



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 12:02 AM UTC

PDB ID : 6T2G / pdb\_00006t2g  
BMRB ID : 34441  
Title : NMR structure of KRAS32R G25T conformer G-quadruplex within KRAS promoter region  
Authors : Marquevielle, J.; Salgado, G.  
Deposited on : 2019-10-08

This is a Full wwPDB NMR 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

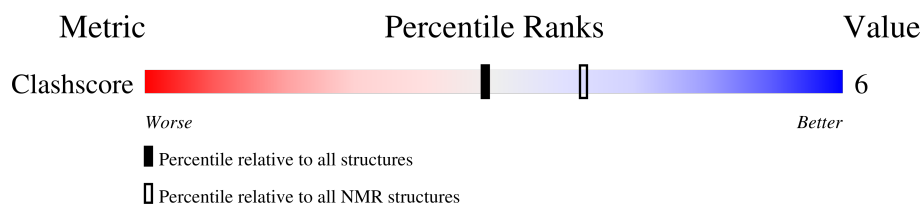
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 45%.

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) | NMR archive<br>(#Entries) |
|------------|-----------------------------|---------------------------|
| Clashscore | 229148                      | 14424                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 32     |                  |

## 2 Ensemble composition and analysis ⓘ

This entry contains 10 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1043 atoms, of which 357 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called KRAS32R G25T.

| Mol | Chain | Residues | Atoms |     |     |     |     |    | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|-------|
| 1   | A     | 32       | Total | C   | H   | N   | O   | P  | 0     |
|     |       |          | 1041  | 319 | 357 | 149 | 185 | 31 |       |

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

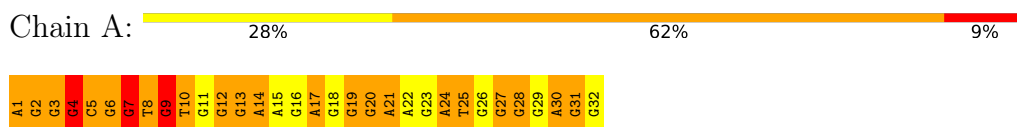
| Mol | Chain | Residues | Atoms |   |
|-----|-------|----------|-------|---|
| 2   | A     | 2        | Total | K |
|     |       |          | 2     | 2 |

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

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: KRAS32R G25T

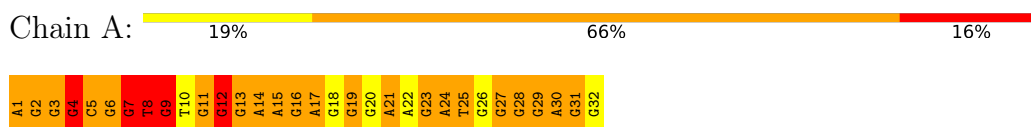


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

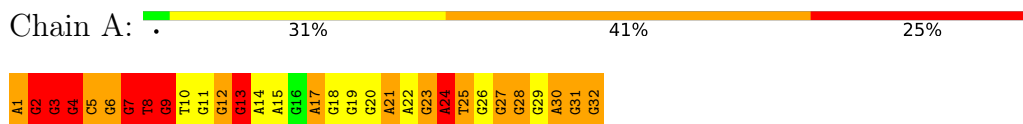
#### 4.2.1 Score per residue for model 1

- Molecule 1: KRAS32R G25T



#### 4.2.2 Score per residue for model 2

- Molecule 1: KRAS32R G25T



#### 4.2.3 Score per residue for model 3

- Molecule 1: KRAS32R G25T

Chain A:  6% 25% 53% 16%



#### 4.2.4 Score per residue for model 4

- Molecule 1: KRAS32R G25T

Chain A:  28% 47% 25%



#### 4.2.5 Score per residue for model 5

- Molecule 1: KRAS32R G25T

Chain A:  34% 44% 19%



#### 4.2.6 Score per residue for model 6

- Molecule 1: KRAS32R G25T

Chain A:  31% 56% 12%



#### 4.2.7 Score per residue for model 7

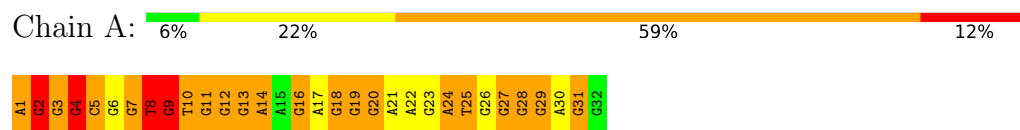
- Molecule 1: KRAS32R G25T

Chain A:  9% 22% 53% 16%



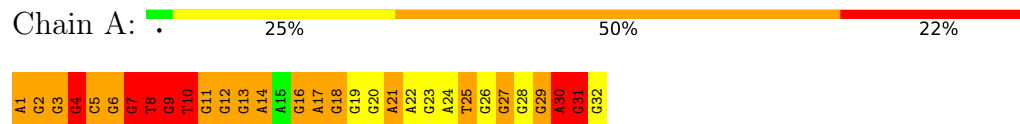
#### 4.2.8 Score per residue for model 8

- Molecule 1: KRAS32R G25T



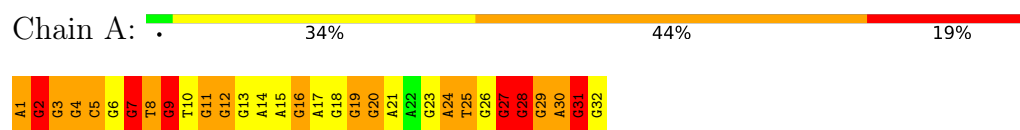
#### 4.2.9 Score per residue for model 9

- Molecule 1: KRAS32R G25T



#### 4.2.10 Score per residue for model 10

- Molecule 1: KRAS32R G25T



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 750 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| Amber         | refinement            | 12      |
| ARIA          | structure calculation |         |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 304            |
| Number of shifts mapped to atoms             | 304            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 45%            |

