 1.99                     | 0.62              |
| 1:H:708:DA:C8   | 1:H:708:DA:H5'' | 2.33                     | 0.61              |
| 1:E:403:DT:H2'' | 1:E:404:DT:C6   | 2.36                     | 0.61              |
| 1:F:513:DT:H2'  | 1:F:514:DC:O4'  | 2.01                     | 0.61              |
| 1:G:600:DG:H4'  | 1:G:601:DA:H2'' | 1.82                     | 0.61              |
| 1:E:419:DT:O4   | 1:F:502:DA:N1   | 2.33                     | 0.60              |
| 1:G:617:DA:H2'' | 1:G:618:DA:C8   | 2.36                     | 0.60              |
| 1:H:701:DA:H3'  | 1:H:702:DA:N7   | 2.15                     | 0.60              |
| 1:G:605:DG:H3'  | 1:G:606:DT:C6   | 2.37                     | 0.60              |
| 1:G:605:DG:H2'  | 1:G:605:DG:N3   | 2.16                     | 0.59              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:609:DG:H2'  | 1:G:610:DC:C6   | 2.37                     | 0.59              |
| 1:H:704:DT:H6   | 1:H:704:DT:OP2  | 1.85                     | 0.59              |
| 1:F:514:DC:H2'  | 1:F:515:DA:C8   | 2.38                     | 0.59              |
| 1:E:400:DG:H2'  | 1:E:401:DA:H8   | 1.66                     | 0.58              |
| 1:G:607:DG:H2'' | 1:G:608:DA:C8   | 2.37                     | 0.58              |
| 1:E:402:DA:H2'  | 1:E:403:DT:C5   | 2.39                     | 0.57              |
| 1:E:403:DT:H2'' | 1:E:404:DT:C5   | 2.39                     | 0.57              |
| 1:E:408:DA:H2   | 1:F:513:DT:H3   | 1.52                     | 0.57              |
| 1:H:711:DG:C2   | 1:H:712:DC:H1'  | 2.39                     | 0.57              |
| 1:E:406:DT:H2'' | 1:E:407:DG:C8   | 2.39                     | 0.57              |
| 1:F:518:DA:N3   | 1:F:519:DT:H1'  | 2.19                     | 0.57              |
| 1:F:502:DA:C6   | 1:F:503:DT:H1'  | 2.39                     | 0.56              |
| 1:E:405:DG:O6   | 1:F:516:DC:N4   | 2.35                     | 0.56              |
| 1:F:515:DA:H2'' | 1:F:516:DC:C5   | 2.41                     | 0.56              |
| 1:G:603:DT:H2'' | 1:G:604:DT:H6   | 1.71                     | 0.56              |
| 1:F:502:DA:C5   | 1:F:503:DT:H1'  | 2.41                     | 0.55              |
| 1:G:619:DT:H2'  | 1:H:701:DA:N1   | 2.21                     | 0.55              |
| 1:E:407:DG:H2'  | 1:E:408:DA:O4'  | 2.06                     | 0.55              |
| 1:F:513:DT:H3'  | 1:F:514:DC:C6   | 2.42                     | 0.55              |
| 1:E:418:DA:N1   | 1:F:503:DT:O2   | 2.39                     | 0.55              |
| 1:G:617:DA:H2'  | 1:G:617:DA:O5'  | 2.06                     | 0.55              |
| 1:H:716:DC:H2'' | 1:H:717:DA:C8   | 2.42                     | 0.55              |
| 1:G:602:DA:C8   | 1:G:602:DA:O5'  | 2.60                     | 0.54              |
| 1:F:513:DT:H3'  | 1:F:514:DC:H6   | 1.72                     | 0.54              |
| 1:G:604:DT:OP1  | 1:G:604:DT:H6   | 1.91                     | 0.53              |
| 1:H:715:DA:H2'  | 1:H:715:DA:OP2  | 2.08                     | 0.53              |
| 1:H:700:DG:H2'' | 1:H:701:DA:H5'' | 1.89                     | 0.53              |