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:  
K

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                      | Bond angles |                        |
|-----|-------|--------------|----------------------|-------------|------------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                   |
| 1   | A     | 1.61±0.03    | 2±2/775 ( 0.3± 0.3%) | 2.35±0.03   | 50±4/1202 ( 4.2± 0.4%) |
| All | All   | 1.61         | 25/7750 ( 0.3%)      | 2.35        | 501/12020 ( 4.2%)      |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 25.7±1.8  |
| All | All   | 0         | 257       |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 4   | DG   | O3'-P   | -7.80 | 1.49        | 1.61     | 1      | 1     |
| 1   | A     | 12  | DG   | O3'-P   | 7.56  | 1.72        | 1.61     | 10     | 2     |
| 1   | A     | 8   | DT   | O3'-P   | -7.24 | 1.50        | 1.61     | 9      | 1     |
| 1   | A     | 7   | DG   | C8-N7   | -6.53 | 1.17        | 1.30     | 3      | 1     |
| 1   | A     | 28  | DG   | C3'-C2' | 6.37  | 1.65        | 1.52     | 4      | 1     |
| 1   | A     | 18  | DG   | O3'-P   | 6.16  | 1.70        | 1.61     | 9      | 1     |
| 1   | A     | 7   | DG   | O3'-P   | 6.08  | 1.70        | 1.61     | 8      | 1     |
| 1   | A     | 19  | DG   | C4'-C3' | 5.83  | 1.64        | 1.52     | 1      | 1     |
| 1   | A     | 15  | DA   | C3'-C2' | 5.80  | 1.64        | 1.52     | 1      | 1     |
| 1   | A     | 27  | DG   | O3'-P   | -5.72 | 1.52        | 1.61     | 9      | 1     |
| 1   | A     | 27  | DG   | C2-N2   | -5.72 | 1.23        | 1.34     | 9      | 1     |
| 1   | A     | 20  | DG   | O3'-P   | -5.54 | 1.52        | 1.61     | 9      | 1     |
| 1   | A     | 25  | DT   | O3'-P   | 5.51  | 1.69        | 1.61     | 3      | 1     |
| 1   | A     | 9   | DG   | P-O5'   | 5.50  | 1.71        | 1.60     | 9      | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 24  | DA   | C5'-C4' | 5.45  | 1.63        | 1.52     | 6      | 1     |
| 1   | A     | 9   | DG   | C2-N2   | -5.44 | 1.23        | 1.34     | 1      | 1     |
| 1   | A     | 15  | DA   | O3'-P   | -5.42 | 1.53        | 1.61     | 3      | 1     |
| 1   | A     | 28  | DG   | O3'-P   | -5.27 | 1.53        | 1.61     | 9      | 1     |
| 1   | A     | 9   | DG   | O3'-P   | 5.26  | 1.69        | 1.61     | 3      | 1     |
| 1   | A     | 6   | DG   | P-O5'   | -5.25 | 1.50        | 1.60     | 2      | 1     |
| 1   | A     | 13  | DG   | N9-C8   | -5.21 | 1.27        | 1.37     | 6      | 1     |
| 1   | A     | 31  | DG   | C1'-N9  | 5.13  | 1.56        | 1.46     | 7      | 1     |
| 1   | A     | 14  | DA   | P-O5'   | -5.07 | 1.50        | 1.60     | 4      | 1     |
| 1   | A     | 29  | DG   | O3'-P   | 5.02  | 1.68        | 1.61     | 3      | 1     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|--------|-------------|----------|--------|-------|
|     |       |     |      |             |        |             |          | Worst  | Total |
| 1   | A     | 27  | DG   | O5'-C5'-C4' | -10.63 | 94.85       | 110.80   | 2      | 1     |
| 1   | A     | 15  | DA   | N1-C6-N6    | -10.52 | 103.22      | 119.00   | 4      | 2     |
| 1   | A     | 23  | DG   | O4'-C1'-N9  | 9.83   | 123.14      | 108.40   | 10     | 3     |
| 1   | A     | 30  | DA   | P-O3'-C3'   | 9.45   | 134.38      | 120.20   | 8      | 9     |
| 1   | A     | 29  | DG   | C5'-C4'-C3' | -9.34  | 100.89      | 114.90   | 9      | 2     |
| 1   | A     | 32  | DG   | C5'-C4'-O4' | -9.32  | 95.42       | 109.40   | 7      | 1     |
| 1   | A     | 17  | DA   | N1-C6-N6    | -9.31  | 105.03      | 119.00   | 10     | 5     |
| 1   | A     | 24  | DA   | O5'-C5'-C4' | 9.29   | 124.74      | 110.80   | 10     | 3     |
| 1   | A     | 27  | DG   | C4-N9-C1'   | -9.21  | 113.19      | 127.00   | 8      | 9     |
| 1   | A     | 5   | DC   | C5'-C4'-C3' | -9.14  | 101.19      | 114.90   | 2      | 1     |
| 1   | A     | 31  | DG   | C4'-C3'-O3' | 8.85   | 123.27      | 110.00   | 8      | 2     |
| 1   | A     | 31  | DG   | O5'-C5'-C4' | 8.84   | 124.06      | 110.80   | 4      | 3     |
| 1   | A     | 27  | DG   | O4'-C1'-N9  | 8.81   | 121.62      | 108.40   | 4      | 5     |
| 1   | A     | 4   | DG   | C5'-C4'-O4' | 8.80   | 122.60      | 109.40   | 6      | 3     |
| 1   | A     | 1   | DA   | C4'-C3'-O3' | 8.71   | 123.06      | 110.00   | 4      | 3     |
| 1   | A     | 31  | DG   | N9-C1'-C2'  | -8.67  | 100.50      | 113.50   | 10     | 3     |
| 1   | A     | 7   | DG   | O4'-C1'-N9  | 8.56   | 121.25      | 108.40   | 1      | 3     |
| 1   | A     | 8   | DT   | C4-C5-C7    | -8.51  | 109.64      | 122.40   | 4      | 2     |
| 1   | A     | 24  | DA   | C5'-C4'-O4' | 8.50   | 122.15      | 109.40   | 6      | 1     |
| 1   | A     | 24  | DA   | N1-C6-N6    | -8.40  | 106.40      | 119.00   | 10     | 4     |
| 1   | A     | 28  | DG   | C2'-C3'-O3' | -8.32  | 99.02       | 111.50   | 6      | 3     |
| 1   | A     | 4   | DG   | C5'-C4'-C3' | -8.30  | 102.44      | 114.90   | 3      | 3     |
| 1   | A     | 12  | DG   | C3'-C2'-C1' | 8.30   | 114.05      | 101.60   | 6      | 7     |
| 1   | A     | 21  | DA   | C4'-C3'-O3' | 8.29   | 122.43      | 110.00   | 10     | 4     |
| 1   | A     | 10  | DT   | C6-C5-C7    | -8.26  | 111.61      | 124.00   | 6      | 4     |
| 1   | A     | 2   | DG   | P-O3'-C3'   | 8.20   | 132.51      | 120.20   | 3      | 4     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 25  | DT   | C6-C5-C7    | -8.17 | 111.74      | 124.00   | 1      | 1     |
| 1   | A     | 12  | DG   | O3'-P-O5'   | 8.15  | 116.22      | 104.00   | 3      | 5     |
| 1   | A     | 25  | DT   | O3'-P-O5'   | 8.15  | 116.22      | 104.00   | 8      | 3     |
| 1   | A     | 7   | DG   | C5'-C4'-O4' | 8.13  | 121.60      | 109.40   | 2      | 1     |
| 1   | A     | 23  | DG   | P-O3'-C3'   | 8.13  | 132.40      | 120.20   | 4      | 1     |
| 1   | A     | 1   | DA   | C2'-C3'-O3' | -8.06 | 99.41       | 111.50   | 5      | 6     |
| 1   | A     | 2   | DG   | O4'-C4'-C3' | -8.02 | 93.37       | 105.40   | 10     | 4     |
| 1   | A     | 16  | DG   | C5'-C4'-C3' | -7.96 | 102.96      | 114.90   | 3      | 1     |
| 1   | A     | 26  | DG   | C1'-O4'-C4' | -7.91 | 97.83       | 109.70   | 6      | 1     |
| 1   | A     | 24  | DA   | C5'-C4'-C3' | -7.89 | 103.07      | 114.90   | 2      | 2     |
| 1   | A     | 3   | DG   | C2'-C3'-O3' | 7.88  | 123.32      | 111.50   | 6      | 2     |
| 1   | A     | 9   | DG   | C8-N9-C1'   | -7.83 | 115.25      | 127.00   | 4      | 4     |
| 1   | A     | 1   | DA   | O5'-C5'-C4' | 7.83  | 122.55      | 110.80   | 1      | 1     |
| 1   | A     | 8   | DT   | C5'-C4'-C3' | 7.79  | 126.59      | 114.90   | 3      | 1     |
| 1   | A     | 6   | DG   | O5'-C5'-C4' | 7.74  | 122.41      | 110.80   | 2      | 2     |
| 1   | A     | 1   | DA   | C5'-C4'-O4' | -7.70 | 97.86       | 109.40   | 1      | 5     |
| 1   | A     | 12  | DG   | O4'-C1'-N9  | 7.69  | 119.93      | 108.40   | 1      | 1     |
| 1   | A     | 11  | DG   | C4-N9-C1'   | 7.67  | 138.50      | 127.00   | 9      | 1     |
| 1   | A     | 4   | DG   | C4'-C3'-O3' | 7.66  | 121.49      | 110.00   | 3      | 1     |
| 1   | A     | 30  | DA   | C2'-C3'-O3' | 7.65  | 122.98      | 111.50   | 2      | 3     |
| 1   | A     | 15  | DA   | O5'-C5'-C4' | 7.54  | 122.12      | 110.80   | 2      | 1     |
| 1   | A     | 3   | DG   | C1'-O4'-C4' | -7.52 | 98.42       | 109.70   | 4      | 4     |
| 1   | A     | 31  | DG   | C3'-C2'-C1' | 7.51  | 112.86      | 101.60   | 1      | 4     |
| 1   | A     | 27  | DG   | O3'-P-O5'   | 7.50  | 115.26      | 104.00   | 5      | 2     |
| 1   | A     | 19  | DG   | O3'-P-O5'   | 7.47  | 115.20      | 104.00   | 10     | 2     |
| 1   | A     | 17  | DA   | C5'-C4'-C3' | -7.47 | 103.70      | 114.90   | 2      | 1     |
| 1   | A     | 9   | DG   | O5'-C5'-C4' | 7.46  | 121.98      | 110.80   | 5      | 2     |
| 1   | A     | 29  | DG   | N3-C2-N2    | -7.44 | 108.54      | 119.70   | 3      | 1     |
| 1   | A     | 21  | DA   | C5'-C4'-O4' | -7.41 | 98.28       | 109.40   | 2      | 1     |
| 1   | A     | 28  | DG   | C4'-C3'-C2' | -7.39 | 91.31       | 102.40   | 2      | 5     |
| 1   | A     | 5   | DC   | C2'-C3'-O3' | 7.34  | 122.51      | 111.50   | 2      | 1     |
| 1   | A     | 29  | DG   | N1-C6-O6    | -7.31 | 109.04      | 120.00   | 6      | 1     |
| 1   | A     | 30  | DA   | P-O5'-C5'   | 7.29  | 130.93      | 120.00   | 4      | 2     |
| 1   | A     | 28  | DG   | O3'-P-O5'   | 7.28  | 114.92      | 104.00   | 4      | 4     |
| 1   | A     | 13  | DG   | O4'-C1'-C2' | -7.26 | 95.51       | 106.40   | 2      | 3     |
| 1   | A     | 9   | DG   | C5'-C4'-O4' | 7.24  | 120.25      | 109.40   | 4      | 2     |
| 1   | A     | 13  | DG   | C4-N9-C1'   | 7.12  | 137.69      | 127.00   | 2      | 3     |
| 1   | A     | 8   | DT   | C5-C4-O4    | 7.12  | 133.28      | 122.60   | 2      | 2     |
| 1   | A     | 25  | DT   | O5'-C5'-C4' | 7.11  | 121.47      | 110.80   | 9      | 1     |
| 1   | A     | 14  | DA   | N1-C6-N6    | -7.09 | 108.36      | 119.00   | 6      | 1     |
| 1   | A     | 5   | DC   | O5'-C5'-C4' | 7.09  | 121.44      | 110.80   | 8      | 2     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 9   | DG   | C4'-C3'-O3' | 7.08  | 120.62      | 110.00   | 1      | 3     |
| 1   | A     | 9   | DG   | O3'-P-O5'   | -7.03 | 93.46       | 104.00   | 4      | 2     |
| 1   | A     | 9   | DG   | C2'-C3'-O3' | -7.01 | 100.98      | 111.50   | 10     | 3     |
| 1   | A     | 30  | DA   | N1-C6-N6    | -7.00 | 108.51      | 119.00   | 8      | 3     |
| 1   | A     | 9   | DG   | N9-C1'-C2'  | -6.99 | 103.02      | 113.50   | 10     | 3     |
| 1   | A     | 17  | DA   | C2'-C3'-O3' | -6.99 | 101.02      | 111.50   | 6      | 3     |
| 1   | A     | 1   | DA   | N1-C6-N6    | -6.98 | 108.53      | 119.00   | 3      | 2     |
| 1   | A     | 3   | DG   | O5'-C5'-C4' | 6.96  | 121.24      | 110.80   | 10     | 5     |
| 1   | A     | 28  | DG   | O4'-C1'-N9  | 6.94  | 118.81      | 108.40   | 5      | 2     |
| 1   | A     | 24  | DA   | C5-C6-N1    | 6.91  | 127.97      | 117.60   | 3      | 1     |
| 1   | A     | 4   | DG   | O5'-C5'-C4' | 6.85  | 121.07      | 110.80   | 10     | 2     |
| 1   | A     | 23  | DG   | N1-C6-O6    | -6.83 | 109.75      | 120.00   | 7      | 1     |
| 1   | A     | 19  | DG   | O5'-C5'-C4' | 6.80  | 121.00      | 110.80   | 10     | 2     |
| 1   | A     | 21  | DA   | O4'-C4'-C3' | 6.79  | 115.59      | 105.40   | 9      | 1     |
| 1   | A     | 27  | DG   | N3-C2-N2    | -6.79 | 109.52      | 119.70   | 5      | 1     |
| 1   | A     | 12  | DG   | O4'-C4'-C3' | 6.77  | 115.56      | 105.40   | 1      | 1     |
| 1   | A     | 13  | DG   | C8-N9-C1'   | -6.76 | 116.86      | 127.00   | 2      | 3     |
| 1   | A     | 13  | DG   | C4'-C3'-O3' | 6.75  | 120.13      | 110.00   | 7      | 1     |
| 1   | A     | 12  | DG   | C4'-C3'-C2' | -6.72 | 92.33       | 102.40   | 9      | 3     |
| 1   | A     | 22  | DA   | N1-C6-N6    | -6.70 | 108.96      | 119.00   | 8      | 2     |
| 1   | A     | 32  | DG   | N3-C2-N2    | -6.66 | 109.70      | 119.70   | 10     | 1     |
| 1   | A     | 9   | DG   | P-O3'-C3'   | 6.65  | 130.18      | 120.20   | 8      | 4     |
| 1   | A     | 31  | DG   | O4'-C1'-N9  | 6.65  | 118.38      | 108.40   | 6      | 3     |
| 1   | A     | 1   | DA   | O3'-P-O5'   | 6.65  | 113.98      | 104.00   | 8      | 1     |
| 1   | A     | 1   | DA   | P-O3'-C3'   | 6.65  | 130.17      | 120.20   | 9      | 2     |
| 1   | A     | 16  | DG   | N1-C6-O6    | -6.63 | 110.05      | 120.00   | 7      | 2     |
| 1   | A     | 1   | DA   | C5'-C4'-C3' | 6.63  | 124.85      | 114.90   | 2      | 2     |
| 1   | A     | 29  | DG   | O4'-C1'-N9  | 6.63  | 118.34      | 108.40   | 6      | 2     |
| 1   | A     | 19  | DG   | O4'-C1'-N9  | 6.62  | 118.32      | 108.40   | 1      | 2     |
| 1   | A     | 13  | DG   | C3'-C2'-C1' | 6.60  | 111.51      | 101.60   | 2      | 2     |
| 1   | A     | 11  | DG   | O4'-C4'-C3' | 6.59  | 115.28      | 105.40   | 8      | 1     |
| 1   | A     | 20  | DG   | C2'-C3'-O3' | -6.58 | 101.63      | 111.50   | 7      | 1     |
| 1   | A     | 6   | DG   | N3-C2-N2    | -6.58 | 109.83      | 119.70   | 7      | 2     |
| 1   | A     | 13  | DG   | P-O5'-C5'   | 6.58  | 129.86      | 120.00   | 9      | 2     |
| 1   | A     | 20  | DG   | O4'-C1'-C2' | -6.52 | 96.61       | 106.40   | 7      | 1     |
| 1   | A     | 5   | DC   | C4'-C3'-O3' | 6.51  | 119.77      | 110.00   | 10     | 1     |
| 1   | A     | 27  | DG   | N1-C2-N2    | 6.50  | 126.06      | 116.30   | 5      | 1     |
| 1   | A     | 3   | DG   | O3'-P-O5'   | -6.47 | 94.30       | 104.00   | 5      | 2     |
| 1   | A     | 9   | DG   | C5-N7-C8    | -6.47 | 94.50       | 104.20   | 5      | 1     |
| 1   | A     | 22  | DA   | C5'-C4'-O4' | 6.45  | 119.08      | 109.40   | 1      | 2     |
| 1   | A     | 25  | DT   | C5'-C4'-C3' | -6.44 | 105.23      | 114.90   | 4      | 3     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 10  | DT   | O5'-C5'-C4' | 6.44  | 120.47      | 110.80   | 2      | 3     |
| 1   | A     | 8   | DT   | P-O5'-C5'   | 6.44  | 129.66      | 120.00   | 10     | 1     |
| 1   | A     | 18  | DG   | O3'-P-O5'   | -6.42 | 94.37       | 104.00   | 10     | 1     |
| 1   | A     | 6   | DG   | P-O5'-C5'   | 6.40  | 129.60      | 120.00   | 5      | 1     |
| 1   | A     | 20  | DG   | C5'-C4'-C3' | -6.40 | 105.30      | 114.90   | 1      | 1     |
| 1   | A     | 10  | DT   | N3-C4-O4    | -6.39 | 113.01      | 122.60   | 7      | 1     |
| 1   | A     | 1   | DA   | C8-N9-C1'   | 6.38  | 136.62      | 127.05   | 7      | 1     |
| 1   | A     | 6   | DG   | C5'-C4'-C3' | -6.38 | 105.33      | 114.90   | 8      | 1     |
| 1   | A     | 29  | DG   | O3'-P-O5'   | -6.37 | 94.45       | 104.00   | 10     | 1     |
| 1   | A     | 8   | DT   | O3'-P-O5'   | 6.35  | 113.53      | 104.00   | 9      | 2     |
| 1   | A     | 15  | DA   | C5-C6-N6    | 6.35  | 132.93      | 123.40   | 4      | 1     |
| 1   | A     | 4   | DG   | P-O5'-C5'   | 6.35  | 129.52      | 120.00   | 4      | 1     |
| 1   | A     | 31  | DG   | O4'-C1'-C2' | -6.35 | 96.88       | 106.40   | 3      | 1     |
| 1   | A     | 5   | DC   | N3-C4-N4    | -6.33 | 108.40      | 117.90   | 1      | 1     |
| 1   | A     | 13  | DG   | C4'-C3'-C2' | -6.33 | 92.90       | 102.40   | 2      | 2     |
| 1   | A     | 27  | DG   | C8-N9-C1'   | 6.30  | 136.46      | 127.00   | 5      | 3     |
| 1   | A     | 3   | DG   | C5'-C4'-O4' | 6.27  | 118.81      | 109.40   | 6      | 1     |
| 1   | A     | 32  | DG   | N1-C2-N2    | 6.27  | 125.70      | 116.30   | 10     | 1     |
| 1   | A     | 2   | DG   | C4'-C3'-O3' | 6.24  | 119.36      | 110.00   | 5      | 7     |
| 1   | A     | 12  | DG   | C4'-C3'-O3' | 6.23  | 119.34      | 110.00   | 5      | 2     |
| 1   | A     | 25  | DT   | C5-C4-O4    | 6.22  | 131.94      | 122.60   | 3      | 1     |
| 1   | A     | 21  | DA   | C3'-C2'-C1' | 6.21  | 110.92      | 101.60   | 3      | 3     |
| 1   | A     | 9   | DG   | N7-C8-N9    | 6.21  | 122.82      | 113.50   | 5      | 1     |
| 1   | A     | 16  | DG   | O4'-C1'-N9  | 6.21  | 117.72      | 108.40   | 10     | 1     |
| 1   | A     | 2   | DG   | N3-C2-N2    | 6.21  | 129.01      | 119.70   | 8      | 2     |
| 1   | A     | 6   | DG   | C5'-C4'-O4' | 6.20  | 118.70      | 109.40   | 7      | 1     |
| 1   | A     | 1   | DA   | C2-N3-C4    | 6.19  | 120.09      | 110.80   | 9      | 1     |
| 1   | A     | 17  | DA   | O5'-C5'-C4' | 6.18  | 120.08      | 110.80   | 7      | 3     |
| 1   | A     | 3   | DG   | O4'-C1'-C2' | -6.16 | 97.16       | 106.40   | 2      | 1     |
| 1   | A     | 5   | DC   | N1-C1'-C2'  | -6.16 | 104.26      | 113.50   | 9      | 4     |
| 1   | A     | 27  | DG   | O4'-C4'-C3' | 6.16  | 114.64      | 105.40   | 7      | 1     |
| 1   | A     | 27  | DG   | C1'-O4'-C4' | -6.14 | 100.49      | 109.70   | 8      | 1     |
| 1   | A     | 17  | DA   | C5-C6-N6    | 6.14  | 132.61      | 123.40   | 6      | 1     |
| 1   | A     | 13  | DG   | N1-C2-N2    | 6.12  | 125.49      | 116.30   | 4      | 1     |
| 1   | A     | 12  | DG   | N1-C2-N2    | 6.10  | 125.45      | 116.30   | 9      | 1     |
| 1   | A     | 7   | DG   | N9-C1'-C2'  | -6.09 | 104.36      | 113.50   | 9      | 3     |
| 1   | A     | 23  | DG   | C2'-C3'-O3' | 6.07  | 120.60      | 111.50   | 4      | 2     |
| 1   | A     | 21  | DA   | C2-N3-C4    | 6.06  | 119.90      | 110.80   | 6      | 1     |
| 1   | A     | 1   | DA   | C4-N9-C1'   | -6.06 | 117.96      | 127.05   | 4      | 3     |
| 1   | A     | 21  | DA   | O5'-C5'-C4' | 6.04  | 119.87      | 110.80   | 1      | 1     |
| 1   | A     | 31  | DG   | C5'-C4'-O4' | 6.04  | 118.46      | 109.40   | 1      | 2     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 27  | DG   | N9-C1'-C2'  | -6.04 | 104.44      | 113.50   | 9      | 2     |
| 1   | A     | 3   | DG   | C5'-C4'-C3' | 6.03  | 123.94      | 114.90   | 5      | 3     |
| 1   | A     | 30  | DA   | C4'-C3'-O3' | -6.00 | 101.00      | 110.00   | 1      | 2     |
| 1   | A     | 31  | DG   | C5-N7-C8    | -5.98 | 95.23       | 104.20   | 8      | 1     |
| 1   | A     | 30  | DA   | C4-C5-C6    | -5.97 | 107.94      | 116.90   | 5      | 1     |
| 1   | A     | 25  | DT   | O4'-C1'-N1  | 5.97  | 117.36      | 108.40   | 7      | 1     |
| 1   | A     | 27  | DG   | C4'-C3'-O3' | 5.95  | 118.93      | 110.00   | 1      | 1     |
| 1   | A     | 8   | DT   | N3-C4-O4    | -5.93 | 113.71      | 122.60   | 2      | 2     |
| 1   | A     | 20  | DG   | O3'-P-O5'   | -5.91 | 95.13       | 104.00   | 10     | 1     |
| 1   | A     | 31  | DG   | C8-N9-C1'   | -5.90 | 118.15      | 127.00   | 3      | 1     |
| 1   | A     | 5   | DC   | P-O3'-C3'   | 5.88  | 129.02      | 120.20   | 9      | 2     |
| 1   | A     | 3   | DG   | P-O5'-C5'   | 5.88  | 128.81      | 120.00   | 5      | 1     |
| 1   | A     | 24  | DA   | O3'-P-O5'   | 5.86  | 112.79      | 104.00   | 4      | 1     |
| 1   | A     | 12  | DG   | C2'-C3'-O3' | -5.85 | 102.73      | 111.50   | 2      | 1     |
| 1   | A     | 28  | DG   | O4'-C4'-C3' | 5.85  | 114.17      | 105.40   | 6      | 1     |
| 1   | A     | 28  | DG   | N9-C1'-C2'  | -5.81 | 104.78      | 113.50   | 5      | 1     |
| 1   | A     | 23  | DG   | O3'-P-O5'   | 5.79  | 112.69      | 104.00   | 7      | 1     |
| 1   | A     | 23  | DG   | N1-C2-N2    | 5.79  | 124.98      | 116.30   | 4      | 1     |
| 1   | A     | 2   | DG   | C4-N9-C1'   | -5.79 | 118.32      | 127.00   | 1      | 1     |
| 1   | A     | 22  | DA   | O3'-P-O5'   | -5.79 | 95.32       | 104.00   | 6      | 2     |
| 1   | A     | 23  | DG   | N3-C2-N2    | -5.77 | 111.05      | 119.70   | 1      | 2     |
| 1   | A     | 13  | DG   | O4'-C1'-N9  | 5.75  | 117.03      | 108.40   | 7      | 1     |
| 1   | A     | 26  | DG   | O3'-P-O5'   | -5.75 | 95.38       | 104.00   | 7      | 1     |
| 1   | A     | 30  | DA   | C5'-C4'-C3' | 5.75  | 123.52      | 114.90   | 1      | 1     |
| 1   | A     | 4   | DG   | P-O3'-C3'   | 5.75  | 128.82      | 120.20   | 8      | 1     |
| 1   | A     | 18  | DG   | C4-N9-C1'   | 5.74  | 135.62      | 127.00   | 8      | 1     |
| 1   | A     | 14  | DA   | P-O3'-C3'   | 5.74  | 128.81      | 120.20   | 8      | 2     |
| 1   | A     | 5   | DC   | O3'-P-O5'   | -5.74 | 95.39       | 104.00   | 10     | 1     |
| 1   | A     | 28  | DG   | C3'-C2'-C1' | 5.73  | 110.19      | 101.60   | 8      | 1     |
| 1   | A     | 5   | DC   | C2-N1-C1'   | -5.71 | 111.14      | 119.70   | 9      | 1     |
| 1   | A     | 11  | DG   | C8-N9-C1'   | -5.69 | 118.47      | 127.00   | 9      | 1     |
| 1   | A     | 23  | DG   | C5'-C4'-C3' | -5.68 | 106.38      | 114.90   | 4      | 1     |
| 1   | A     | 16  | DG   | O3'-P-O5'   | 5.67  | 112.51      | 104.00   | 9      | 1     |
| 1   | A     | 6   | DG   | C4'-C3'-O3' | 5.67  | 118.50      | 110.00   | 9      | 1     |
| 1   | A     | 13  | DG   | O5'-C5'-C4' | -5.66 | 102.32      | 110.80   | 2      | 1     |
| 1   | A     | 18  | DG   | O5'-C5'-C4' | -5.66 | 102.32      | 110.80   | 5      | 1     |
| 1   | A     | 25  | DT   | C1'-O4'-C4' | -5.66 | 101.22      | 109.70   | 9      | 1     |
| 1   | A     | 23  | DG   | C5-C6-O6    | 5.65  | 136.77      | 128.30   | 7      | 1     |
| 1   | A     | 31  | DG   | C4-N9-C1'   | 5.64  | 135.47      | 127.00   | 6      | 1     |
| 1   | A     | 7   | DG   | C5'-C4'-C3' | -5.64 | 106.44      | 114.90   | 9      | 2     |
| 1   | A     | 1   | DA   | C5-C6-N1    | 5.62  | 126.03      | 117.60   | 7      | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 22  | DA   | C4-N9-C1'   | -5.58 | 118.68      | 127.05   | 8      | 1     |
| 1   | A     | 17  | DA   | C8-N9-C1'   | -5.57 | 118.70      | 127.05   | 4      | 1     |
| 1   | A     | 30  | DA   | C3'-C2'-C1' | -5.57 | 93.25       | 101.60   | 5      | 1     |
| 1   | A     | 11  | DG   | C5'-C4'-C3' | -5.56 | 106.56      | 114.90   | 10     | 2     |
| 1   | A     | 5   | DC   | O4'-C1'-C2' | -5.56 | 98.06       | 106.40   | 4      | 1     |
| 1   | A     | 13  | DG   | P-O3'-C3'   | 5.56  | 128.54      | 120.20   | 3      | 1     |
| 1   | A     | 31  | DG   | O3'-P-O5'   | 5.56  | 112.34      | 104.00   | 7      | 2     |
| 1   | A     | 32  | DG   | C4'-C3'-O3' | 5.56  | 118.33      | 110.00   | 5      | 1     |
| 1   | A     | 30  | DA   | C4'-C3'-C2' | -5.56 | 94.07       | 102.40   | 9      | 2     |
| 1   | A     | 7   | DG   | C2'-C3'-O3' | 5.55  | 119.83      | 111.50   | 4      | 1     |
| 1   | A     | 17  | DA   | C5-C6-N1    | 5.55  | 125.93      | 117.60   | 10     | 1     |
| 1   | A     | 31  | DG   | C8-N9-C4    | -5.54 | 97.69       | 106.00   | 6      | 1     |
| 1   | A     | 7   | DG   | O5'-C5'-C4' | 5.54  | 119.10      | 110.80   | 8      | 1     |
| 1   | A     | 25  | DT   | C4'-C3'-O3' | 5.53  | 118.30      | 110.00   | 10     | 4     |
| 1   | A     | 29  | DG   | P-O5'-C5'   | 5.52  | 128.28      | 120.00   | 10     | 1     |
| 1   | A     | 16  | DG   | C5-C6-O6    | 5.51  | 136.57      | 128.30   | 7      | 1     |
| 1   | A     | 16  | DG   | C4'-C3'-C2' | -5.51 | 94.14       | 102.40   | 4      | 1     |
| 1   | A     | 6   | DG   | C2'-C3'-O3' | -5.50 | 103.26      | 111.50   | 1      | 2     |
| 1   | A     | 1   | DA   | C6-C5-N7    | 5.49  | 140.54      | 132.30   | 9      | 1     |
| 1   | A     | 9   | DG   | C4-N9-C1'   | 5.49  | 135.23      | 127.00   | 3      | 2     |
| 1   | A     | 19  | DG   | N9-C1'-C2'  | -5.49 | 105.27      | 113.50   | 1      | 1     |
| 1   | A     | 5   | DC   | C6-N1-C1'   | -5.48 | 111.47      | 119.70   | 8      | 3     |
| 1   | A     | 14  | DA   | C5-C6-N6    | -5.48 | 115.18      | 123.40   | 9      | 1     |
| 1   | A     | 10  | DT   | C5-C4-O4    | 5.46  | 130.80      | 122.60   | 2      | 1     |
| 1   | A     | 20  | DG   | O5'-C5'-C4' | 5.46  | 119.00      | 110.80   | 5      | 2     |
| 1   | A     | 13  | DG   | N3-C2-N2    | -5.45 | 111.52      | 119.70   | 4      | 1     |
| 1   | A     | 29  | DG   | C4'-C3'-C2' | -5.44 | 94.24       | 102.40   | 3      | 1     |
| 1   | A     | 6   | DG   | C8-N9-C1'   | 5.43  | 135.15      | 127.00   | 10     | 1     |
| 1   | A     | 2   | DG   | N1-C6-O6    | -5.43 | 111.86      | 120.00   | 3      | 1     |
| 1   | A     | 2   | DG   | C2'-C3'-O3' | -5.43 | 103.36      | 111.50   | 7      | 1     |
| 1   | A     | 25  | DT   | N1-C1'-C2'  | 5.42  | 121.63      | 113.50   | 10     | 1     |
| 1   | A     | 30  | DA   | O4'-C1'-C2' | -5.40 | 98.30       | 106.40   | 9      | 1     |
| 1   | A     | 20  | DG   | C4'-C3'-O3' | 5.40  | 118.10      | 110.00   | 4      | 1     |
| 1   | A     | 8   | DT   | C4'-C3'-O3' | 5.40  | 118.09      | 110.00   | 2      | 1     |
| 1   | A     | 30  | DA   | O5'-C5'-C4' | -5.39 | 102.72      | 110.80   | 9      | 1     |
| 1   | A     | 13  | DG   | C5'-C4'-O4' | 5.39  | 117.48      | 109.40   | 7      | 1     |
| 1   | A     | 9   | DG   | N1-C2-N2    | 5.39  | 124.38      | 116.30   | 8      | 1     |
| 1   | A     | 3   | DG   | N3-C2-N2    | -5.38 | 111.63      | 119.70   | 1      | 1     |
| 1   | A     | 31  | DG   | O4'-C4'-C3' | 5.37  | 113.46      | 105.40   | 8      | 1     |
| 1   | A     | 13  | DG   | C2'-C3'-O3' | -5.35 | 103.47      | 111.50   | 7      | 1     |
| 1   | A     | 29  | DG   | P-O3'-C3'   | 5.35  | 128.23      | 120.20   | 1      | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 22  | DA   | C2'-C3'-O3' | -5.35 | 103.48      | 111.50   | 8      | 1     |
| 1   | A     | 20  | DG   | O4'-C1'-N9  | 5.34  | 116.42      | 108.40   | 9      | 1     |
| 1   | A     | 12  | DG   | O5'-C5'-C4' | 5.33  | 118.80      | 110.80   | 8      | 1     |
| 1   | A     | 6   | DG   | C3'-C2'-C1' | -5.32 | 93.62       | 101.60   | 1      | 1     |
| 1   | A     | 9   | DG   | O4'-C1'-N9  | 5.32  | 116.38      | 108.40   | 7      | 1     |
| 1   | A     | 13  | DG   | N7-C8-N9    | 5.32  | 121.48      | 113.50   | 2      | 1     |
| 1   | A     | 29  | DG   | O5'-C5'-C4' | 5.32  | 118.78      | 110.80   | 6      | 1     |
| 1   | A     | 19  | DG   | C2'-C3'-O3' | -5.30 | 103.55      | 111.50   | 9      | 1     |
| 1   | A     | 13  | DG   | O3'-P-O5'   | -5.30 | 96.05       | 104.00   | 5      | 1     |
| 1   | A     | 4   | DG   | O4'-C1'-N9  | 5.30  | 116.35      | 108.40   | 9      | 2     |
| 1   | A     | 18  | DG   | C2'-C3'-O3' | -5.30 | 103.55      | 111.50   | 6      | 1     |
| 1   | A     | 8   | DT   | C6-N1-C2    | -5.28 | 113.38      | 121.30   | 10     | 1     |
| 1   | A     | 12  | DG   | C5'-C4'-C3' | 5.27  | 122.80      | 114.90   | 10     | 1     |
| 1   | A     | 11  | DG   | O5'-C5'-C4' | 5.26  | 118.70      | 110.80   | 8      | 1     |
| 1   | A     | 20  | DG   | C8-N9-C1'   | 5.26  | 134.89      | 127.00   | 1      | 1     |
| 1   | A     | 23  | DG   | C3'-C2'-C1' | 5.25  | 109.47      | 101.60   | 4      | 1     |
| 1   | A     | 6   | DG   | P-O3'-C3'   | 5.24  | 128.06      | 120.20   | 2      | 1     |
| 1   | A     | 17  | DA   | P-O5'-C5'   | 5.24  | 127.86      | 120.00   | 6      | 1     |
| 1   | A     | 19  | DG   | C5'-C4'-O4' | -5.24 | 101.55      | 109.40   | 8      | 1     |
| 1   | A     | 14  | DA   | C2'-C3'-O3' | -5.23 | 103.65      | 111.50   | 5      | 1     |
| 1   | A     | 16  | DG   | C5'-C4'-O4' | -5.23 | 101.56      | 109.40   | 1      | 1     |
| 1   | A     | 5   | DC   | C2-N3-C4    | -5.22 | 112.17      | 120.00   | 9      | 1     |
| 1   | A     | 3   | DG   | O4'-C1'-N9  | 5.22  | 116.23      | 108.40   | 2      | 1     |
| 1   | A     | 11  | DG   | C3'-C2'-C1' | 5.21  | 109.42      | 101.60   | 1      | 1     |
| 1   | A     | 21  | DA   | C5-C6-N1    | 5.21  | 125.42      | 117.60   | 1      | 1     |
| 1   | A     | 20  | DG   | N9-C1'-C2'  | 5.21  | 121.31      | 113.50   | 10     | 1     |
| 1   | A     | 17  | DA   | O3'-P-O5'   | 5.21  | 111.81      | 104.00   | 9      | 1     |
| 1   | A     | 1   | DA   | N9-C1'-C2'  | 5.20  | 121.30      | 113.50   | 2      | 1     |
| 1   | A     | 24  | DA   | C6-N1-C2    | -5.20 | 111.00      | 118.80   | 3      | 1     |
| 1   | A     | 14  | DA   | C4'-C3'-C2' | -5.20 | 94.60       | 102.40   | 9      | 1     |
| 1   | A     | 22  | DA   | C5-C6-N6    | 5.19  | 131.18      | 123.40   | 9      | 1     |
| 1   | A     | 15  | DA   | O3'-P-O5'   | 5.18  | 111.78      | 104.00   | 6      | 1     |
| 1   | A     | 30  | DA   | O3'-P-O5'   | 5.18  | 111.77      | 104.00   | 1      | 1     |
| 1   | A     | 23  | DG   | O5'-C5'-C4' | 5.18  | 118.56      | 110.80   | 3      | 1     |
| 1   | A     | 5   | DC   | C3'-C2'-C1' | 5.17  | 109.36      | 101.60   | 3      | 2     |
| 1   | A     | 24  | DA   | P-O5'-C5'   | 5.17  | 127.75      | 120.00   | 8      | 1     |
| 1   | A     | 10  | DT   | C4-C5-C6    | 5.16  | 126.94      | 119.20   | 1      | 1     |
| 1   | A     | 28  | DG   | C5'-C4'-O4' | 5.16  | 117.14      | 109.40   | 4      | 1     |
| 1   | A     | 2   | DG   | N1-C2-N2    | -5.15 | 108.57      | 116.30   | 3      | 1     |
| 1   | A     | 26  | DG   | C5'-C4'-C3' | -5.15 | 107.18      | 114.90   | 7      | 1     |
| 1   | A     | 15  | DA   | C4'-C3'-O3' | -5.12 | 102.32      | 110.00   | 5      | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 30  | DA   | O4'-C1'-N9  | -5.12 | 100.72      | 108.40   | 9      | 1     |
| 1   | A     | 25  | DT   | N3-C4-O4    | -5.11 | 114.94      | 122.60   | 3      | 1     |
| 1   | A     | 31  | DG   | C5'-C4'-C3' | -5.11 | 107.24      | 114.90   | 5      | 1     |
| 1   | A     | 17  | DA   | C4-N9-C1'   | 5.09  | 134.69      | 127.05   | 4      | 1     |
| 1   | A     | 1   | DA   | O4'-C1'-N9  | 5.09  | 116.04      | 108.40   | 3      | 1     |
| 1   | A     | 5   | DC   | N3-C2-O2    | -5.08 | 114.28      | 121.90   | 10     | 1     |
| 1   | A     | 1   | DA   | C5-C6-N6    | 5.08  | 131.02      | 123.40   | 3      | 1     |
| 1   | A     | 2   | DG   | O5'-C5'-C4' | 5.08  | 118.42      | 110.80   | 8      | 1     |
| 1   | A     | 15  | DA   | O4'-C1'-C2' | 5.07  | 114.01      | 106.40   | 1      | 1     |
| 1   | A     | 30  | DA   | C5'-C4'-O4' | 5.06  | 116.99      | 109.40   | 6      | 1     |
| 1   | A     | 26  | DG   | N3-C2-N2    | -5.06 | 112.11      | 119.70   | 7      | 1     |
| 1   | A     | 24  | DA   | N9-C1'-C2'  | -5.06 | 105.92      | 113.50   | 1      | 1     |
| 1   | A     | 7   | DG   | N1-C2-N2    | -5.05 | 108.73      | 116.30   | 5      | 1     |
| 1   | A     | 29  | DG   | C6-C5-N7    | 5.04  | 137.67      | 130.10   | 2      | 1     |
| 1   | A     | 29  | DG   | C4'-C3'-O3' | 5.04  | 117.55      | 110.00   | 2      | 1     |
| 1   | A     | 26  | DG   | P-O5'-C5'   | 5.03  | 127.55      | 120.00   | 10     | 1     |
| 1   | A     | 32  | DG   | C1'-O4'-C4' | 5.03  | 117.25      | 109.70   | 2      | 1     |
| 1   | A     | 10  | DT   | C2'-C3'-O3' | 5.03  | 119.04      | 111.50   | 3      | 1     |
| 1   | A     | 3   | DG   | C4'-C3'-C2' | -5.02 | 94.88       | 102.40   | 1      | 1     |
| 1   | A     | 4   | DG   | C2'-C3'-O3' | -5.01 | 103.98      | 111.50   | 7      | 1     |
| 1   | A     | 24  | DA   | C5-C6-N6    | 5.01  | 130.91      | 123.40   | 10     | 1     |
| 1   | A     | 20  | DG   | N3-C2-N2    | -5.00 | 112.20      | 119.70   | 5      | 1     |
| 1   | A     | 24  | DA   | C4'-C3'-O3' | 5.00  | 117.50      | 110.00   | 3      | 1     |
| 1   | A     | 14  | DA   | C5'-C4'-C3' | -5.00 | 107.40      | 114.90   | 8      | 1     |

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 5   | DC   | Sidechain | 10             |
| 1   | A     | 9   | DG   | Sidechain | 10             |
| 1   | A     | 11  | DG   | Sidechain | 10             |
| 1   | A     | 12  | DG   | Sidechain | 10             |
| 1   | A     | 13  | DG   | Sidechain | 10             |
| 1   | A     | 31  | DG   | Sidechain | 10             |
| 1   | A     | 1   | DA   | Sidechain | 9              |
| 1   | A     | 2   | DG   | Sidechain | 9              |
| 1   | A     | 4   | DG   | Sidechain | 9              |
| 1   | A     | 7   | DG   | Sidechain | 9              |
| 1   | A     | 8   | DT   | Sidechain | 9              |

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| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 14  | DA   | Sidechain | 9              |
| 1   | A     | 24  | DA   | Sidechain | 9              |
| 1   | A     | 27  | DG   | Sidechain | 9              |
| 1   | A     | 3   | DG   | Sidechain | 8              |
| 1   | A     | 6   | DG   | Sidechain | 8              |
| 1   | A     | 16  | DG   | Sidechain | 8              |
| 1   | A     | 17  | DA   | Sidechain | 8              |
| 1   | A     | 19  | DG   | Sidechain | 8              |
| 1   | A     | 23  | DG   | Sidechain | 8              |
| 1   | A     | 28  | DG   | Sidechain | 8              |
| 1   | A     | 32  | DG   | Sidechain | 8              |
| 1   | A     | 10  | DT   | Sidechain | 8              |
| 1   | A     | 25  | DT   | Sidechain | 8              |
| 1   | A     | 18  | DG   | Sidechain | 7              |
| 1   | A     | 21  | DA   | Sidechain | 7              |
| 1   | A     | 29  | DG   | Sidechain | 7              |
| 1   | A     | 20  | DG   | Sidechain | 7              |
| 1   | A     | 26  | DG   | Sidechain | 6              |
| 1   | A     | 22  | DA   | Sidechain | 4              |
| 1   | A     | 30  | DA   | Sidechain | 4              |
| 1   | A     | 15  | DA   | Sidechain | 3              |

## 6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 684   | 357      | 333      | 6±2     |
| All | All   | 6860  | 3570     | 3373     | 59      |

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 6.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1        | Atom-2       | Clash(Å) | Distance(Å) | Models |       |
|---------------|--------------|----------|-------------|--------|-------|
|               |              |          |             | Worst  | Total |
| 1:A:7:DG:H2'' | 1:A:9:DG:C8  | 0.72     | 2.19        | 7      | 7     |
| 1:A:8:DT:H72  | 1:A:30:DA:C8 | 0.64     | 2.26        | 1      | 3     |

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| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:A:2:DG:C4    | 1:A:3:DG:C8    | 0.59     | 2.90        | 7      | 4     |
| 1:A:2:DG:H1'   | 1:A:3:DG:C8    | 0.57     | 2.35        | 4      | 1     |
| 1:A:4:DG:C6    | 1:A:8:DT:H73   | 0.55     | 2.36        | 1      | 2     |
| 1:A:6:DG:H2''  | 1:A:7:DG:C8    | 0.55     | 2.37        | 4      | 3     |
| 1:A:9:DG:H1'   | 1:A:10:DT:C5'  | 0.53     | 2.34        | 6      | 3     |
| 1:A:4:DG:C6    | 1:A:8:DT:H72   | 0.53     | 2.39        | 9      | 3     |
| 1:A:8:DT:H72   | 1:A:30:DA:C5   | 0.51     | 2.41        | 7      | 1     |
| 1:A:13:DG:H5'' | 1:A:13:DG:C8   | 0.51     | 2.41        | 2      | 2     |
| 1:A:27:DG:H2'' | 1:A:28:DG:C8   | 0.50     | 2.40        | 10     | 2     |
| 1:A:12:DG:C4   | 1:A:13:DG:C8   | 0.49     | 3.00        | 5      | 4     |
| 1:A:12:DG:H1'  | 1:A:25:DT:C7   | 0.49     | 2.38        | 5      | 1     |
| 1:A:30:DA:O3'  | 1:A:31:DG:C8   | 0.48     | 2.66        | 9      | 2     |
| 1:A:4:DG:H4'   | 1:A:5:DC:H4'   | 0.47     | 1.86        | 6      | 1     |
| 1:A:4:DG:C5    | 1:A:8:DT:H72   | 0.47     | 2.44        | 9      | 3     |
| 1:A:7:DG:C2'   | 1:A:9:DG:C8    | 0.47     | 2.97        | 2      | 2     |
| 1:A:3:DG:C6    | 1:A:4:DG:C5    | 0.47     | 3.03        | 4      | 1     |
| 1:A:1:DA:H1'   | 1:A:2:DG:C8    | 0.46     | 2.46        | 10     | 1     |
| 1:A:20:DG:H3'  | 1:A:21:DA:C8   | 0.46     | 2.46        | 8      | 2     |
| 1:A:1:DA:H4'   | 1:A:2:DG:OP1   | 0.43     | 2.13        | 4      | 1     |
| 1:A:17:DA:H5'' | 1:A:19:DG:C6   | 0.43     | 2.48        | 6      | 1     |
| 1:A:24:DA:H5'' | 1:A:25:DT:C5   | 0.43     | 2.49        | 4      | 1     |
| 1:A:24:DA:H3'  | 1:A:25:DT:H5'' | 0.42     | 1.90        | 2      | 1     |
| 1:A:25:DT:H3'  | 1:A:26:DG:H5'' | 0.42     | 1.90        | 1      | 1     |
| 1:A:8:DT:C7    | 1:A:30:DA:C8   | 0.42     | 3.03        | 5      | 2     |
| 1:A:12:DG:H2'' | 1:A:13:DG:C5'  | 0.41     | 2.45        | 4      | 1     |
| 1:A:4:DG:C6    | 1:A:8:DT:C7    | 0.41     | 3.03        | 1      | 1     |
| 1:A:8:DT:H71   | 1:A:30:DA:C8   | 0.41     | 2.50        | 9      | 1     |
| 1:A:2:DG:C8    | 1:A:2:DG:H5'   | 0.40     | 2.52        | 10     | 1     |

## 6.3 Torsion angles [i](#)

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

There are no protein molecules in this entry.

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

There are no protein molecules in this entry.

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 45% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 304 |
| Number of shifts mapped to atoms        | 304 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

#### 7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 45%, i.e. 295 atoms were assigned a chemical shift out of a possible 654. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|         | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|---------|---------------|----------------|-----------------|-----------------|
| Sugar   | 202/384 (53%) | 202/224 (90%)  | 0/160 (0%)      | 0/0 (—%)        |
| Base    | 93/270 (34%)  | 47/174 (27%)   | 34/44 (77%)     | 12/52 (23%)     |
| Overall | 295/654 (45%) | 249/398 (63%)  | 34/204 (17%)    | 12/52 (23%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 45%, i.e. 295 atoms were assigned a chemical shift out of a possible 654. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|         | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|---------|---------------|----------------|-----------------|-----------------|
| Sugar   | 202/384 (53%) | 202/224 (90%)  | 0/160 (0%)      | 0/0 (—%)        |
| Base    | 93/270 (34%)  | 47/174 (27%)   | 34/44 (77%)     | 12/52 (23%)     |
| Overall | 295/654 (45%) | 249/398 (63%)  | 34/204 (17%)    | 12/52 (23%)     |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots ⓘ

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 552   |
| Intra-residue ( $ i-j =0$ )                              | 376   |
| Sequential ( $ i-j =1$ )                                 | 103   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 36    |
| Long range ( $ i-j \geq 5$ )                             | 37    |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 16.2  |
| Number of long range restraints per residue <sup>1</sup> | 1.1   |

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 52.0                                   | 0.2     |
| 0.2-0.5 (Medium) | 66.7                                   | 0.5     |
| >0.5 (Large)     | 34.9                                   | 6.0     |

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis ⓘ

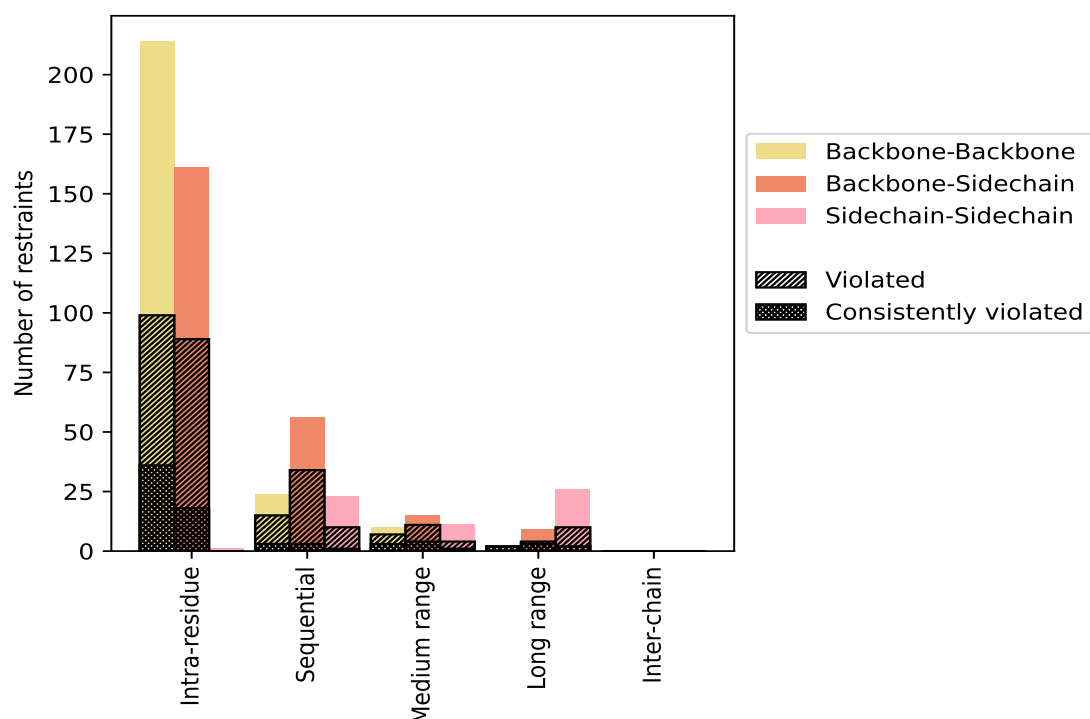
### 9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restrains type                                             | Count               | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                      |                      |
|------------------------------------------------------------|---------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|----------------------|
|                                                            |                     |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>       | % <sup>1</sup>       |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">376</a> | <a href="#">68.1</a>  | <a href="#">188</a>   | <a href="#">50.0</a> | <a href="#">34.1</a> | <a href="#">54</a>                 | <a href="#">14.4</a> | <a href="#">9.8</a>  |
| Backbone-Backbone                                          | 214                 | 38.8                  | 99                    | 46.3                 | 17.9                 | 36                                 | 16.8                 | 6.5                  |
| Backbone-Sidechain                                         | 161                 | 29.2                  | 89                    | 55.3                 | 16.1                 | 18                                 | 11.2                 | 3.3                  |
| Sidechain-Sidechain                                        | 1                   | 0.2                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">103</a> | <a href="#">18.7</a>  | <a href="#">59</a>    | <a href="#">57.3</a> | <a href="#">10.7</a> | <a href="#">7</a>                  | <a href="#">6.8</a>  | <a href="#">1.3</a>  |
| Backbone-Backbone                                          | 24                  | 4.3                   | 15                    | 62.5                 | 2.7                  | 3                                  | 12.5                 | 0.5                  |
| Backbone-Sidechain                                         | 56                  | 10.1                  | 34                    | 60.7                 | 6.2                  | 3                                  | 5.4                  | 0.5                  |
| Sidechain-Sidechain                                        | 23                  | 4.2                   | 10                    | 43.5                 | 1.8                  | 1                                  | 4.3                  | 0.2                  |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">36</a>  | <a href="#">6.5</a>   | <a href="#">22</a>    | <a href="#">61.1</a> | <a href="#">4.0</a>  | <a href="#">8</a>                  | <a href="#">22.2</a> | <a href="#">1.4</a>  |
| Backbone-Backbone                                          | 10                  | 1.8                   | 7                     | 70.0                 | 1.3                  | 3                                  | 30.0                 | 0.5                  |
| Backbone-Sidechain                                         | 15                  | 2.7                   | 11                    | 73.3                 | 2.0                  | 4                                  | 26.7                 | 0.7                  |
| Sidechain-Sidechain                                        | 11                  | 2.0                   | 4                     | 36.4                 | 0.7                  | 1                                  | 9.1                  | 0.2                  |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">37</a>  | <a href="#">6.7</a>   | <a href="#">16</a>    | <a href="#">43.2</a> | <a href="#">2.9</a>  | <a href="#">7</a>                  | <a href="#">18.9</a> | <a href="#">1.3</a>  |
| Backbone-Backbone                                          | 2                   | 0.4                   | 2                     | 100.0                | 0.4                  | 2                                  | 100.0                | 0.4                  |
| Backbone-Sidechain                                         | 9                   | 1.6                   | 4                     | 44.4                 | 0.7                  | 3                                  | 33.3                 | 0.5                  |
| Sidechain-Sidechain                                        | 26                  | 4.7                   | 10                    | 38.5                 | 1.8                  | 2                                  | 7.7                  | 0.4                  |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Backbone-Sidechain                                         | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Sidechain-Sidechain                                        | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| <a href="#">Total</a>                                      | <a href="#">552</a> | <a href="#">100.0</a> | <a href="#">285</a>   | <a href="#">51.6</a> | <a href="#">51.6</a> | <a href="#">76</a>                 | <a href="#">13.8</a> | <a href="#">13.8</a> |
| Backbone-Backbone                                          | 250                 | 45.3                  | 123                   | 49.2                 | 22.3                 | 44                                 | 17.6                 | 8.0                  |
| Backbone-Sidechain                                         | 241                 | 43.7                  | 138                   | 57.3                 | 25.0                 | 28                                 | 11.6                 | 5.1                  |
| Sidechain-Sidechain                                        | 61                  | 11.1                  | 24                    | 39.3                 | 4.3                  | 4                                  | 6.6                  | 0.7                  |

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

### 9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

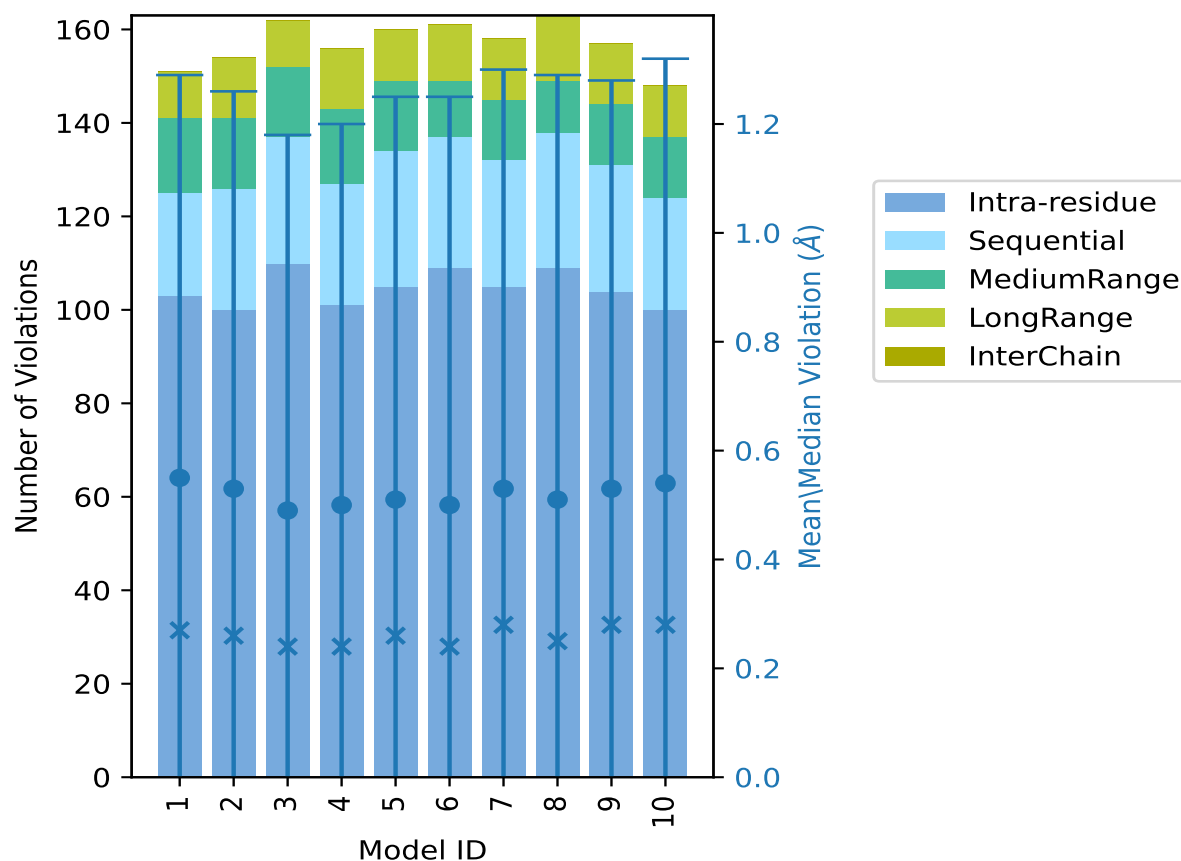
## 9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 103                  | 22              | 16              | 10              | 0               | 151   | 0.55     | 5.03    | 0.74                | 0.27       |
| 2        | 100                  | 26              | 15              | 13              | 0               | 154   | 0.53     | 4.96    | 0.73                | 0.26       |
| 3        | 110                  | 27              | 15              | 10              | 0               | 162   | 0.49     | 5.88    | 0.69                | 0.24       |
| 4        | 101                  | 26              | 16              | 13              | 0               | 156   | 0.5      | 5.38    | 0.7                 | 0.24       |
| 5        | 105                  | 29              | 15              | 11              | 0               | 160   | 0.51     | 5.64    | 0.74                | 0.26       |
| 6        | 109                  | 28              | 12              | 12              | 0               | 161   | 0.5      | 5.67    | 0.75                | 0.24       |
| 7        | 105                  | 27              | 13              | 13              | 0               | 158   | 0.53     | 5.82    | 0.77                | 0.28       |
| 8        | 109                  | 29              | 11              | 14              | 0               | 163   | 0.51     | 6.0     | 0.78                | 0.25       |
| 9        | 104                  | 27              | 13              | 13              | 0               | 157   | 0.53     | 5.7     | 0.75                | 0.28       |
| 10       | 100                  | 24              | 13              | 11              | 0               | 148   | 0.54     | 5.94    | 0.78                | 0.28       |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot), median(x) and the standard deviation are shown in blue with respect to the y axis on the right