| 1:F:511:DG:C2   | 1:F:512:DC:H1'  | 2.43                     | 0.52              |
| 1:G:608:DA:N1   | 1:H:713:DT:O4   | 2.42                     | 0.52              |
| 1:E:417:DA:H2'  | 1:E:417:DA:OP2  | 2.09                     | 0.52              |
| 1:E:416:DC:N4   | 1:F:505:DG:H1   | 2.04                     | 0.52              |
| 1:H:703:DT:H3'  | 2:D:30:VAL:CA   | 2.40                     | 0.52              |
| 1:G:619:DT:N3   | 1:H:702:DA:H2   | 2.08                     | 0.52              |
| 1:E:419:DT:P    | 1:E:419:DT:H73  | 2.51                     | 0.51              |
| 1:F:506:DT:C2'  | 1:F:507:DG:H5'  | 2.39                     | 0.51              |
| 1:E:406:DT:H6   | 1:E:406:DT:OP2  | 1.94                     | 0.50              |
| 1:F:501:DA:H3'  | 1:F:501:DA:H8   | 1.76                     | 0.50              |
| 1:F:501:DA:C8   | 1:F:501:DA:H3'  | 2.46                     | 0.50              |
| 1:H:700:DG:N2   | 1:H:702:DA:N1   | 2.60                     | 0.50              |
| 1:F:504:DT:OP2  | 1:F:504:DT:H6   | 1.95                     | 0.50              |
| 1:G:600:DG:H4'  | 1:G:601:DA:C2'  | 2.41                     | 0.50              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:604:DT:O4   | 1:H:717:DA:N1   | 2.45                     | 0.50              |
| 1:F:519:DT:H2'  | 1:F:520:DT:C4'  | 2.41                     | 0.50              |
| 1:E:419:DT:H3'  | 1:E:420:DT:C3'  | 2.41                     | 0.49              |
| 1:F:500:DG:H2'' | 1:F:501:DA:C8   | 2.47                     | 0.49              |
| 1:F:518:DA:C2   | 1:F:519:DT:H1'  | 2.47                     | 0.49              |
| 1:H:719:DT:H6   | 1:H:719:DT:OP1  | 1.96                     | 0.49              |
| 1:E:413:DT:H3'  | 1:E:414:DC:C5   | 2.48                     | 0.49              |
| 1:F:508:DA:H1'  | 1:F:509:DG:H5'  | 1.95                     | 0.48              |
| 1:G:616:DC:H2'' | 1:G:617:DA:C8   | 2.49                     | 0.48              |
| 1:H:703:DT:H2'' | 1:H:704:DT:OP2  | 2.13                     | 0.47              |
| 1:F:515:DA:H2'' | 1:F:516:DC:H5   | 1.80                     | 0.47              |
| 1:G:604:DT:O4'  | 1:G:604:DT:OP2  | 2.32                     | 0.47              |
| 1:H:704:DT:OP2  | 1:H:704:DT:C6   | 2.66                     | 0.47              |
| 1:G:602:DA:C2   | 1:H:720:DT:O4'  | 2.68                     | 0.47              |
| 1:G:613:DT:H3   | 1:H:708:DA:H2   | 1.61                     | 0.47              |
| 1:F:518:DA:H2'' | 1:F:519:DT:C4'  | 2.44                     | 0.46              |
| 1:G:601:DA:H3'  | 1:G:602:DA:C5   | 2.50                     | 0.46              |
| 1:E:402:DA:H3'  | 1:E:403:DT:O4'  | 2.14                     | 0.46              |
| 1:F:501:DA:C3'  | 1:F:501:DA:C8   | 2.99                     | 0.46              |
| 1:H:708:DA:H2'  | 1:H:709:DG:C8   | 2.51                     | 0.46              |
| 1:H:712:DC:H2'  | 1:H:713:DT:C5   | 2.51                     | 0.46              |
| 1:E:419:DT:OP2  | 1:E:419:DT:H73  | 2.17                     | 0.45              |