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 267(IR:188, SQ:44, MR:14, LR:21, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |      |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %    |
| 38                            | 8               | 1               | 1               | 0               | 48    | 1                        | 10.0 |
| 22                            | 11              | 2               | 0               | 0               | 35    | 2                        | 20.0 |
| 12                            | 13              | 4               | 1               | 0               | 30    | 3                        | 30.0 |

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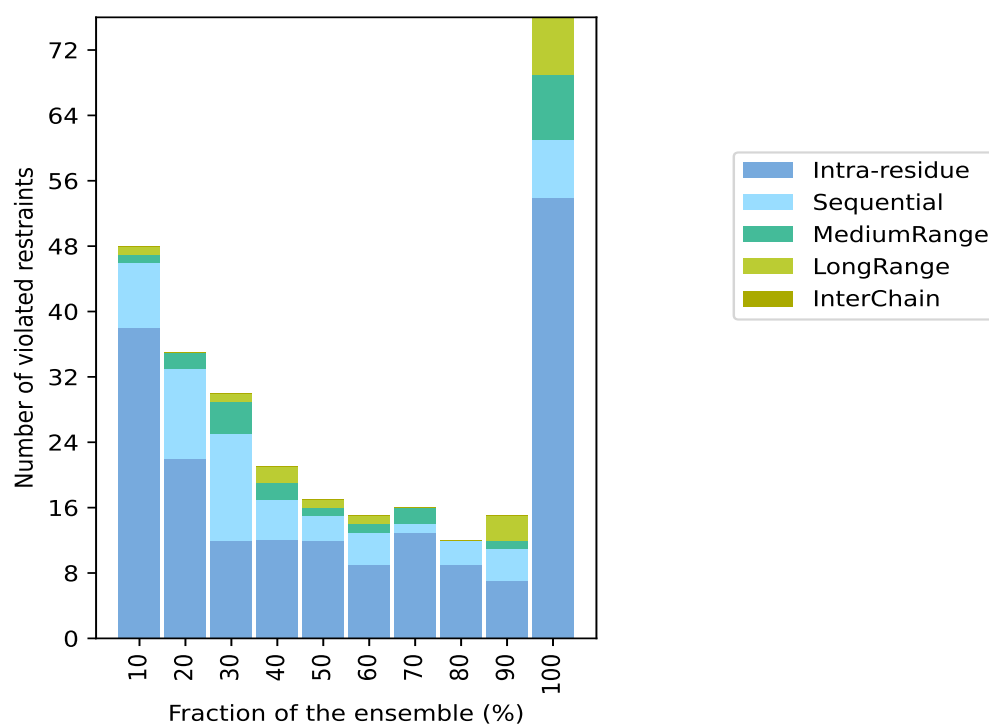
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 12                            | 5               | 2               | 2               | 0               | 21    | 4                        | 40.0  |
| 12                            | 3               | 1               | 1               | 0               | 17    | 5                        | 50.0  |
| 9                             | 4               | 1               | 1               | 0               | 15    | 6                        | 60.0  |
| 13                            | 1               | 2               | 0               | 0               | 16    | 7                        | 70.0  |
| 9                             | 3               | 0               | 0               | 0               | 12    | 8                        | 80.0  |
| 7                             | 4               | 1               | 3               | 0               | 15    | 9                        | 90.0  |
| 54                            | 7               | 8               | 7               | 0               | 76    | 10                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

### 9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

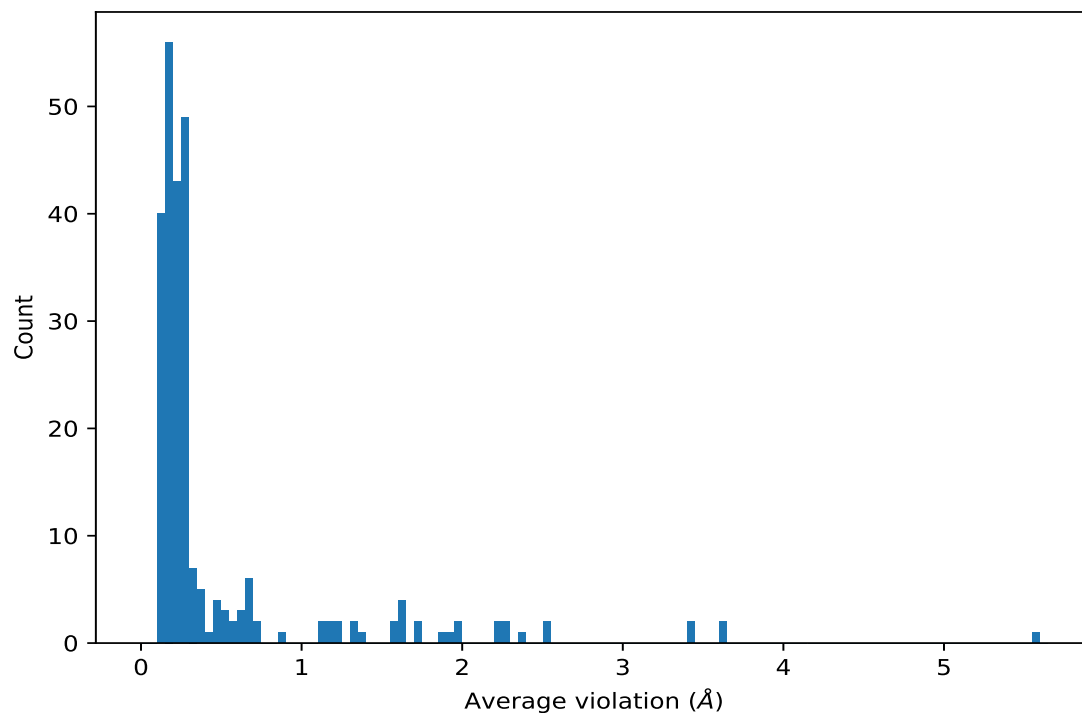


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



#### 9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key     | Atom-1         | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,380) | 1:10:A:DT:H6   | 1:8:A:DT:H6   | 10                  | 5.6      | 0.35                | 5.68       |
| (1,348) | 1:8:A:DT:H5'   | 1:4:A:DG:H8   | 10                  | 3.65     | 0.34                | 3.68       |
| (1,348) | 1:8:A:DT:H5''  | 1:4:A:DG:H8   | 10                  | 3.65     | 0.34                | 3.68       |
| (1,361) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'  | 10                  | 3.44     | 0.55                | 3.66       |
| (1,361) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'  | 10                  | 3.44     | 0.55                | 3.66       |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8  | 10                  | 2.54     | 0.6                 | 2.64       |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8  | 10                  | 2.54     | 0.6                 | 2.64       |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8   | 10                  | 2.39     | 0.29                | 2.49       |
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'  | 10                  | 2.3      | 0.4                 | 2.41       |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'  | 10                  | 2.3      | 0.4                 | 2.41       |
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1' | 10                  | 2.22     | 0.43                | 2.28       |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1' | 10                  | 2.22     | 0.43                | 2.28       |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'' | 10                  | 1.99     | 0.46                | 2.08       |
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'' | 10                  | 1.99     | 0.46                | 2.08       |
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'  | 10                  | 1.91     | 0.07                | 1.89       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 10                  | 1.89     | 0.07                | 1.9        |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 10                  | 1.74     | 0.24                | 1.77       |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 10                  | 1.74     | 0.24                | 1.77       |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 10                  | 1.6      | 0.31                | 1.52       |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 10                  | 1.6      | 0.31                | 1.52       |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 10                  | 1.55     | 0.09                | 1.54       |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 10                  | 1.55     | 0.09                | 1.54       |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 10                  | 1.36     | 0.19                | 1.4        |
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 10                  | 1.31     | 0.31                | 1.31       |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 10                  | 1.3      | 0.27                | 1.34       |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 10                  | 1.24     | 0.08                | 1.23       |
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 10                  | 1.22     | 0.08                | 1.2        |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 10                  | 1.18     | 0.35                | 1.28       |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 10                  | 1.18     | 0.35                | 1.28       |
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 10                  | 1.1      | 0.1                 | 1.06       |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 10                  | 1.1      | 0.07                | 1.08       |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 10                  | 0.88     | 0.04                | 0.88       |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 10                  | 0.73     | 0.03                | 0.72       |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 10                  | 0.72     | 0.09                | 0.74       |
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 10                  | 0.69     | 0.09                | 0.69       |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 10                  | 0.66     | 0.07                | 0.66       |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 10                  | 0.66     | 0.07                | 0.66       |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 10                  | 0.66     | 0.13                | 0.67       |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 10                  | 0.62     | 0.19                | 0.57       |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 10                  | 0.62     | 0.08                | 0.6        |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 10                  | 0.61     | 0.05                | 0.64       |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 10                  | 0.59     | 0.08                | 0.6        |
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 10                  | 0.56     | 0.06                | 0.55       |
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 10                  | 0.51     | 0.06                | 0.48       |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 10                  | 0.5      | 0.04                | 0.5        |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 10                  | 0.5      | 0.1                 | 0.5        |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 10                  | 0.47     | 0.06                | 0.46       |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 10                  | 0.46     | 0.11                | 0.46       |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 10                  | 0.46     | 0.06                | 0.44       |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 10                  | 0.45     | 0.07                | 0.44       |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 10                  | 0.4      | 0.12                | 0.42       |
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 10                  | 0.39     | 0.1                 | 0.4        |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 10                  | 0.39     | 0.08                | 0.38       |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 10                  | 0.38     | 0.16                | 0.33       |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 10                  | 0.37     | 0.08                | 0.38       |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 10                  | 0.36     | 0.08                | 0.37       |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 10                  | 0.33     | 0.1                 | 0.33       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 10                  | 0.33     | 0.07                | 0.33       |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 10                  | 0.32     | 0.07                | 0.32       |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 10                  | 0.29     | 0.03                | 0.3        |
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 10                  | 0.29     | 0.05                | 0.3        |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 10                  | 0.28     | 0.04                | 0.28       |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 10                  | 0.28     | 0.09                | 0.32       |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 10                  | 0.28     | 0.06                | 0.27       |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 10                  | 0.28     | 0.05                | 0.28       |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 10                  | 0.28     | 0.09                | 0.29       |
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 10                  | 0.28     | 0.08                | 0.29       |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 10                  | 0.28     | 0.07                | 0.26       |
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 10                  | 0.28     | 0.09                | 0.28       |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 10                  | 0.27     | 0.1                 | 0.29       |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 10                  | 0.27     | 0.09                | 0.27       |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 10                  | 0.27     | 0.08                | 0.3        |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 10                  | 0.27     | 0.07                | 0.26       |
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 10                  | 0.26     | 0.08                | 0.26       |
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 10                  | 0.26     | 0.09                | 0.25       |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 10                  | 0.26     | 0.03                | 0.26       |
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 10                  | 0.25     | 0.1                 | 0.26       |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 10                  | 0.25     | 0.04                | 0.23       |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 10                  | 0.25     | 0.04                | 0.25       |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 10                  | 0.24     | 0.06                | 0.23       |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 10                  | 0.22     | 0.05                | 0.22       |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 10                  | 0.22     | 0.04                | 0.22       |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 10                  | 0.21     | 0.05                | 0.2        |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 10                  | 0.2      | 0.05                | 0.19       |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 10                  | 0.2      | 0.05                | 0.18       |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 10                  | 0.19     | 0.05                | 0.18       |
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 10                  | 0.17     | 0.05                | 0.14       |
| (1,35)  | 1:28:A:DG:H1   | 1:3:A:DG:H8    | 9                   | 0.35     | 0.09                | 0.37       |
| (1,459) | 1:3:A:DG:H1    | 1:5:A:DC:H1'   | 9                   | 0.34     | 0.11                | 0.33       |
| (1,468) | 1:12:A:DG:H2'  | 1:13:A:DG:H1'  | 9                   | 0.33     | 0.11                | 0.28       |
| (1,298) | 1:8:A:DT:H6    | 1:30:A:DA:H8   | 9                   | 0.3      | 0.09                | 0.29       |
| (1,320) | 1:31:A:DG:H8   | 1:31:A:DG:H3'  | 9                   | 0.28     | 0.07                | 0.28       |
| (1,171) | 1:7:A:DG:H1    | 1:13:A:DG:H8   | 9                   | 0.26     | 0.1                 | 0.24       |
| (1,337) | 1:26:A:DG:H1   | 1:27:A:DG:H1'  | 9                   | 0.26     | 0.1                 | 0.24       |
| (1,351) | 1:25:A:DT:H5'  | 1:24:A:DA:H1'  | 9                   | 0.26     | 0.08                | 0.29       |
| (1,351) | 1:25:A:DT:H5'' | 1:24:A:DA:H1'  | 9                   | 0.26     | 0.08                | 0.29       |
| (1,388) | 1:22:A:DA:H8   | 1:22:A:DA:H3'  | 9                   | 0.25     | 0.07                | 0.26       |
| (1,226) | 1:9:A:DG:H3'   | 1:9:A:DG:H2'   | 9                   | 0.25     | 0.09                | 0.23       |
| (1,156) | 1:8:A:DT:H6    | 1:8:A:DT:H2'   | 9                   | 0.24     | 0.08                | 0.22       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,279) | 1:1:A:DA:H8    | 1:1:A:DA:H3'   | 9                   | 0.24     | 0.06                | 0.22       |
| (1,486) | 1:30:A:DA:H1'  | 1:30:A:DA:H5'  | 9                   | 0.22     | 0.07                | 0.2        |
| (1,475) | 1:25:A:DT:H2'' | 1:24:A:DA:H5'' | 9                   | 0.2      | 0.06                | 0.22       |
| (1,552) | 1:8:A:DT:H2'   | 1:8:A:DT:H2''  | 9                   | 0.17     | 0.05                | 0.16       |
| (1,216) | 1:7:A:DG:H2''  | 1:7:A:DG:H8    | 8                   | 0.28     | 0.1                 | 0.34       |
| (1,189) | 1:5:A:DC:H5    | 1:5:A:DC:H3'   | 8                   | 0.28     | 0.11                | 0.24       |
| (1,487) | 1:30:A:DA:H8   | 1:30:A:DA:H4'  | 8                   | 0.26     | 0.08                | 0.26       |
| (1,46)  | 1:3:A:DG:H8    | 1:2:A:DG:H1'   | 8                   | 0.24     | 0.07                | 0.22       |
| (1,514) | 1:16:A:DG:H2'  | 1:16:A:DG:H3'  | 8                   | 0.23     | 0.06                | 0.24       |
| (1,535) | 1:29:A:DG:H2'' | 1:29:A:DG:H4'  | 8                   | 0.22     | 0.06                | 0.24       |
| (1,311) | 1:32:A:DG:H1'  | 1:32:A:DG:H5'  | 8                   | 0.21     | 0.06                | 0.18       |
| (1,497) | 1:1:A:DA:H2    | 1:2:A:DG:H5''  | 8                   | 0.19     | 0.06                | 0.18       |
| (1,22)  | 1:25:A:DT:H6   | 1:24:A:DA:H1'  | 8                   | 0.18     | 0.07                | 0.15       |
| (1,301) | 1:30:A:DA:H8   | 1:30:A:DA:H2'' | 8                   | 0.18     | 0.06                | 0.18       |
| (1,101) | 1:29:A:DG:H1'  | 1:29:A:DG:H2'' | 8                   | 0.17     | 0.05                | 0.16       |
| (1,90)  | 1:7:A:DG:H2'   | 1:7:A:DG:H2''  | 8                   | 0.13     | 0.02                | 0.12       |
| (1,354) | 1:10:A:DT:H5'  | 1:7:A:DG:H3'   | 7                   | 1.61     | 0.97                | 1.86       |
| (1,354) | 1:10:A:DT:H5'' | 1:7:A:DG:H3'   | 7                   | 1.61     | 0.97                | 1.86       |
| (1,52)  | 1:4:A:DG:H8    | 1:4:A:DG:H3'   | 7                   | 0.29     | 0.1                 | 0.29       |
| (1,225) | 1:9:A:DG:H3'   | 1:9:A:DG:H2''  | 7                   | 0.27     | 0.09                | 0.23       |
| (1,244) | 1:11:A:DG:H8   | 1:11:A:DG:H2'' | 7                   | 0.26     | 0.15                | 0.18       |
| (1,259) | 1:13:A:DG:H8   | 1:12:A:DG:H3'  | 7                   | 0.25     | 0.04                | 0.26       |
| (1,215) | 1:7:A:DG:H2'   | 1:7:A:DG:H8    | 7                   | 0.21     | 0.07                | 0.2        |
| (1,331) | 1:14:A:DA:H8   | 1:14:A:DA:H1'  | 7                   | 0.2      | 0.08                | 0.23       |
| (1,47)  | 1:3:A:DG:H8    | 1:3:A:DG:H3'   | 7                   | 0.2      | 0.06                | 0.22       |
| (1,419) | 1:17:A:DA:H8   | 1:17:A:DA:H3'  | 7                   | 0.2      | 0.06                | 0.2        |
| (1,423) | 1:5:A:DC:H6    | 1:5:A:DC:H4'   | 7                   | 0.19     | 0.04                | 0.19       |
| (1,390) | 1:22:A:DA:H8   | 1:22:A:DA:H2'' | 7                   | 0.19     | 0.07                | 0.19       |
| (1,520) | 1:17:A:DA:H4'  | 1:17:A:DA:H5'  | 7                   | 0.18     | 0.05                | 0.16       |
| (1,80)  | 1:25:A:DT:H1'  | 1:25:A:DT:H5'  | 7                   | 0.18     | 0.04                | 0.18       |
| (1,7)   | 1:7:A:DG:H1    | 1:11:A:DG:H1   | 7                   | 0.17     | 0.05                | 0.16       |
| (1,276) | 1:23:A:DG:H1'  | 1:23:A:DG:H2'' | 7                   | 0.17     | 0.05                | 0.18       |
| (1,193) | 1:3:A:DG:H1'   | 1:3:A:DG:H4'   | 7                   | 0.17     | 0.05                | 0.15       |
| (1,318) | 1:29:A:DG:H1'  | 1:31:A:DG:H8   | 6                   | 0.29     | 0.07                | 0.29       |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'  | 6                   | 0.24     | 0.04                | 0.23       |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'' | 6                   | 0.24     | 0.04                | 0.23       |
| (1,526) | 1:32:A:DG:H5'  | 1:31:A:DG:H5'  | 6                   | 0.23     | 0.06                | 0.24       |
| (1,25)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'' | 6                   | 0.22     | 0.03                | 0.2        |
| (1,124) | 1:4:A:DG:H8    | 1:3:A:DG:H2'   | 6                   | 0.22     | 0.06                | 0.2        |
| (1,76)  | 1:13:A:DG:H1   | 1:28:A:DG:H8   | 6                   | 0.19     | 0.07                | 0.22       |
| (1,372) | 1:19:A:DG:H8   | 1:19:A:DG:H1'  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,51)  | 1:3:A:DG:H8    | 1:2:A:DG:H2''  | 6                   | 0.19     | 0.06                | 0.19       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,425) | 1:17:A:DA:H8   | 1:17:A:DA:H4'  | 6                   | 0.19     | 0.06                | 0.18       |
| (1,412) | 1:19:A:DG:H8   | 1:19:A:DG:H2'  | 6                   | 0.19     | 0.03                | 0.18       |
| (1,123) | 1:4:A:DG:H8    | 1:3:A:DG:H2''  | 6                   | 0.18     | 0.06                | 0.16       |
| (1,224) | 1:9:A:DG:H1'   | 1:9:A:DG:H2''  | 6                   | 0.17     | 0.04                | 0.16       |
| (1,105) | 1:29:A:DG:H8   | 1:29:A:DG:H3'  | 6                   | 0.16     | 0.05                | 0.16       |
| (1,451) | 1:14:A:DA:H1'  | 1:14:A:DA:H2'  | 6                   | 0.16     | 0.03                | 0.15       |
| (1,251) | 1:11:A:DG:H2'' | 1:11:A:DG:H3'  | 6                   | 0.14     | 0.04                | 0.12       |
| (1,513) | 1:21:A:DA:H1'  | 1:20:A:DG:H5'  | 5                   | 0.32     | 0.12                | 0.33       |
| (1,359) | 1:25:A:DT:H5'  | 1:24:A:DA:H2'  | 5                   | 0.29     | 0.16                | 0.26       |
| (1,359) | 1:25:A:DT:H5'' | 1:24:A:DA:H2'  | 5                   | 0.29     | 0.16                | 0.26       |
| (1,407) | 1:20:A:DG:H1'  | 1:19:A:DG:H5'  | 5                   | 0.24     | 0.09                | 0.28       |
| (1,280) | 1:1:A:DA:H8    | 1:1:A:DA:H5'   | 5                   | 0.24     | 0.1                 | 0.22       |
| (1,28)  | 1:26:A:DG:H8   | 1:26:A:DG:H2'' | 5                   | 0.21     | 0.07                | 0.19       |
| (1,491) | 1:13:A:DG:H5'  | 1:31:A:DG:H8   | 5                   | 0.21     | 0.05                | 0.2        |
| (1,548) | 1:32:A:DG:H2'  | 1:32:A:DG:H5'  | 5                   | 0.2      | 0.08                | 0.15       |
| (1,199) | 1:6:A:DG:H3'   | 1:6:A:DG:H2'   | 5                   | 0.19     | 0.1                 | 0.14       |
| (1,227) | 1:9:A:DG:H8    | 1:9:A:DG:H4'   | 5                   | 0.19     | 0.04                | 0.2        |
| (1,385) | 1:28:A:DG:H1   | 1:30:A:DA:H8   | 5                   | 0.16     | 0.03                | 0.16       |
| (1,103) | 1:28:A:DG:H8   | 1:28:A:DG:H3'  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,48)  | 1:2:A:DG:H8    | 1:2:A:DG:H2''  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,41)  | 1:2:A:DG:H8    | 1:2:A:DG:H3'   | 5                   | 0.15     | 0.05                | 0.13       |
| (1,145) | 1:5:A:DC:H2''  | 1:5:A:DC:H2'   | 5                   | 0.15     | 0.04                | 0.14       |
| (1,479) | 1:30:A:DA:H8   | 1:30:A:DA:H3'  | 5                   | 0.14     | 0.03                | 0.13       |
| (1,119) | 1:2:A:DG:H3'   | 1:2:A:DG:H2''  | 5                   | 0.14     | 0.03                | 0.13       |
| (1,265) | 1:13:A:DG:H1'  | 1:13:A:DG:H2'' | 5                   | 0.12     | 0.02                | 0.11       |
| (1,228) | 1:9:A:DG:H1'   | 1:7:A:DG:H3'   | 4                   | 0.28     | 0.09                | 0.3        |
| (1,544) | 1:22:A:DA:H2'' | 1:21:A:DA:H5'' | 4                   | 0.28     | 0.07                | 0.29       |
| (1,539) | 1:21:A:DA:H2'  | 1:21:A:DA:H5'' | 4                   | 0.25     | 0.08                | 0.29       |
| (1,313) | 1:32:A:DG:H8   | 1:32:A:DG:H4'  | 4                   | 0.22     | 0.03                | 0.22       |
| (1,511) | 1:25:A:DT:H6   | 1:12:A:DG:H8   | 4                   | 0.21     | 0.09                | 0.22       |
| (1,448) | 1:15:A:DA:H8   | 1:15:A:DA:H2'' | 4                   | 0.21     | 0.06                | 0.19       |
| (1,6)   | 1:11:A:DG:H1   | 1:26:A:DG:H1   | 4                   | 0.21     | 0.08                | 0.21       |
| (1,210) | 1:7:A:DG:H2''  | 1:7:A:DG:H1'   | 4                   | 0.21     | 0.07                | 0.18       |
| (1,408) | 1:19:A:DG:H1'  | 1:19:A:DG:H5'' | 4                   | 0.19     | 0.03                | 0.2        |
| (1,498) | 1:1:A:DA:H2    | 1:2:A:DG:H5'   | 4                   | 0.19     | 0.05                | 0.21       |
| (1,441) | 1:7:A:DG:H1'   | 1:9:A:DG:H1'   | 4                   | 0.18     | 0.05                | 0.2        |
| (1,250) | 1:11:A:DG:H1'  | 1:11:A:DG:H2'' | 4                   | 0.18     | 0.04                | 0.2        |
| (1,290) | 1:1:A:DA:H5'   | 1:1:A:DA:H2'   | 4                   | 0.18     | 0.07                | 0.18       |
| (1,481) | 1:2:A:DG:H8    | 1:1:A:DA:H3'   | 4                   | 0.18     | 0.06                | 0.15       |
| (1,324) | 1:32:A:DG:H8   | 1:31:A:DG:H2'' | 4                   | 0.17     | 0.06                | 0.16       |
| (1,64)  | 1:8:A:DT:H5'   | 1:8:A:DT:H1'   | 4                   | 0.16     | 0.04                | 0.15       |
| (1,64)  | 1:8:A:DT:H5''  | 1:8:A:DT:H1'   | 4                   | 0.16     | 0.04                | 0.15       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,139) | 1:5:A:DC:H6    | 1:5:A:DC:H2'   | 4                   | 0.16     | 0.05                | 0.13       |
| (1,314) | 1:32:A:DG:H8   | 1:32:A:DG:H5'  | 4                   | 0.15     | 0.02                | 0.16       |
| (1,384) | 1:28:A:DG:H1   | 1:27:A:DG:H8   | 4                   | 0.15     | 0.02                | 0.15       |
| (1,78)  | 1:25:A:DT:H1'  | 1:25:A:DT:H2'' | 4                   | 0.15     | 0.02                | 0.14       |
| (1,84)  | 1:26:A:DG:H1'  | 1:26:A:DG:H2'' | 4                   | 0.14     | 0.03                | 0.12       |
| (1,154) | 1:25:A:DT:H5'  | 1:27:A:DG:H8   | 3                   | 0.7      | 0.32                | 0.79       |
| (1,154) | 1:25:A:DT:H5'' | 1:27:A:DG:H8   | 3                   | 0.7      | 0.32                | 0.79       |
| (1,30)  | 1:25:A:DT:H5'  | 1:24:A:DA:H8   | 3                   | 0.27     | 0.1                 | 0.24       |
| (1,30)  | 1:25:A:DT:H5'' | 1:24:A:DA:H8   | 3                   | 0.27     | 0.1                 | 0.24       |
| (1,254) | 1:12:A:DG:H8   | 1:11:A:DG:H2'' | 3                   | 0.27     | 0.07                | 0.22       |
| (1,494) | 1:3:A:DG:H8    | 1:2:A:DG:H5''  | 3                   | 0.26     | 0.04                | 0.25       |
| (1,180) | 1:9:A:DG:H8    | 1:7:A:DG:H1'   | 3                   | 0.25     | 0.09                | 0.3        |
| (1,527) | 1:21:A:DA:H5'  | 1:17:A:DA:H5'  | 3                   | 0.24     | 0.07                | 0.28       |
| (1,110) | 1:29:A:DG:H8   | 1:28:A:DG:H2'' | 3                   | 0.24     | 0.09                | 0.26       |
| (1,383) | 1:26:A:DG:H1   | 1:1:A:DA:H8    | 3                   | 0.24     | 0.01                | 0.24       |
| (1,24)  | 1:24:A:DA:H8   | 1:23:A:DG:H1'  | 3                   | 0.22     | 0.07                | 0.23       |
| (1,411) | 1:19:A:DG:H8   | 1:19:A:DG:H2'' | 3                   | 0.21     | 0.05                | 0.19       |
| (1,219) | 1:7:A:DG:H2'   | 1:9:A:DG:H8    | 3                   | 0.2      | 0.04                | 0.22       |
| (1,482) | 1:30:A:DA:H8   | 1:30:A:DA:H5'' | 3                   | 0.19     | 0.05                | 0.19       |
| (1,443) | 1:15:A:DA:H1'  | 1:15:A:DA:H5'  | 3                   | 0.19     | 0.08                | 0.14       |
| (1,129) | 1:10:A:DT:H6   | 1:10:A:DT:H2'  | 3                   | 0.19     | 0.02                | 0.18       |
| (1,49)  | 1:2:A:DG:H8    | 1:2:A:DG:H2'   | 3                   | 0.18     | 0.05                | 0.18       |
| (1,449) | 1:15:A:DA:H1'  | 1:15:A:DA:H2'' | 3                   | 0.18     | 0.04                | 0.19       |
| (1,549) | 1:30:A:DA:H2'  | 1:30:A:DA:H5'  | 3                   | 0.17     | 0.03                | 0.19       |
| (1,332) | 1:27:A:DG:H8   | 1:28:A:DG:H8   | 3                   | 0.17     | 0.06                | 0.14       |
| (1,377) | 1:10:A:DT:H6   | 1:9:A:DG:H8    | 3                   | 0.17     | 0.04                | 0.17       |
| (1,368) | 1:20:A:DG:H1'  | 1:21:A:DA:H8   | 3                   | 0.16     | 0.04                | 0.18       |
| (1,155) | 1:8:A:DT:H6    | 1:8:A:DT:H2''  | 3                   | 0.16     | 0.02                | 0.16       |
| (1,237) | 1:6:A:DG:H8    | 1:6:A:DG:H5''  | 3                   | 0.15     | 0.05                | 0.14       |
| (1,336) | 1:2:A:DG:H1    | 1:3:A:DG:H1'   | 3                   | 0.15     | 0.02                | 0.16       |
| (1,370) | 1:17:A:DA:H1'  | 1:18:A:DG:H8   | 3                   | 0.15     | 0.03                | 0.14       |
| (1,496) | 1:3:A:DG:H1'   | 1:3:A:DG:H5''  | 3                   | 0.15     | 0.04                | 0.13       |
| (1,418) | 1:18:A:DG:H8   | 1:18:A:DG:H2'  | 3                   | 0.14     | 0.02                | 0.14       |
| (1,68)  | 1:27:A:DG:H8   | 1:26:A:DG:H3'  | 3                   | 0.13     | 0.03                | 0.12       |
| (1,113) | 1:29:A:DG:H2'' | 1:29:A:DG:H2'  | 3                   | 0.13     | 0.01                | 0.14       |
| (1,260) | 1:13:A:DG:H8   | 1:12:A:DG:H2'  | 3                   | 0.13     | 0.02                | 0.14       |
| (1,74)  | 1:28:A:DG:H1'  | 1:29:A:DG:H8   | 3                   | 0.12     | 0.02                | 0.13       |
| (1,402) | 1:20:A:DG:H1'  | 1:21:A:DA:H5'' | 2                   | 0.29     | 0.08                | 0.29       |
| (1,295) | 1:12:A:DG:H8   | 1:13:A:DG:H8   | 2                   | 0.28     | 0.02                | 0.28       |
| (1,234) | 1:7:A:DG:H8    | 1:7:A:DG:H3'   | 2                   | 0.27     | 0.02                | 0.27       |
| (1,21)  | 1:8:A:DT:H6    | 1:8:A:DT:H1'   | 2                   | 0.22     | 0.07                | 0.22       |
| (1,363) | 1:11:A:DG:H8   | 1:12:A:DG:H8   | 2                   | 0.22     | 0.07                | 0.22       |

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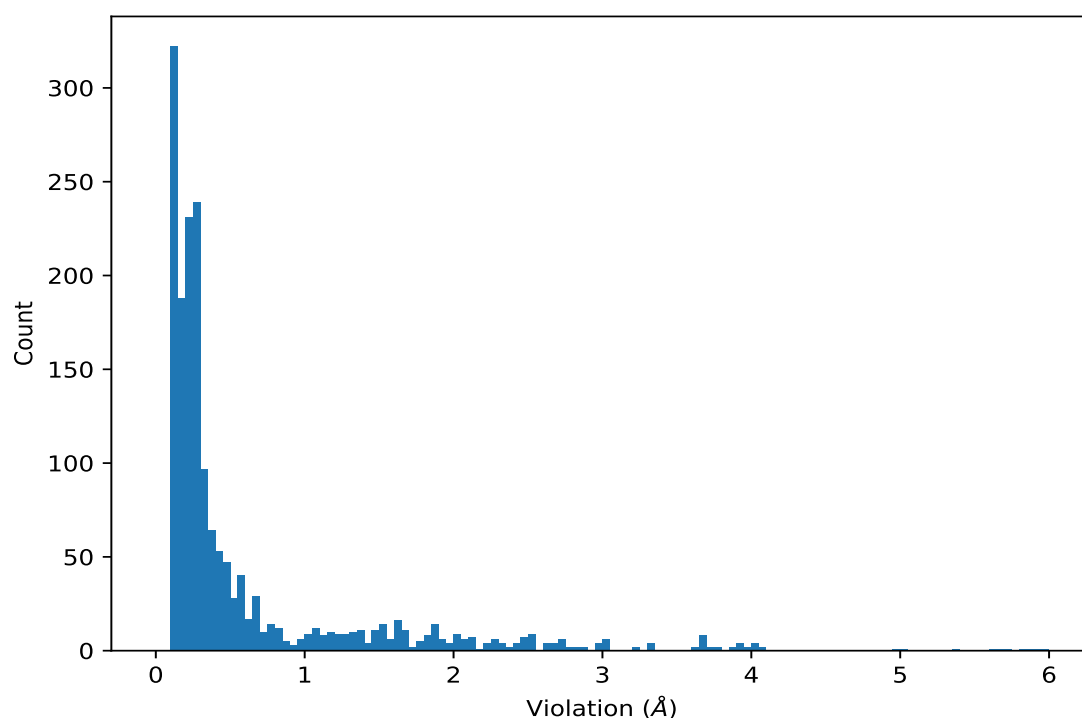
| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,281) | 1:2:A:DG:H8    | 1:1:A:DA:H5'   | 2                   | 0.22     | 0.06                | 0.22       |
| (1,69)  | 1:27:A:DG:H8   | 1:27:A:DG:H3'  | 2                   | 0.2      | 0.03                | 0.2        |
| (1,277) | 1:23:A:DG:H8   | 1:23:A:DG:H3'  | 2                   | 0.19     | 0.09                | 0.19       |
| (1,507) | 1:3:A:DG:H4'   | 1:1:A:DA:H2    | 2                   | 0.18     | 0.03                | 0.18       |
| (1,109) | 1:29:A:DG:H8   | 1:28:A:DG:H2'  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,524) | 1:16:A:DG:H4'  | 1:16:A:DG:H5'  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,95)  | 1:28:A:DG:H1'  | 1:28:A:DG:H2'' | 2                   | 0.17     | 0.03                | 0.17       |
| (1,230) | 1:9:A:DG:H1'   | 1:9:A:DG:H5''  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,386) | 1:13:A:DG:H1'  | 1:14:A:DA:H8   | 2                   | 0.16     | 0.01                | 0.16       |
| (1,508) | 1:12:A:DG:H8   | 1:12:A:DG:H5'  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,241) | 1:6:A:DG:H8    | 1:6:A:DG:H2''  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,509) | 1:12:A:DG:H1'  | 1:12:A:DG:H5'  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,436) | 1:16:A:DG:H8   | 1:16:A:DG:H2'  | 2                   | 0.15     | 0.04                | 0.15       |
| (1,440) | 1:15:A:DA:H8   | 1:15:A:DA:H3'  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,240) | 1:11:A:DG:H8   | 1:11:A:DG:H3'  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,288) | 1:1:A:DA:H1'   | 1:1:A:DA:H4'   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,308) | 1:32:A:DG:H8   | 1:32:A:DG:H2'  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,32)  | 1:25:A:DT:H6   | 1:26:A:DG:H8   | 2                   | 0.13     | 0.03                | 0.13       |
| (1,204) | 1:6:A:DG:H3'   | 1:6:A:DG:H5'   | 2                   | 0.13     | 0.02                | 0.13       |
| (1,220) | 1:7:A:DG:H2''  | 1:9:A:DG:H8    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,375) | 1:16:A:DG:H8   | 1:15:A:DA:H1'  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,447) | 1:15:A:DA:H8   | 1:15:A:DA:H2'  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,401) | 1:20:A:DG:H1'  | 1:21:A:DA:H5'  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,538) | 1:25:A:DT:H2'' | 1:25:A:DT:H5'  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,414) | 1:18:A:DG:H8   | 1:18:A:DG:H3'  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,480) | 1:13:A:DG:H5'  | 1:14:A:DA:H2   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,504) | 1:11:A:DG:H1'  | 1:11:A:DG:H5'  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,547) | 1:32:A:DG:H2'' | 1:32:A:DG:H5'  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,27)  | 1:26:A:DG:H8   | 1:25:A:DT:H2'' | 2                   | 0.12     | 0.02                | 0.12       |
| (1,389) | 1:22:A:DA:H8   | 1:22:A:DA:H2'  | 2                   | 0.12     | 0.02                | 0.12       |

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

### 9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



### 9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,380) | 1:10:A:DT:H6  | 1:8:A:DT:H6  | 8        | 6.0           |
| (1,380) | 1:10:A:DT:H6  | 1:8:A:DT:H6  | 10       | 5.94          |
| (1,380) | 1:10:A:DT:H6  | 1:8:A:DT:H6  | 3        | 5.88          |
| (1,380) | 1:10:A:DT:H6  | 1:8:A:DT:H6  | 7        | 5.82          |
| (1,380) | 1:10:A:DT:H6  | 1:8:A:DT:H6  | 9        | 5.7           |
| (1,380) | 1:10:A:DT:H6  | 1:8:A:DT:H6  | 6        | 5.67          |
| (1,380) | 1:10:A:DT:H6  | 1:8:A:DT:H6  | 5        | 5.64          |
| (1,380) | 1:10:A:DT:H6  | 1:8:A:DT:H6  | 4        | 5.38          |
| (1,380) | 1:10:A:DT:H6  | 1:8:A:DT:H6  | 1        | 5.03          |
| (1,380) | 1:10:A:DT:H6  | 1:8:A:DT:H6  | 2        | 4.96          |
| (1,348) | 1:8:A:DT:H5'  | 1:4:A:DG:H8  | 8        | 4.05          |
| (1,348) | 1:8:A:DT:H5'' | 1:4:A:DG:H8  | 8        | 4.05          |
| (1,361) | 1:8:A:DT:H5'  | 1:4:A:DG:H2' | 7        | 4.03          |
| (1,361) | 1:8:A:DT:H5'' | 1:4:A:DG:H2' | 7        | 4.03          |
| (1,361) | 1:8:A:DT:H5'  | 1:4:A:DG:H2' | 8        | 4.0           |
| (1,361) | 1:8:A:DT:H5'' | 1:4:A:DG:H2' | 8        | 4.0           |

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| Key     | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,348) | 1:8:A:DT:H5'   | 1:4:A:DG:H8   | 6        | 3.98          |
| (1,348) | 1:8:A:DT:H5''  | 1:4:A:DG:H8   | 6        | 3.98          |
| (1,361) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'  | 6        | 3.93          |
| (1,361) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'  | 6        | 3.93          |
| (1,348) | 1:8:A:DT:H5'   | 1:4:A:DG:H8   | 1        | 3.92          |
| (1,348) | 1:8:A:DT:H5''  | 1:4:A:DG:H8   | 1        | 3.92          |
| (1,361) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'  | 10       | 3.9           |
| (1,361) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'  | 10       | 3.9           |
| (1,348) | 1:8:A:DT:H5'   | 1:4:A:DG:H8   | 9        | 3.75          |
| (1,348) | 1:8:A:DT:H5''  | 1:4:A:DG:H8   | 9        | 3.75          |
| (1,348) | 1:8:A:DT:H5'   | 1:4:A:DG:H8   | 10       | 3.7           |
| (1,348) | 1:8:A:DT:H5''  | 1:4:A:DG:H8   | 10       | 3.7           |
| (1,361) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'  | 5        | 3.67          |
| (1,361) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'  | 5        | 3.67          |
| (1,348) | 1:8:A:DT:H5'   | 1:4:A:DG:H8   | 2        | 3.67          |
| (1,348) | 1:8:A:DT:H5''  | 1:4:A:DG:H8   | 2        | 3.67          |
| (1,361) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'  | 9        | 3.66          |
| (1,361) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'  | 9        | 3.66          |
| (1,348) | 1:8:A:DT:H5'   | 1:4:A:DG:H8   | 5        | 3.66          |
| (1,348) | 1:8:A:DT:H5''  | 1:4:A:DG:H8   | 5        | 3.66          |
| (1,348) | 1:8:A:DT:H5'   | 1:4:A:DG:H8   | 7        | 3.64          |
| (1,348) | 1:8:A:DT:H5''  | 1:4:A:DG:H8   | 7        | 3.64          |
| (1,348) | 1:8:A:DT:H5'   | 1:4:A:DG:H8   | 4        | 3.34          |
| (1,348) | 1:8:A:DT:H5''  | 1:4:A:DG:H8   | 4        | 3.34          |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8  | 5        | 3.33          |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8  | 5        | 3.33          |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8  | 3        | 3.23          |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8  | 3        | 3.23          |
| (1,361) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'  | 2        | 3.05          |
| (1,361) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'  | 2        | 3.05          |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8  | 4        | 3.04          |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8  | 4        | 3.04          |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8  | 2        | 3.01          |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8  | 2        | 3.01          |
| (1,361) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'  | 1        | 2.98          |
| (1,361) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'  | 1        | 2.98          |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8  | 1        | 2.96          |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8  | 1        | 2.96          |
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1' | 7        | 2.86          |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1' | 7        | 2.86          |
| (1,348) | 1:8:A:DT:H5'   | 1:4:A:DG:H8   | 3        | 2.83          |
| (1,348) | 1:8:A:DT:H5''  | 1:4:A:DG:H8   | 3        | 2.83          |