| 1:E:404:DT:OP2  | 1:E:404:DT:H6   | 1.99                     | 0.45              |
| 1:E:403:DT:OP2  | 1:E:403:DT:C6   | 2.65                     | 0.45              |
| 1:E:415:DA:H2'' | 1:E:416:DC:C6   | 2.49                     | 0.45              |
| 1:G:618:DA:N1   | 1:H:703:DT:O4   | 2.50                     | 0.45              |
| 1:F:516:DC:H3'  | 1:F:516:DC:OP2  | 2.17                     | 0.44              |
| 1:G:615:DA:OP2  | 1:G:615:DA:H8   | 2.00                     | 0.44              |
| 1:H:713:DT:C6   | 1:H:713:DT:H5'' | 2.53                     | 0.44              |
| 1:F:502:DA:N3   | 1:F:502:DA:H2'  | 2.33                     | 0.44              |
| 1:G:606:DT:C2'  | 1:G:607:DG:H5'  | 2.48                     | 0.44              |
| 1:G:613:DT:H2'  | 1:G:614:DC:C6   | 2.53                     | 0.44              |
| 1:E:417:DA:N1   | 1:F:504:DT:O4   | 2.51                     | 0.44              |
| 1:G:601:DA:H3'  | 1:G:602:DA:C8   | 2.52                     | 0.43              |
| 1:E:412:DC:H5'' | 1:E:413:DT:OP2  | 2.18                     | 0.43              |
| 1:H:712:DC:H5'' | 1:H:713:DT:OP2  | 2.19                     | 0.43              |
| 1:G:620:DT:O4   | 1:H:700:DG:C2   | 2.72                     | 0.43              |
| 1:H:714:DC:H6   | 1:H:714:DC:O5'  | 2.02                     | 0.42              |
| 1:G:603:DT:H6   | 1:G:603:DT:OP2  | 2.02                     | 0.41              |
| 1:E:402:DA:N3   | 1:F:519:DT:O4   | 2.52                     | 0.41              |
| 1:E:408:DA:H5'' | 1:E:408:DA:C8   | 2.47                     | 0.41              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:E:401:DA:H2'' | 1:E:402:DA:C1' | 2.50                     | 0.41              |
| 1:G:604:DT:O4'  | 1:G:604:DT:P   | 2.78                     | 0.41              |
| 1:G:602:DA:C8   | 1:G:602:DA:P   | 3.13                     | 0.41              |
| 1:G:612:DC:H2'  | 1:G:613:DT:C6  | 2.55                     | 0.41              |
| 1:G:618:DA:H2   | 1:H:703:DT:H3  | 1.68                     | 0.41              |
| 1:F:511:DG:H4'  | 1:F:512:DC:OP1 | 2.20                     | 0.41              |
| 1:E:408:DA:H2'  | 1:E:409:DG:N9  | 2.36                     | 0.40              |
| 1:G:608:DA:H2'' | 1:G:609:DG:C8  | 2.57                     | 0.40              |

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------------|--------------------------|-------------------|
| 1:G:600:DG:N7 | 2:D:351:ARG:CA[1_455] | 0.37                     | 1.83              |
| 1:G:600:DG:C5 | 2:D:351:ARG:CA[1_455] | 1.25                     | 0.95              |
| 1:G:600:DG:O6 | 2:D:350:ALA:CA[1_455] | 1.38                     | 0.82              |
| 1:G:600:DG:C8 | 2:D:351:ARG:CA[1_455] | 1.46                     | 0.74              |
| 1:G:600:DG:C6 | 2:D:350:ALA:CA[1_455] | 2.06                     | 0.14              |
| 1:G:600:DG:C4 | 2:D:351:ARG:CA[1_455] | 2.18                     | 0.02              |

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 carbohydrates 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 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.