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| Key     | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'  | 8        | 2.77          |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'  | 8        | 2.77          |
| (1,361) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'  | 4        | 2.72          |
| (1,361) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'  | 4        | 2.72          |
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'  | 1        | 2.72          |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'  | 1        | 2.72          |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8   | 6        | 2.7           |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8   | 7        | 2.7           |
| (1,354) | 1:10:A:DT:H5'  | 1:7:A:DG:H3'  | 3        | 2.67          |
| (1,354) | 1:10:A:DT:H5'' | 1:7:A:DG:H3'  | 3        | 2.67          |
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1' | 10       | 2.66          |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1' | 10       | 2.66          |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8   | 9        | 2.64          |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8   | 8        | 2.63          |
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'  | 6        | 2.62          |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'  | 6        | 2.62          |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'' | 7        | 2.54          |
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'' | 7        | 2.54          |
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1' | 9        | 2.52          |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1' | 9        | 2.52          |
| (1,361) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'  | 3        | 2.5           |
| (1,361) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'  | 3        | 2.5           |
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'  | 9        | 2.5           |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'  | 9        | 2.5           |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8   | 1        | 2.5           |
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1' | 2        | 2.49          |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1' | 2        | 2.49          |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8   | 2        | 2.47          |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'' | 8        | 2.46          |
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'' | 8        | 2.46          |
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'  | 2        | 2.46          |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'  | 2        | 2.46          |
| (1,354) | 1:10:A:DT:H5'  | 1:7:A:DG:H3'  | 4        | 2.44          |
| (1,354) | 1:10:A:DT:H5'' | 1:7:A:DG:H3'  | 4        | 2.44          |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2'' | 6        | 2.41          |
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2'' | 6        | 2.41          |
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'  | 7        | 2.35          |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'  | 7        | 2.35          |
| (1,354) | 1:10:A:DT:H5'  | 1:7:A:DG:H3'  | 1        | 2.33          |
| (1,354) | 1:10:A:DT:H5'' | 1:7:A:DG:H3'  | 1        | 2.33          |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8  | 10       | 2.31          |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8  | 10       | 2.31          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1'  | 8        | 2.3           |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1'  | 8        | 2.3           |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2''  | 10       | 2.29          |
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2''  | 10       | 2.29          |
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1'  | 6        | 2.27          |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1'  | 6        | 2.27          |
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1'  | 1        | 2.24          |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1'  | 1        | 2.24          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 2        | 2.21          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 2        | 2.21          |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8    | 10       | 2.17          |
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'   | 4        | 2.13          |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'   | 4        | 2.13          |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8    | 4        | 2.12          |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2''  | 9        | 2.11          |
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2''  | 9        | 2.11          |
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'   | 5        | 2.11          |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'   | 5        | 2.11          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 1        | 2.08          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 1        | 2.08          |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8   | 8        | 2.07          |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8   | 8        | 2.07          |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2''  | 5        | 2.06          |
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2''  | 5        | 2.06          |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8    | 5        | 2.04          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 8        | 2.04          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 8        | 2.04          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 2        | 2.03          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 2        | 2.03          |
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'   | 1        | 2.01          |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8   | 7        | 2.01          |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8   | 7        | 2.01          |
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'   | 2        | 2.0           |
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 7        | 1.99          |
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'   | 6        | 1.97          |
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 1        | 1.97          |
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'   | 5        | 1.96          |
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 8        | 1.94          |
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 9        | 1.93          |
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 10       | 1.93          |
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'   | 10       | 1.92          |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'   | 10       | 1.92          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'   | 10       | 1.91          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 10       | 1.9           |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 10       | 1.9           |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 1        | 1.89          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 1        | 1.89          |
| (1,166) | 1:3:A:DG:H1    | 1:9:A:DG:H8    | 3        | 1.88          |
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'   | 3        | 1.87          |
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'   | 9        | 1.87          |
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'   | 4        | 1.86          |
| (1,354) | 1:10:A:DT:H5'  | 1:7:A:DG:H3'   | 5        | 1.86          |
| (1,354) | 1:10:A:DT:H5'' | 1:7:A:DG:H3'   | 5        | 1.86          |
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 3        | 1.86          |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2''  | 2        | 1.85          |
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2''  | 2        | 1.85          |
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 5        | 1.85          |
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'   | 8        | 1.84          |
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 2        | 1.84          |
| (1,502) | 1:2:A:DG:H1'   | 1:2:A:DG:H4'   | 7        | 1.8           |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8   | 9        | 1.8           |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8   | 9        | 1.8           |
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 6        | 1.8           |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 7        | 1.8           |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 7        | 1.8           |
| (1,107) | 1:28:A:DG:H2'  | 1:28:A:DG:H3'  | 4        | 1.79          |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 10       | 1.77          |
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 7        | 1.75          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 9        | 1.75          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 9        | 1.75          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 6        | 1.74          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 6        | 1.74          |
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1'  | 3        | 1.7           |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1'  | 3        | 1.7           |
| (1,490) | 1:8:A:DT:H5'   | 1:31:A:DG:H8   | 6        | 1.69          |
| (1,490) | 1:8:A:DT:H5''  | 1:31:A:DG:H8   | 6        | 1.69          |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 2        | 1.69          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 9        | 1.69          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 9        | 1.69          |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 9        | 1.67          |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 9        | 1.67          |
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1'  | 4        | 1.66          |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1'  | 4        | 1.66          |
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 8        | 1.64          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 10       | 1.64          |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 6        | 1.64          |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 6        | 1.64          |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 8        | 1.64          |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 8        | 1.64          |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 5        | 1.63          |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 5        | 1.63          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 5        | 1.63          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 5        | 1.63          |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2''  | 1        | 1.61          |
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2''  | 1        | 1.61          |
| (1,354) | 1:10:A:DT:H5'  | 1:7:A:DG:H3'   | 2        | 1.61          |
| (1,354) | 1:10:A:DT:H5'' | 1:7:A:DG:H3'   | 2        | 1.61          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 5        | 1.61          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 5        | 1.61          |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 7        | 1.57          |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 7        | 1.57          |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 5        | 1.57          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 4        | 1.55          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 4        | 1.55          |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 4        | 1.55          |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 4        | 1.54          |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 4        | 1.54          |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 9        | 1.54          |
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 6        | 1.53          |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 2        | 1.52          |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 2        | 1.52          |
| (1,350) | 1:25:A:DT:H5'  | 1:11:A:DG:H1'  | 5        | 1.51          |
| (1,350) | 1:25:A:DT:H5'' | 1:11:A:DG:H1'  | 5        | 1.51          |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 3        | 1.51          |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 1        | 1.5           |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 1        | 1.5           |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 8        | 1.5           |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 8        | 1.5           |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 6        | 1.5           |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 10       | 1.49          |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 10       | 1.49          |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 3        | 1.49          |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 3        | 1.49          |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 7        | 1.49          |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 7        | 1.49          |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2''  | 4        | 1.48          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2''  | 4        | 1.48          |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 3        | 1.47          |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 3        | 1.47          |
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 9        | 1.46          |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 9        | 1.42          |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 9        | 1.42          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 7        | 1.42          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 7        | 1.42          |
| (1,349) | 1:8:A:DT:H5'   | 1:4:A:DG:H1'   | 3        | 1.4           |
| (1,349) | 1:8:A:DT:H5''  | 1:4:A:DG:H1'   | 3        | 1.4           |
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 3        | 1.39          |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 5        | 1.39          |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 1        | 1.38          |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 5        | 1.37          |
| (1,357) | 1:25:A:DT:H5'  | 1:25:A:DT:H2'  | 4        | 1.37          |
| (1,357) | 1:25:A:DT:H5'' | 1:25:A:DT:H2'  | 4        | 1.37          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 10       | 1.37          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 10       | 1.37          |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 3        | 1.35          |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 4        | 1.33          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 4        | 1.33          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 4        | 1.33          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5'   | 3        | 1.32          |
| (1,17)  | 1:8:A:DT:H6    | 1:8:A:DT:H5''  | 3        | 1.32          |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 9        | 1.31          |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 2        | 1.31          |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 6        | 1.3           |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 6        | 1.3           |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 8        | 1.3           |
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 2        | 1.29          |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 3        | 1.29          |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 10       | 1.29          |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 8        | 1.29          |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 8        | 1.29          |
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 10       | 1.27          |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 6        | 1.27          |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 6        | 1.27          |
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 6        | 1.25          |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 8        | 1.24          |
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 5        | 1.23          |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 2        | 1.23          |
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 7        | 1.22          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 10       | 1.22          |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 4        | 1.22          |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 7        | 1.22          |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 3        | 1.22          |
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 8        | 1.21          |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 6        | 1.2           |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'  | 3        | 1.2           |
| (1,342) | 1:11:A:DG:H1   | 1:25:A:DT:H5'' | 3        | 1.2           |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 2        | 1.2           |
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 5        | 1.19          |
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 8        | 1.18          |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 1        | 1.17          |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 10       | 1.17          |
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 1        | 1.16          |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 9        | 1.16          |
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 1        | 1.15          |
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 9        | 1.14          |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 4        | 1.14          |
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 4        | 1.12          |
| (1,471) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'  | 4        | 1.12          |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 5        | 1.11          |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 5        | 1.11          |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 10       | 1.1           |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 7        | 1.09          |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 10       | 1.08          |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 10       | 1.08          |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 7        | 1.08          |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 8        | 1.08          |
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 1        | 1.07          |
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 4        | 1.07          |
| (1,360) | 1:8:A:DT:H5'   | 1:4:A:DG:H2''  | 3        | 1.07          |
| (1,360) | 1:8:A:DT:H5''  | 1:4:A:DG:H2''  | 3        | 1.07          |
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 9        | 1.06          |
| (1,470) | 1:15:A:DA:H3'  | 1:15:A:DA:H2'' | 1        | 1.06          |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 9        | 1.05          |
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 7        | 1.04          |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 1        | 1.04          |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 6        | 1.04          |
| (1,154) | 1:25:A:DT:H5'  | 1:27:A:DG:H8   | 2        | 1.04          |
| (1,154) | 1:25:A:DT:H5'' | 1:27:A:DG:H8   | 2        | 1.04          |
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 6        | 1.03          |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 6        | 1.02          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 2        | 1.0           |
| (1,338) | 1:27:A:DG:H1   | 1:27:A:DG:H1'  | 5        | 1.0           |
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 2        | 0.99          |
| (1,223) | 1:9:A:DG:H8    | 1:9:A:DG:H2''  | 7        | 0.99          |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 6        | 0.99          |
| (1,501) | 1:2:A:DG:H1'   | 1:2:A:DG:H5''  | 3        | 0.96          |
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 3        | 0.96          |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 6        | 0.96          |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 1        | 0.92          |
| (1,488) | 1:28:A:DG:H1   | 1:30:A:DA:H4'  | 5        | 0.9           |
| (1,466) | 1:7:A:DG:H2''  | 1:9:A:DG:H1    | 8        | 0.9           |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 7        | 0.89          |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 1        | 0.88          |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 2        | 0.88          |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 8        | 0.88          |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 4        | 0.87          |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 9        | 0.85          |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 3        | 0.85          |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 10       | 0.85          |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 9        | 0.84          |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 9        | 0.84          |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 5        | 0.84          |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 3        | 0.83          |
| (1,120) | 1:2:A:DG:H3'   | 1:2:A:DG:H2'   | 9        | 0.83          |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 3        | 0.82          |
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 3        | 0.82          |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 1        | 0.81          |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 5        | 0.8           |
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 9        | 0.79          |
| (1,154) | 1:25:A:DT:H5'  | 1:27:A:DG:H8   | 1        | 0.79          |
| (1,154) | 1:25:A:DT:H5'' | 1:27:A:DG:H8   | 1        | 0.79          |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 3        | 0.78          |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 4        | 0.78          |
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 2        | 0.77          |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 1        | 0.77          |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 5        | 0.76          |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 6        | 0.76          |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 6        | 0.76          |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 10       | 0.76          |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 4        | 0.76          |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 3        | 0.75          |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 10       | 0.75          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 6        | 0.74          |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 8        | 0.73          |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 8        | 0.73          |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 4        | 0.72          |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 9        | 0.72          |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 4        | 0.72          |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 10       | 0.71          |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 10       | 0.71          |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 1        | 0.71          |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 3        | 0.71          |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 7        | 0.7           |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 8        | 0.7           |
| (1,317) | 1:32:A:DG:H2'' | 1:32:A:DG:H2'  | 2        | 0.69          |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 2        | 0.69          |
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 4        | 0.69          |
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 7        | 0.69          |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 1        | 0.68          |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 1        | 0.68          |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 4        | 0.68          |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 4        | 0.68          |
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 1        | 0.67          |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 2        | 0.67          |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 2        | 0.67          |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 1        | 0.67          |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 7        | 0.67          |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 5        | 0.67          |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 6        | 0.67          |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 10       | 0.67          |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 7        | 0.66          |
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 8        | 0.66          |
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 5        | 0.65          |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 5        | 0.65          |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 5        | 0.65          |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 8        | 0.65          |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 8        | 0.65          |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 1        | 0.65          |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 9        | 0.65          |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 5        | 0.65          |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 9        | 0.65          |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 3        | 0.64          |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 5        | 0.64          |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 8        | 0.64          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 2        | 0.64          |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 7        | 0.63          |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 2        | 0.63          |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 10       | 0.63          |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 3        | 0.63          |
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 3        | 0.62          |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 2        | 0.62          |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 2        | 0.62          |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 7        | 0.62          |
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 5        | 0.62          |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 5        | 0.62          |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 10       | 0.61          |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 3        | 0.61          |
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 9        | 0.61          |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 5        | 0.6           |
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 10       | 0.6           |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 2        | 0.6           |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 6        | 0.6           |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 9        | 0.59          |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 2        | 0.59          |
| (1,359) | 1:25:A:DT:H5'  | 1:24:A:DA:H2'  | 4        | 0.59          |
| (1,359) | 1:25:A:DT:H5'' | 1:24:A:DA:H2'  | 4        | 0.59          |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 6        | 0.59          |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 6        | 0.59          |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 7        | 0.59          |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 7        | 0.59          |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 2        | 0.59          |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 10       | 0.59          |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 4        | 0.59          |
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 8        | 0.58          |
| (1,459) | 1:3:A:DG:H1    | 1:5:A:DC:H1'   | 2        | 0.58          |
| (1,352) | 1:25:A:DT:H5'  | 1:25:A:DT:H1'  | 3        | 0.58          |
| (1,352) | 1:25:A:DT:H5'' | 1:25:A:DT:H1'  | 3        | 0.58          |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 5        | 0.58          |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 2        | 0.58          |
| (1,264) | 1:13:A:DG:H8   | 1:13:A:DG:H2'' | 5        | 0.58          |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 10       | 0.58          |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 1        | 0.57          |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 5        | 0.57          |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 8        | 0.57          |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 6        | 0.57          |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 2        | 0.57          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 7        | 0.56          |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 4        | 0.56          |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 10       | 0.56          |
| (1,244) | 1:11:A:DG:H8   | 1:11:A:DG:H2'' | 1        | 0.56          |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 8        | 0.56          |
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 10       | 0.56          |
| (1,468) | 1:12:A:DG:H2'  | 1:13:A:DG:H1'  | 1        | 0.55          |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 8        | 0.55          |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 8        | 0.55          |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 6        | 0.55          |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 1        | 0.55          |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 10       | 0.55          |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 3        | 0.54          |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 9        | 0.54          |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 9        | 0.53          |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 10       | 0.53          |
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 9        | 0.53          |
| (1,252) | 1:11:A:DG:H2'  | 1:11:A:DG:H3'  | 1        | 0.53          |
| (1,213) | 1:7:A:DG:H2'   | 1:7:A:DG:H3'   | 7        | 0.53          |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 4        | 0.53          |
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 10       | 0.52          |
| (1,337) | 1:26:A:DG:H1   | 1:27:A:DG:H1'  | 7        | 0.52          |
| (1,298) | 1:8:A:DT:H6    | 1:30:A:DA:H8   | 8        | 0.52          |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 8        | 0.52          |
| (1,35)  | 1:28:A:DG:H1   | 1:3:A:DG:H8    | 8        | 0.52          |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 2        | 0.51          |
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 2        | 0.51          |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 4        | 0.51          |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 4        | 0.51          |
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 5        | 0.51          |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 3        | 0.5           |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 4        | 0.5           |
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 6        | 0.5           |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 1        | 0.5           |
| (1,356) | 1:10:A:DT:H5'  | 1:10:A:DT:H2'  | 1        | 0.5           |
| (1,356) | 1:10:A:DT:H5'' | 1:10:A:DT:H2'  | 1        | 0.5           |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 6        | 0.5           |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 8        | 0.5           |
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 3        | 0.5           |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 3        | 0.5           |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 8        | 0.49          |
| (1,300) | 1:13:A:DG:H5'' | 1:13:A:DG:H5'  | 4        | 0.49          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 5        | 0.49          |
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 7        | 0.49          |
| (1,513) | 1:21:A:DA:H1'  | 1:20:A:DG:H5'  | 9        | 0.48          |
| (1,469) | 1:12:A:DG:H3'  | 1:12:A:DG:H2'  | 4        | 0.48          |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 10       | 0.48          |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 6        | 0.48          |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 1        | 0.48          |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 9        | 0.48          |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 2        | 0.48          |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 7        | 0.48          |
| (1,189) | 1:5:A:DC:H5    | 1:5:A:DC:H3'   | 1        | 0.48          |
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 9        | 0.48          |
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 6        | 0.48          |
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 8        | 0.48          |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 7        | 0.47          |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 8        | 0.47          |
| (1,468) | 1:12:A:DG:H2'  | 1:13:A:DG:H1'  | 4        | 0.47          |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 9        | 0.47          |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 7        | 0.47          |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 7        | 0.47          |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 5        | 0.47          |
| (1,225) | 1:9:A:DG:H3'   | 1:9:A:DG:H2''  | 9        | 0.47          |
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 4        | 0.47          |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 6        | 0.46          |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 1        | 0.46          |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 8        | 0.46          |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 10       | 0.46          |
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 6        | 0.46          |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 2        | 0.46          |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 9        | 0.46          |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 9        | 0.46          |
| (1,192) | 1:4:A:DG:H3'   | 1:4:A:DG:H2'   | 1        | 0.46          |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 2        | 0.46          |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 9        | 0.45          |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 1        | 0.45          |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 3        | 0.45          |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 7        | 0.45          |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 5        | 0.45          |
| (1,263) | 1:13:A:DG:H8   | 1:13:A:DG:H2'  | 7        | 0.45          |
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 1        | 0.45          |
| (1,140) | 1:5:A:DC:H6    | 1:5:A:DC:H2''  | 10       | 0.45          |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 5        | 0.45          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 3        | 0.45          |
| (1,52)  | 1:4:A:DG:H8    | 1:4:A:DG:H3'   | 1        | 0.45          |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 4        | 0.45          |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 2        | 0.44          |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 2        | 0.44          |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 6        | 0.44          |
| (1,459) | 1:3:A:DG:H1    | 1:5:A:DC:H1'   | 1        | 0.44          |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 3        | 0.44          |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 7        | 0.44          |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 10       | 0.44          |
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 7        | 0.44          |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 7        | 0.44          |
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 7        | 0.44          |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 10       | 0.44          |
| (1,528) | 1:21:A:DA:H5'' | 1:21:A:DA:H5'  | 4        | 0.43          |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 6        | 0.43          |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 2        | 0.43          |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 3        | 0.43          |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 3        | 0.43          |
| (1,280) | 1:1:A:DA:H8    | 1:1:A:DA:H5'   | 9        | 0.43          |
| (1,156) | 1:8:A:DT:H6    | 1:8:A:DT:H2'   | 9        | 0.43          |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 2        | 0.43          |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 7        | 0.42          |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 7        | 0.42          |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 4        | 0.42          |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 9        | 0.42          |
| (1,320) | 1:31:A:DG:H8   | 1:31:A:DG:H3'  | 10       | 0.42          |
| (1,171) | 1:7:A:DG:H1    | 1:13:A:DG:H8   | 7        | 0.42          |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 9        | 0.42          |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 3        | 0.41          |
| (1,513) | 1:21:A:DA:H1'  | 1:20:A:DG:H5'  | 7        | 0.41          |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 10       | 0.41          |
| (1,487) | 1:30:A:DA:H8   | 1:30:A:DA:H4'  | 4        | 0.41          |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 2        | 0.41          |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 3        | 0.41          |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 10       | 0.41          |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 4        | 0.41          |
| (1,226) | 1:9:A:DG:H3'   | 1:9:A:DG:H2'   | 9        | 0.41          |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 6        | 0.41          |
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 2        | 0.41          |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 8        | 0.41          |
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 9        | 0.41          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,35)  | 1:28:A:DG:H1   | 1:3:A:DG:H8    | 7        | 0.41          |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 1        | 0.4           |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 5        | 0.4           |
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 2        | 0.4           |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 1        | 0.4           |
| (1,309) | 1:32:A:DG:H1'  | 1:32:A:DG:H2'' | 10       | 0.4           |
| (1,216) | 1:7:A:DG:H2''  | 1:7:A:DG:H8    | 6        | 0.4           |
| (1,171) | 1:7:A:DG:H1    | 1:13:A:DG:H8   | 2        | 0.4           |
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 1        | 0.4           |
| (1,46)  | 1:3:A:DG:H8    | 1:2:A:DG:H1'   | 4        | 0.4           |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 1        | 0.4           |
| (1,30)  | 1:25:A:DT:H5'  | 1:24:A:DA:H8   | 5        | 0.4           |
| (1,30)  | 1:25:A:DT:H5'' | 1:24:A:DA:H8   | 5        | 0.4           |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 9        | 0.4           |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 8        | 0.39          |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 3        | 0.39          |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 3        | 0.39          |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 2        | 0.39          |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 1        | 0.39          |
| (1,228) | 1:9:A:DG:H1'   | 1:7:A:DG:H3'   | 1        | 0.39          |
| (1,226) | 1:9:A:DG:H3'   | 1:9:A:DG:H2'   | 8        | 0.39          |
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 8        | 0.39          |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 6        | 0.39          |
| (1,52)  | 1:4:A:DG:H8    | 1:4:A:DG:H3'   | 3        | 0.39          |
| (1,35)  | 1:28:A:DG:H1   | 1:3:A:DG:H8    | 9        | 0.39          |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 5        | 0.38          |
| (1,467) | 1:30:A:DA:H2'' | 1:31:A:DG:H1'  | 4        | 0.38          |
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 10       | 0.38          |
| (1,318) | 1:29:A:DG:H1'  | 1:31:A:DG:H8   | 6        | 0.38          |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 4        | 0.38          |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 9        | 0.38          |
| (1,244) | 1:11:A:DG:H8   | 1:11:A:DG:H2'' | 3        | 0.38          |
| (1,199) | 1:6:A:DG:H3'   | 1:6:A:DG:H2'   | 7        | 0.38          |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 10       | 0.38          |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 7        | 0.38          |
| (1,35)  | 1:28:A:DG:H1   | 1:3:A:DG:H8    | 1        | 0.38          |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 1        | 0.38          |
| (1,486) | 1:30:A:DA:H1'  | 1:30:A:DA:H5'  | 6        | 0.37          |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 8        | 0.37          |
| (1,402) | 1:20:A:DG:H1'  | 1:21:A:DA:H5'' | 7        | 0.37          |
| (1,351) | 1:25:A:DT:H5'  | 1:24:A:DA:H1'  | 4        | 0.37          |
| (1,351) | 1:25:A:DT:H5'' | 1:24:A:DA:H1'  | 4        | 0.37          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 1        | 0.37          |
| (1,318) | 1:29:A:DG:H1'  | 1:31:A:DG:H8   | 10       | 0.37          |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 9        | 0.37          |
| (1,254) | 1:12:A:DG:H8   | 1:11:A:DG:H2'' | 2        | 0.37          |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 2        | 0.37          |
| (1,189) | 1:5:A:DC:H5    | 1:5:A:DC:H3'   | 10       | 0.37          |
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 6        | 0.37          |
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 8        | 0.37          |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 7        | 0.37          |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 1        | 0.37          |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 1        | 0.37          |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 4        | 0.37          |
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 5        | 0.37          |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 4        | 0.37          |
| (1,35)  | 1:28:A:DG:H1   | 1:3:A:DG:H8    | 5        | 0.37          |
| (1,35)  | 1:28:A:DG:H1   | 1:3:A:DG:H8    | 10       | 0.37          |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 9        | 0.36          |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 2        | 0.36          |
| (1,468) | 1:12:A:DG:H2'  | 1:13:A:DG:H1'  | 10       | 0.36          |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 8        | 0.36          |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 9        | 0.36          |
| (1,407) | 1:20:A:DG:H1'  | 1:19:A:DG:H5'  | 6        | 0.36          |
| (1,388) | 1:22:A:DA:H8   | 1:22:A:DA:H3'  | 1        | 0.36          |
| (1,320) | 1:31:A:DG:H8   | 1:31:A:DG:H3'  | 2        | 0.36          |
| (1,305) | 1:30:A:DA:H2'' | 1:30:A:DA:H2'  | 2        | 0.36          |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 4        | 0.36          |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 9        | 0.36          |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 10       | 0.36          |
| (1,216) | 1:7:A:DG:H2''  | 1:7:A:DG:H8    | 2        | 0.36          |
| (1,216) | 1:7:A:DG:H2''  | 1:7:A:DG:H8    | 10       | 0.36          |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 3        | 0.36          |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 8        | 0.36          |
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 1        | 0.36          |
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 10       | 0.36          |
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 8        | 0.36          |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 5        | 0.36          |
| (1,544) | 1:22:A:DA:H2'' | 1:21:A:DA:H5'' | 4        | 0.35          |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 8        | 0.35          |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 5        | 0.35          |
| (1,459) | 1:3:A:DG:H1    | 1:5:A:DC:H1'   | 7        | 0.35          |
| (1,459) | 1:3:A:DG:H1    | 1:5:A:DC:H1'   | 10       | 0.35          |
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 5        | 0.35          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 9        | 0.35          |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 8        | 0.35          |
| (1,134) | 1:10:A:DT:H3'  | 1:10:A:DT:H2'  | 1        | 0.35          |
| (1,35)  | 1:28:A:DG:H1   | 1:3:A:DG:H8    | 4        | 0.35          |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 8        | 0.34          |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 4        | 0.34          |
| (1,216) | 1:7:A:DG:H2''  | 1:7:A:DG:H8    | 8        | 0.34          |
| (1,189) | 1:5:A:DC:H5    | 1:5:A:DC:H3'   | 7        | 0.34          |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 5        | 0.34          |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 5        | 0.34          |
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 9        | 0.34          |
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 4        | 0.34          |
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 6        | 0.34          |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 8        | 0.34          |
| (1,544) | 1:22:A:DA:H2'' | 1:21:A:DA:H5'' | 3        | 0.33          |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 9        | 0.33          |
| (1,513) | 1:21:A:DA:H1'  | 1:20:A:DG:H5'  | 8        | 0.33          |
| (1,497) | 1:1:A:DA:H2    | 1:2:A:DG:H5''  | 3        | 0.33          |
| (1,487) | 1:30:A:DA:H8   | 1:30:A:DA:H4'  | 10       | 0.33          |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 10       | 0.33          |
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 8        | 0.33          |
| (1,459) | 1:3:A:DG:H1    | 1:5:A:DC:H1'   | 9        | 0.33          |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 6        | 0.33          |
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 10       | 0.33          |
| (1,331) | 1:14:A:DA:H8   | 1:14:A:DA:H1'  | 9        | 0.33          |
| (1,279) | 1:1:A:DA:H8    | 1:1:A:DA:H3'   | 10       | 0.33          |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 5        | 0.33          |
| (1,225) | 1:9:A:DG:H3'   | 1:9:A:DG:H2''  | 8        | 0.33          |
| (1,216) | 1:7:A:DG:H2''  | 1:7:A:DG:H8    | 7        | 0.33          |
| (1,180) | 1:9:A:DG:H8    | 1:7:A:DG:H1'   | 7        | 0.33          |
| (1,171) | 1:7:A:DG:H1    | 1:13:A:DG:H8   | 5        | 0.33          |
| (1,124) | 1:4:A:DG:H8    | 1:3:A:DG:H2'   | 5        | 0.33          |
| (1,110) | 1:29:A:DG:H8   | 1:28:A:DG:H2'' | 7        | 0.33          |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 6        | 0.33          |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 5        | 0.32          |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 10       | 0.32          |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 9        | 0.32          |
| (1,514) | 1:16:A:DG:H2'  | 1:16:A:DG:H3'  | 9        | 0.32          |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 7        | 0.32          |
| (1,494) | 1:3:A:DG:H8    | 1:2:A:DG:H5''  | 2        | 0.32          |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 1        | 0.32          |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 8        | 0.32          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 2        | 0.32          |
| (1,459) | 1:3:A:DG:H1    | 1:5:A:DC:H1'   | 3        | 0.32          |
| (1,372) | 1:19:A:DG:H8   | 1:19:A:DG:H1'  | 3        | 0.32          |
| (1,351) | 1:25:A:DT:H5'  | 1:24:A:DA:H1'  | 9        | 0.32          |
| (1,351) | 1:25:A:DT:H5'' | 1:24:A:DA:H1'  | 9        | 0.32          |
| (1,337) | 1:26:A:DG:H1   | 1:27:A:DG:H1'  | 10       | 0.32          |
| (1,318) | 1:29:A:DG:H1'  | 1:31:A:DG:H8   | 9        | 0.32          |
| (1,311) | 1:32:A:DG:H1'  | 1:32:A:DG:H5'  | 9        | 0.32          |
| (1,298) | 1:8:A:DT:H6    | 1:30:A:DA:H8   | 7        | 0.32          |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 5        | 0.32          |
| (1,279) | 1:1:A:DA:H8    | 1:1:A:DA:H3'   | 4        | 0.32          |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 4        | 0.32          |
| (1,228) | 1:9:A:DG:H1'   | 1:7:A:DG:H3'   | 5        | 0.32          |
| (1,210) | 1:7:A:DG:H2''  | 1:7:A:DG:H1'   | 7        | 0.32          |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 9        | 0.32          |
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 6        | 0.32          |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 5        | 0.32          |
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 5        | 0.32          |
| (1,52)  | 1:4:A:DG:H8    | 1:4:A:DG:H3'   | 7        | 0.32          |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 6        | 0.32          |
| (1,548) | 1:32:A:DG:H2'  | 1:32:A:DG:H5'  | 7        | 0.31          |
| (1,539) | 1:21:A:DA:H2'  | 1:21:A:DA:H5'' | 9        | 0.31          |
| (1,526) | 1:32:A:DG:H5'  | 1:31:A:DG:H5'  | 7        | 0.31          |
| (1,511) | 1:25:A:DT:H6   | 1:12:A:DG:H8   | 2        | 0.31          |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 6        | 0.31          |
| (1,487) | 1:30:A:DA:H8   | 1:30:A:DA:H4'  | 6        | 0.31          |
| (1,464) | 1:4:A:DG:H1    | 1:6:A:DG:H2''  | 1        | 0.31          |
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 9        | 0.31          |
| (1,448) | 1:15:A:DA:H8   | 1:15:A:DA:H2'' | 5        | 0.31          |
| (1,359) | 1:25:A:DT:H5'  | 1:24:A:DA:H2'  | 1        | 0.31          |
| (1,359) | 1:25:A:DT:H5'' | 1:24:A:DA:H2'  | 1        | 0.31          |
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 5        | 0.31          |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 6        | 0.31          |
| (1,298) | 1:8:A:DT:H6    | 1:30:A:DA:H8   | 2        | 0.31          |
| (1,298) | 1:8:A:DT:H6    | 1:30:A:DA:H8   | 6        | 0.31          |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 10       | 0.31          |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 9        | 0.31          |
| (1,215) | 1:7:A:DG:H2'   | 1:7:A:DG:H8    | 1        | 0.31          |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 1        | 0.31          |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 7        | 0.31          |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 1        | 0.31          |
| (1,171) | 1:7:A:DG:H1    | 1:13:A:DG:H8   | 9        | 0.31          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 3        | 0.31          |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 2        | 0.31          |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 7        | 0.31          |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 6        | 0.31          |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 1        | 0.31          |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 7        | 0.31          |
| (1,46)  | 1:3:A:DG:H8    | 1:2:A:DG:H1'   | 9        | 0.31          |
| (1,539) | 1:21:A:DA:H2'  | 1:21:A:DA:H5'' | 7        | 0.3           |
| (1,535) | 1:29:A:DG:H2'' | 1:29:A:DG:H4'  | 9        | 0.3           |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 8        | 0.3           |
| (1,527) | 1:21:A:DA:H5'  | 1:17:A:DA:H5'  | 7        | 0.3           |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 6        | 0.3           |
| (1,511) | 1:25:A:DT:H6   | 1:12:A:DG:H8   | 10       | 0.3           |
| (1,486) | 1:30:A:DA:H1'  | 1:30:A:DA:H5'  | 9        | 0.3           |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 7        | 0.3           |
| (1,468) | 1:12:A:DG:H2'  | 1:13:A:DG:H1'  | 2        | 0.3           |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 5        | 0.3           |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 7        | 0.3           |
| (1,443) | 1:15:A:DA:H1'  | 1:15:A:DA:H5'  | 10       | 0.3           |
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 1        | 0.3           |
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 2        | 0.3           |
| (1,390) | 1:22:A:DA:H8   | 1:22:A:DA:H2'' | 6        | 0.3           |
| (1,388) | 1:22:A:DA:H8   | 1:22:A:DA:H3'  | 2        | 0.3           |
| (1,388) | 1:22:A:DA:H8   | 1:22:A:DA:H3'  | 8        | 0.3           |
| (1,351) | 1:25:A:DT:H5'  | 1:24:A:DA:H1'  | 8        | 0.3           |
| (1,351) | 1:25:A:DT:H5'' | 1:24:A:DA:H1'  | 8        | 0.3           |
| (1,341) | 1:13:A:DG:H1   | 1:13:A:DG:H1'  | 6        | 0.3           |
| (1,337) | 1:26:A:DG:H1   | 1:27:A:DG:H1'  | 8        | 0.3           |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 7        | 0.3           |
| (1,320) | 1:31:A:DG:H8   | 1:31:A:DG:H3'  | 6        | 0.3           |
| (1,311) | 1:32:A:DG:H1'  | 1:32:A:DG:H5'  | 2        | 0.3           |
| (1,295) | 1:12:A:DG:H8   | 1:13:A:DG:H8   | 8        | 0.3           |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 8        | 0.3           |
| (1,259) | 1:13:A:DG:H8   | 1:12:A:DG:H3'  | 4        | 0.3           |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 7        | 0.3           |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 9        | 0.3           |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 2        | 0.3           |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 5        | 0.3           |
| (1,180) | 1:9:A:DG:H8    | 1:7:A:DG:H1'   | 3        | 0.3           |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 5        | 0.3           |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 3        | 0.3           |
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 4        | 0.3           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 7        | 0.3           |
| (1,28)  | 1:26:A:DG:H8   | 1:26:A:DG:H2'' | 9        | 0.3           |
| (1,24)  | 1:24:A:DA:H8   | 1:23:A:DG:H1'  | 9        | 0.3           |
| (1,22)  | 1:25:A:DT:H6   | 1:24:A:DA:H1'  | 7        | 0.3           |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'  | 6        | 0.3           |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'' | 6        | 0.3           |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'  | 8        | 0.3           |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'' | 8        | 0.3           |
| (1,548) | 1:32:A:DG:H2'  | 1:32:A:DG:H5'  | 9        | 0.29          |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 1        | 0.29          |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 4        | 0.29          |
| (1,491) | 1:13:A:DG:H5'  | 1:31:A:DG:H8   | 5        | 0.29          |
| (1,481) | 1:2:A:DG:H8    | 1:1:A:DA:H3'   | 9        | 0.29          |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 1        | 0.29          |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 5        | 0.29          |
| (1,477) | 1:12:A:DG:H1'  | 1:13:A:DG:H5'  | 4        | 0.29          |
| (1,475) | 1:25:A:DT:H2'' | 1:24:A:DA:H5'' | 5        | 0.29          |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 10       | 0.29          |
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 6        | 0.29          |
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 8        | 0.29          |
| (1,388) | 1:22:A:DA:H8   | 1:22:A:DA:H3'  | 4        | 0.29          |
| (1,363) | 1:11:A:DG:H8   | 1:12:A:DG:H8   | 7        | 0.29          |
| (1,351) | 1:25:A:DT:H5'  | 1:24:A:DA:H1'  | 1        | 0.29          |
| (1,351) | 1:25:A:DT:H5'' | 1:24:A:DA:H1'  | 1        | 0.29          |
| (1,351) | 1:25:A:DT:H5'  | 1:24:A:DA:H1'  | 10       | 0.29          |
| (1,351) | 1:25:A:DT:H5'' | 1:24:A:DA:H1'  | 10       | 0.29          |
| (1,320) | 1:31:A:DG:H8   | 1:31:A:DG:H3'  | 5        | 0.29          |
| (1,298) | 1:8:A:DT:H6    | 1:30:A:DA:H8   | 4        | 0.29          |
| (1,298) | 1:8:A:DT:H6    | 1:30:A:DA:H8   | 10       | 0.29          |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 7        | 0.29          |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 4        | 0.29          |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 5        | 0.29          |
| (1,259) | 1:13:A:DG:H8   | 1:12:A:DG:H3'  | 10       | 0.29          |
| (1,234) | 1:7:A:DG:H8    | 1:7:A:DG:H3'   | 5        | 0.29          |
| (1,215) | 1:7:A:DG:H2'   | 1:7:A:DG:H8    | 4        | 0.29          |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 3        | 0.29          |
| (1,156) | 1:8:A:DT:H6    | 1:8:A:DT:H2'   | 10       | 0.29          |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 3        | 0.29          |
| (1,101) | 1:29:A:DG:H1'  | 1:29:A:DG:H2'' | 10       | 0.29          |
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 2        | 0.29          |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 2        | 0.29          |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 7        | 0.29          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 1        | 0.29          |
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 3        | 0.29          |
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 6        | 0.29          |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 2        | 0.29          |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 6        | 0.29          |
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 10       | 0.29          |
| (1,52)  | 1:4:A:DG:H8    | 1:4:A:DG:H3'   | 2        | 0.29          |
| (1,21)  | 1:8:A:DT:H6    | 1:8:A:DT:H1'   | 6        | 0.29          |
| (1,6)   | 1:11:A:DG:H1   | 1:26:A:DG:H1   | 6        | 0.29          |
| (1,6)   | 1:11:A:DG:H1   | 1:26:A:DG:H1   | 9        | 0.29          |
| (1,539) | 1:21:A:DA:H2'  | 1:21:A:DA:H5'' | 10       | 0.28          |
| (1,527) | 1:21:A:DA:H5'  | 1:17:A:DA:H5'  | 6        | 0.28          |
| (1,526) | 1:32:A:DG:H5'  | 1:31:A:DG:H5'  | 8        | 0.28          |
| (1,514) | 1:16:A:DG:H2'  | 1:16:A:DG:H3'  | 2        | 0.28          |
| (1,468) | 1:12:A:DG:H2'  | 1:13:A:DG:H1'  | 5        | 0.28          |
| (1,468) | 1:12:A:DG:H2'  | 1:13:A:DG:H1'  | 7        | 0.28          |
| (1,459) | 1:3:A:DG:H1    | 1:5:A:DC:H1'   | 5        | 0.28          |
| (1,425) | 1:17:A:DA:H8   | 1:17:A:DA:H4'  | 5        | 0.28          |
| (1,423) | 1:5:A:DC:H6    | 1:5:A:DC:H4'   | 7        | 0.28          |
| (1,419) | 1:17:A:DA:H8   | 1:17:A:DA:H3'  | 8        | 0.28          |
| (1,411) | 1:19:A:DG:H8   | 1:19:A:DG:H2'' | 7        | 0.28          |
| (1,407) | 1:20:A:DG:H1'  | 1:19:A:DG:H5'  | 8        | 0.28          |
| (1,407) | 1:20:A:DG:H1'  | 1:19:A:DG:H5'  | 9        | 0.28          |
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 8        | 0.28          |
| (1,320) | 1:31:A:DG:H8   | 1:31:A:DG:H3'  | 8        | 0.28          |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 1        | 0.28          |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 5        | 0.28          |
| (1,279) | 1:1:A:DA:H8    | 1:1:A:DA:H3'   | 9        | 0.28          |
| (1,277) | 1:23:A:DG:H8   | 1:23:A:DG:H3'  | 1        | 0.28          |
| (1,259) | 1:13:A:DG:H8   | 1:12:A:DG:H3'  | 6        | 0.28          |
| (1,244) | 1:11:A:DG:H8   | 1:11:A:DG:H2'' | 5        | 0.28          |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 4        | 0.28          |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 1        | 0.28          |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 7        | 0.28          |
| (1,228) | 1:9:A:DG:H1'   | 1:7:A:DG:H3'   | 3        | 0.28          |
| (1,226) | 1:9:A:DG:H3'   | 1:9:A:DG:H2'   | 6        | 0.28          |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 8        | 0.28          |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 9        | 0.28          |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 7        | 0.28          |
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 10       | 0.28          |
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 2        | 0.28          |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 3        | 0.28          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,28)  | 1:26:A:DG:H8   | 1:26:A:DG:H2'' | 7        | 0.28          |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 4        | 0.28          |
| (1,25)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'' | 10       | 0.28          |
| (1,22)  | 1:25:A:DT:H6   | 1:24:A:DA:H1'  | 10       | 0.28          |
| (1,7)   | 1:7:A:DG:H1    | 1:11:A:DG:H1   | 7        | 0.28          |
| (1,535) | 1:29:A:DG:H2'' | 1:29:A:DG:H4'  | 6        | 0.27          |
| (1,526) | 1:32:A:DG:H5'  | 1:31:A:DG:H5'  | 10       | 0.27          |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 3        | 0.27          |
| (1,495) | 1:3:A:DG:H8    | 1:3:A:DG:H4'   | 5        | 0.27          |
| (1,468) | 1:12:A:DG:H2'  | 1:13:A:DG:H1'  | 3        | 0.27          |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 6        | 0.27          |
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 1        | 0.27          |
| (1,459) | 1:3:A:DG:H1    | 1:5:A:DC:H1'   | 6        | 0.27          |
| (1,390) | 1:22:A:DA:H8   | 1:22:A:DA:H2'' | 4        | 0.27          |
| (1,351) | 1:25:A:DT:H5'  | 1:24:A:DA:H1'  | 5        | 0.27          |
| (1,351) | 1:25:A:DT:H5'' | 1:24:A:DA:H1'  | 5        | 0.27          |
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 4        | 0.27          |
| (1,331) | 1:14:A:DA:H8   | 1:14:A:DA:H1'  | 5        | 0.27          |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 10       | 0.27          |
| (1,281) | 1:2:A:DG:H8    | 1:1:A:DA:H5'   | 2        | 0.27          |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 10       | 0.27          |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 9        | 0.27          |
| (1,170) | 1:12:A:DG:H8   | 1:9:A:DG:H1    | 1        | 0.27          |
| (1,154) | 1:25:A:DT:H5'  | 1:27:A:DG:H8   | 4        | 0.27          |
| (1,154) | 1:25:A:DT:H5'' | 1:27:A:DG:H8   | 4        | 0.27          |
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 5        | 0.27          |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 4        | 0.27          |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 10       | 0.27          |
| (1,123) | 1:4:A:DG:H8    | 1:3:A:DG:H2''  | 10       | 0.27          |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 1        | 0.27          |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 6        | 0.27          |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 8        | 0.27          |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 9        | 0.27          |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 3        | 0.27          |
| (1,76)  | 1:13:A:DG:H1   | 1:28:A:DG:H8   | 6        | 0.27          |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 8        | 0.27          |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 9        | 0.27          |
| (1,51)  | 1:3:A:DG:H8    | 1:2:A:DG:H2''  | 9        | 0.27          |
| (1,47)  | 1:3:A:DG:H8    | 1:3:A:DG:H3'   | 2        | 0.27          |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 8        | 0.27          |
| (1,552) | 1:8:A:DT:H2'   | 1:8:A:DT:H2''  | 10       | 0.26          |
| (1,520) | 1:17:A:DA:H4'  | 1:17:A:DA:H5'  | 7        | 0.26          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,514) | 1:16:A:DG:H2'  | 1:16:A:DG:H3'  | 1        | 0.26          |
| (1,487) | 1:30:A:DA:H8   | 1:30:A:DA:H4'  | 2        | 0.26          |
| (1,475) | 1:25:A:DT:H2'' | 1:24:A:DA:H5'' | 2        | 0.26          |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 10       | 0.26          |
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 4        | 0.26          |
| (1,430) | 1:17:A:DA:H8   | 1:17:A:DA:H2'  | 8        | 0.26          |
| (1,419) | 1:17:A:DA:H8   | 1:17:A:DA:H3'  | 1        | 0.26          |
| (1,388) | 1:22:A:DA:H8   | 1:22:A:DA:H3'  | 5        | 0.26          |
| (1,359) | 1:25:A:DT:H5'  | 1:24:A:DA:H2'  | 2        | 0.26          |
| (1,359) | 1:25:A:DT:H5'' | 1:24:A:DA:H2'  | 2        | 0.26          |
| (1,331) | 1:14:A:DA:H8   | 1:14:A:DA:H1'  | 2        | 0.26          |
| (1,320) | 1:31:A:DG:H8   | 1:31:A:DG:H3'  | 9        | 0.26          |
| (1,313) | 1:32:A:DG:H8   | 1:32:A:DG:H4'  | 1        | 0.26          |
| (1,301) | 1:30:A:DA:H8   | 1:30:A:DA:H2'' | 9        | 0.26          |
| (1,295) | 1:12:A:DG:H8   | 1:13:A:DG:H8   | 9        | 0.26          |
| (1,290) | 1:1:A:DA:H5'   | 1:1:A:DA:H2'   | 1        | 0.26          |
| (1,259) | 1:13:A:DG:H8   | 1:12:A:DG:H3'  | 8        | 0.26          |
| (1,226) | 1:9:A:DG:H3'   | 1:9:A:DG:H2'   | 3        | 0.26          |
| (1,215) | 1:7:A:DG:H2'   | 1:7:A:DG:H8    | 9        | 0.26          |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 6        | 0.26          |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 4        | 0.26          |
| (1,193) | 1:3:A:DG:H1'   | 1:3:A:DG:H4'   | 5        | 0.26          |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 3        | 0.26          |
| (1,156) | 1:8:A:DT:H6    | 1:8:A:DT:H2'   | 7        | 0.26          |
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 2        | 0.26          |
| (1,110) | 1:29:A:DG:H8   | 1:28:A:DG:H2'' | 8        | 0.26          |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 5        | 0.26          |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 10       | 0.26          |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 9        | 0.26          |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 5        | 0.26          |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 7        | 0.26          |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 2        | 0.26          |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 3        | 0.26          |
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 2        | 0.26          |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 3        | 0.26          |
| (1,544) | 1:22:A:DA:H2'' | 1:21:A:DA:H5'' | 5        | 0.25          |
| (1,535) | 1:29:A:DG:H2'' | 1:29:A:DG:H4'  | 1        | 0.25          |
| (1,535) | 1:29:A:DG:H2'' | 1:29:A:DG:H4'  | 8        | 0.25          |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 10       | 0.25          |
| (1,514) | 1:16:A:DG:H2'  | 1:16:A:DG:H3'  | 6        | 0.25          |
| (1,494) | 1:3:A:DG:H8    | 1:2:A:DG:H5''  | 1        | 0.25          |
| (1,487) | 1:30:A:DA:H8   | 1:30:A:DA:H4'  | 7        | 0.25          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,486) | 1:30:A:DA:H1'  | 1:30:A:DA:H5'  | 8        | 0.25          |
| (1,482) | 1:30:A:DA:H8   | 1:30:A:DA:H5'' | 3        | 0.25          |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 9        | 0.25          |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 1        | 0.25          |
| (1,383) | 1:26:A:DG:H1   | 1:1:A:DA:H8    | 8        | 0.25          |
| (1,372) | 1:19:A:DG:H8   | 1:19:A:DG:H1'  | 7        | 0.25          |
| (1,337) | 1:26:A:DG:H1   | 1:27:A:DG:H1'  | 9        | 0.25          |
| (1,332) | 1:27:A:DG:H8   | 1:28:A:DG:H8   | 5        | 0.25          |
| (1,324) | 1:32:A:DG:H8   | 1:31:A:DG:H2'' | 7        | 0.25          |
| (1,318) | 1:29:A:DG:H1'  | 1:31:A:DG:H8   | 2        | 0.25          |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 6        | 0.25          |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 3        | 0.25          |
| (1,279) | 1:1:A:DA:H8    | 1:1:A:DA:H3'   | 5        | 0.25          |
| (1,234) | 1:7:A:DG:H8    | 1:7:A:DG:H3'   | 3        | 0.25          |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 3        | 0.25          |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 10       | 0.25          |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 6        | 0.25          |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 10       | 0.25          |
| (1,189) | 1:5:A:DC:H5    | 1:5:A:DC:H3'   | 8        | 0.25          |
| (1,156) | 1:8:A:DT:H6    | 1:8:A:DT:H2'   | 8        | 0.25          |
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 3        | 0.25          |
| (1,124) | 1:4:A:DG:H8    | 1:3:A:DG:H2'   | 1        | 0.25          |
| (1,123) | 1:4:A:DG:H8    | 1:3:A:DG:H2''  | 4        | 0.25          |
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 10       | 0.25          |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 4        | 0.25          |
| (1,105) | 1:29:A:DG:H8   | 1:29:A:DG:H3'  | 10       | 0.25          |
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 8        | 0.25          |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 2        | 0.25          |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 10       | 0.25          |
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 3        | 0.25          |
| (1,51)  | 1:3:A:DG:H8    | 1:2:A:DG:H2''  | 3        | 0.25          |
| (1,49)  | 1:2:A:DG:H8    | 1:2:A:DG:H2'   | 9        | 0.25          |
| (1,47)  | 1:3:A:DG:H8    | 1:3:A:DG:H3'   | 6        | 0.25          |
| (1,47)  | 1:3:A:DG:H8    | 1:3:A:DG:H3'   | 8        | 0.25          |
| (1,25)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'' | 3        | 0.25          |
| (1,1)   | 1:27:A:DG:H1   | 1:28:A:DG:H1   | 3        | 0.25          |
| (1,520) | 1:17:A:DA:H4'  | 1:17:A:DA:H5'  | 6        | 0.24          |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 1        | 0.24          |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 5        | 0.24          |
| (1,514) | 1:16:A:DG:H2'  | 1:16:A:DG:H3'  | 7        | 0.24          |
| (1,513) | 1:21:A:DA:H1'  | 1:20:A:DG:H5'  | 10       | 0.24          |
| (1,437) | 1:16:A:DG:H8   | 1:16:A:DG:H5'' | 10       | 0.24          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,425) | 1:17:A:DA:H8   | 1:17:A:DA:H4'  | 7        | 0.24          |
| (1,412) | 1:19:A:DG:H8   | 1:19:A:DG:H2'  | 3        | 0.24          |
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 4        | 0.24          |
| (1,388) | 1:22:A:DA:H8   | 1:22:A:DA:H3'  | 3        | 0.24          |
| (1,383) | 1:26:A:DG:H1   | 1:1:A:DA:H8    | 3        | 0.24          |
| (1,351) | 1:25:A:DT:H5'  | 1:24:A:DA:H1'  | 2        | 0.24          |
| (1,351) | 1:25:A:DT:H5'' | 1:24:A:DA:H1'  | 2        | 0.24          |
| (1,337) | 1:26:A:DG:H1   | 1:27:A:DG:H1'  | 2        | 0.24          |
| (1,301) | 1:30:A:DA:H8   | 1:30:A:DA:H2'' | 1        | 0.24          |
| (1,301) | 1:30:A:DA:H8   | 1:30:A:DA:H2'' | 2        | 0.24          |
| (1,298) | 1:8:A:DT:H6    | 1:30:A:DA:H8   | 9        | 0.24          |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 1        | 0.24          |
| (1,290) | 1:1:A:DA:H5'   | 1:1:A:DA:H2'   | 10       | 0.24          |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 1        | 0.24          |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 5        | 0.24          |
| (1,259) | 1:13:A:DG:H8   | 1:12:A:DG:H3'  | 2        | 0.24          |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 6        | 0.24          |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 6        | 0.24          |
| (1,227) | 1:9:A:DG:H8    | 1:9:A:DG:H4'   | 1        | 0.24          |
| (1,219) | 1:7:A:DG:H2'   | 1:9:A:DG:H8    | 1        | 0.24          |
| (1,181) | 1:11:A:DG:H1'  | 1:12:A:DG:H8   | 5        | 0.24          |
| (1,171) | 1:7:A:DG:H1    | 1:13:A:DG:H8   | 4        | 0.24          |
| (1,144) | 1:5:A:DC:H3'   | 1:5:A:DC:H2'   | 4        | 0.24          |
| (1,139) | 1:5:A:DC:H6    | 1:5:A:DC:H2'   | 6        | 0.24          |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 3        | 0.24          |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 6        | 0.24          |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 2        | 0.24          |
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 10       | 0.24          |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 5        | 0.24          |
| (1,80)  | 1:25:A:DT:H1'  | 1:25:A:DT:H5'  | 8        | 0.24          |
| (1,76)  | 1:13:A:DG:H1   | 1:28:A:DG:H8   | 5        | 0.24          |
| (1,69)  | 1:27:A:DG:H8   | 1:27:A:DG:H3'  | 8        | 0.24          |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 9        | 0.24          |
| (1,52)  | 1:4:A:DG:H8    | 1:4:A:DG:H3'   | 5        | 0.24          |
| (1,46)  | 1:3:A:DG:H8    | 1:2:A:DG:H1'   | 3        | 0.24          |
| (1,46)  | 1:3:A:DG:H8    | 1:2:A:DG:H1'   | 7        | 0.24          |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 3        | 0.24          |
| (1,41)  | 1:2:A:DG:H8    | 1:2:A:DG:H3'   | 5        | 0.24          |
| (1,30)  | 1:25:A:DT:H5'  | 1:24:A:DA:H8   | 3        | 0.24          |
| (1,30)  | 1:25:A:DT:H5'' | 1:24:A:DA:H8   | 3        | 0.24          |
| (1,22)  | 1:25:A:DT:H6   | 1:24:A:DA:H1'  | 6        | 0.24          |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'  | 9        | 0.24          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'' | 9        | 0.24          |
| (1,535) | 1:29:A:DG:H2'' | 1:29:A:DG:H4'  | 5        | 0.23          |
| (1,498) | 1:1:A:DA:H2    | 1:2:A:DG:H5'   | 6        | 0.23          |
| (1,497) | 1:1:A:DA:H2    | 1:2:A:DG:H5''  | 7        | 0.23          |
| (1,486) | 1:30:A:DA:H1'  | 1:30:A:DA:H5'  | 7        | 0.23          |
| (1,475) | 1:25:A:DT:H2'' | 1:24:A:DA:H5'' | 6        | 0.23          |
| (1,475) | 1:25:A:DT:H2'' | 1:24:A:DA:H5'' | 10       | 0.23          |
| (1,468) | 1:12:A:DG:H2'  | 1:13:A:DG:H1'  | 6        | 0.23          |
| (1,449) | 1:15:A:DA:H1'  | 1:15:A:DA:H2'' | 1        | 0.23          |
| (1,441) | 1:7:A:DG:H1'   | 1:9:A:DG:H1'   | 5        | 0.23          |
| (1,419) | 1:17:A:DA:H8   | 1:17:A:DA:H3'  | 9        | 0.23          |
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 3        | 0.23          |
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 6        | 0.23          |
| (1,331) | 1:14:A:DA:H8   | 1:14:A:DA:H1'  | 8        | 0.23          |
| (1,320) | 1:31:A:DG:H8   | 1:31:A:DG:H3'  | 1        | 0.23          |
| (1,298) | 1:8:A:DT:H6    | 1:30:A:DA:H8   | 1        | 0.23          |
| (1,280) | 1:1:A:DA:H8    | 1:1:A:DA:H5'   | 5        | 0.23          |
| (1,276) | 1:23:A:DG:H1'  | 1:23:A:DG:H2'' | 4        | 0.23          |
| (1,226) | 1:9:A:DG:H3'   | 1:9:A:DG:H2'   | 2        | 0.23          |
| (1,225) | 1:9:A:DG:H3'   | 1:9:A:DG:H2''  | 7        | 0.23          |
| (1,225) | 1:9:A:DG:H3'   | 1:9:A:DG:H2''  | 10       | 0.23          |
| (1,224) | 1:9:A:DG:H1'   | 1:9:A:DG:H2''  | 3        | 0.23          |
| (1,216) | 1:7:A:DG:H2''  | 1:7:A:DG:H8    | 9        | 0.23          |
| (1,206) | 1:6:A:DG:H2''  | 1:6:A:DG:H2'   | 4        | 0.23          |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 7        | 0.23          |
| (1,193) | 1:3:A:DG:H1'   | 1:3:A:DG:H4'   | 2        | 0.23          |
| (1,189) | 1:5:A:DC:H5    | 1:5:A:DC:H3'   | 3        | 0.23          |
| (1,189) | 1:5:A:DC:H5    | 1:5:A:DC:H3'   | 6        | 0.23          |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 7        | 0.23          |
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 9        | 0.23          |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 9        | 0.23          |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 6        | 0.23          |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 4        | 0.23          |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 9        | 0.23          |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 1        | 0.23          |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 6        | 0.23          |
| (1,24)  | 1:24:A:DA:H8   | 1:23:A:DG:H1'  | 6        | 0.23          |
| (1,552) | 1:8:A:DT:H2'   | 1:8:A:DT:H2''  | 7        | 0.22          |
| (1,546) | 1:22:A:DA:H2'  | 1:21:A:DA:H5'  | 1        | 0.22          |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 2        | 0.22          |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 3        | 0.22          |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 2        | 0.22          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,498) | 1:1:A:DA:H2    | 1:2:A:DG:H5'   | 8        | 0.22          |
| (1,494) | 1:3:A:DG:H8    | 1:2:A:DG:H5''  | 6        | 0.22          |
| (1,491) | 1:13:A:DG:H5'  | 1:31:A:DG:H8   | 8        | 0.22          |
| (1,475) | 1:25:A:DT:H2'' | 1:24:A:DA:H5'' | 8        | 0.22          |
| (1,408) | 1:19:A:DG:H1'  | 1:19:A:DG:H5'' | 10       | 0.22          |
| (1,383) | 1:26:A:DG:H1   | 1:1:A:DA:H8    | 7        | 0.22          |
| (1,377) | 1:10:A:DT:H6   | 1:9:A:DG:H8    | 10       | 0.22          |
| (1,337) | 1:26:A:DG:H1   | 1:27:A:DG:H1'  | 1        | 0.22          |
| (1,327) | 1:31:A:DG:H8   | 1:31:A:DG:H2'' | 8        | 0.22          |
| (1,318) | 1:29:A:DG:H1'  | 1:31:A:DG:H8   | 8        | 0.22          |
| (1,313) | 1:32:A:DG:H8   | 1:32:A:DG:H4'  | 10       | 0.22          |
| (1,311) | 1:32:A:DG:H1'  | 1:32:A:DG:H5'  | 10       | 0.22          |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 3        | 0.22          |
| (1,280) | 1:1:A:DA:H8    | 1:1:A:DA:H5'   | 3        | 0.22          |
| (1,279) | 1:1:A:DA:H8    | 1:1:A:DA:H3'   | 6        | 0.22          |
| (1,276) | 1:23:A:DG:H1'  | 1:23:A:DG:H2'' | 1        | 0.22          |
| (1,254) | 1:12:A:DG:H8   | 1:11:A:DG:H2'' | 7        | 0.22          |
| (1,237) | 1:6:A:DG:H8    | 1:6:A:DG:H5''  | 7        | 0.22          |
| (1,232) | 1:9:A:DG:H2'   | 1:9:A:DG:H2''  | 8        | 0.22          |
| (1,226) | 1:9:A:DG:H3'   | 1:9:A:DG:H2'   | 7        | 0.22          |
| (1,224) | 1:9:A:DG:H1'   | 1:9:A:DG:H2''  | 5        | 0.22          |
| (1,219) | 1:7:A:DG:H2'   | 1:9:A:DG:H8    | 3        | 0.22          |
| (1,205) | 1:6:A:DG:H3'   | 1:6:A:DG:H5''  | 8        | 0.22          |
| (1,199) | 1:6:A:DG:H3'   | 1:6:A:DG:H2'   | 8        | 0.22          |
| (1,171) | 1:7:A:DG:H1    | 1:13:A:DG:H8   | 10       | 0.22          |
| (1,156) | 1:8:A:DT:H6    | 1:8:A:DT:H2'   | 5        | 0.22          |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 7        | 0.22          |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 8        | 0.22          |
| (1,103) | 1:28:A:DG:H8   | 1:28:A:DG:H3'  | 2        | 0.22          |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 6        | 0.22          |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 10       | 0.22          |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 3        | 0.22          |
| (1,76)  | 1:13:A:DG:H1   | 1:28:A:DG:H8   | 2        | 0.22          |
| (1,76)  | 1:13:A:DG:H1   | 1:28:A:DG:H8   | 7        | 0.22          |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 7        | 0.22          |
| (1,55)  | 1:3:A:DG:H8    | 1:3:A:DG:H2'   | 8        | 0.22          |
| (1,52)  | 1:4:A:DG:H8    | 1:4:A:DG:H3'   | 10       | 0.22          |
| (1,48)  | 1:2:A:DG:H8    | 1:2:A:DG:H2''  | 10       | 0.22          |
| (1,47)  | 1:3:A:DG:H8    | 1:3:A:DG:H3'   | 5        | 0.22          |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 2        | 0.22          |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'  | 3        | 0.22          |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'' | 3        | 0.22          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,526) | 1:32:A:DG:H5'  | 1:31:A:DG:H5'  | 6        | 0.21          |
| (1,507) | 1:3:A:DG:H4'   | 1:1:A:DA:H2    | 2        | 0.21          |
| (1,496) | 1:3:A:DG:H1'   | 1:3:A:DG:H5''  | 4        | 0.21          |
| (1,468) | 1:12:A:DG:H2'  | 1:13:A:DG:H1'  | 8        | 0.21          |
| (1,451) | 1:14:A:DA:H1'  | 1:14:A:DA:H2'  | 9        | 0.21          |
| (1,421) | 1:5:A:DC:H1'   | 1:5:A:DC:H4'   | 4        | 0.21          |
| (1,390) | 1:22:A:DA:H8   | 1:22:A:DA:H2'' | 10       | 0.21          |
| (1,385) | 1:28:A:DG:H1   | 1:30:A:DA:H8   | 5        | 0.21          |
| (1,337) | 1:26:A:DG:H1   | 1:27:A:DG:H1'  | 6        | 0.21          |
| (1,320) | 1:31:A:DG:H8   | 1:31:A:DG:H3'  | 4        | 0.21          |
| (1,318) | 1:29:A:DG:H1'  | 1:31:A:DG:H8   | 5        | 0.21          |
| (1,313) | 1:32:A:DG:H8   | 1:32:A:DG:H4'  | 2        | 0.21          |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 4        | 0.21          |
| (1,279) | 1:1:A:DA:H8    | 1:1:A:DA:H3'   | 1        | 0.21          |
| (1,254) | 1:12:A:DG:H8   | 1:11:A:DG:H2'' | 10       | 0.21          |
| (1,251) | 1:11:A:DG:H2'' | 1:11:A:DG:H3'  | 9        | 0.21          |
| (1,250) | 1:11:A:DG:H1'  | 1:11:A:DG:H2'' | 6        | 0.21          |
| (1,250) | 1:11:A:DG:H1'  | 1:11:A:DG:H2'' | 7        | 0.21          |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 5        | 0.21          |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 10       | 0.21          |
| (1,230) | 1:9:A:DG:H1'   | 1:9:A:DG:H5''  | 4        | 0.21          |
| (1,227) | 1:9:A:DG:H8    | 1:9:A:DG:H4'   | 7        | 0.21          |
| (1,226) | 1:9:A:DG:H3'   | 1:9:A:DG:H2'   | 1        | 0.21          |
| (1,225) | 1:9:A:DG:H3'   | 1:9:A:DG:H2''  | 1        | 0.21          |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 5        | 0.21          |
| (1,156) | 1:8:A:DT:H6    | 1:8:A:DT:H2'   | 6        | 0.21          |
| (1,145) | 1:5:A:DC:H2''  | 1:5:A:DC:H2'   | 3        | 0.21          |
| (1,129) | 1:10:A:DT:H6   | 1:10:A:DT:H2'  | 9        | 0.21          |
| (1,124) | 1:4:A:DG:H8    | 1:3:A:DG:H2'   | 8        | 0.21          |
| (1,109) | 1:29:A:DG:H8   | 1:28:A:DG:H2'  | 3        | 0.21          |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 2        | 0.21          |
| (1,101) | 1:29:A:DG:H1'  | 1:29:A:DG:H2'' | 7        | 0.21          |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 1        | 0.21          |
| (1,88)  | 1:26:A:DG:H2'' | 1:26:A:DG:H2'  | 8        | 0.21          |
| (1,80)  | 1:25:A:DT:H1'  | 1:25:A:DT:H5'  | 1        | 0.21          |
| (1,80)  | 1:25:A:DT:H1'  | 1:25:A:DT:H5'  | 7        | 0.21          |
| (1,64)  | 1:8:A:DT:H5'   | 1:8:A:DT:H1'   | 3        | 0.21          |
| (1,64)  | 1:8:A:DT:H5''  | 1:8:A:DT:H1'   | 3        | 0.21          |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 1        | 0.21          |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 5        | 0.21          |
| (1,35)  | 1:28:A:DG:H1   | 1:3:A:DG:H8    | 3        | 0.21          |
| (1,25)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'' | 8        | 0.21          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'  | 7        | 0.21          |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'' | 7        | 0.21          |
| (1,549) | 1:30:A:DA:H2'  | 1:30:A:DA:H5'  | 2        | 0.2           |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 4        | 0.2           |
| (1,521) | 1:30:A:DA:H5'  | 1:30:A:DA:H4'  | 10       | 0.2           |
| (1,520) | 1:17:A:DA:H4'  | 1:17:A:DA:H5'  | 3        | 0.2           |
| (1,498) | 1:1:A:DA:H2    | 1:2:A:DG:H5'   | 2        | 0.2           |
| (1,491) | 1:13:A:DG:H5'  | 1:31:A:DG:H8   | 7        | 0.2           |
| (1,486) | 1:30:A:DA:H1'  | 1:30:A:DA:H5'  | 1        | 0.2           |
| (1,486) | 1:30:A:DA:H1'  | 1:30:A:DA:H5'  | 10       | 0.2           |
| (1,475) | 1:25:A:DT:H2'' | 1:24:A:DA:H5'' | 1        | 0.2           |
| (1,448) | 1:15:A:DA:H8   | 1:15:A:DA:H2'' | 4        | 0.2           |
| (1,441) | 1:7:A:DG:H1'   | 1:9:A:DG:H1'   | 1        | 0.2           |
| (1,441) | 1:7:A:DG:H1'   | 1:9:A:DG:H1'   | 4        | 0.2           |
| (1,425) | 1:17:A:DA:H8   | 1:17:A:DA:H4'  | 2        | 0.2           |
| (1,419) | 1:17:A:DA:H8   | 1:17:A:DA:H3'  | 4        | 0.2           |
| (1,412) | 1:19:A:DG:H8   | 1:19:A:DG:H2'  | 9        | 0.2           |
| (1,408) | 1:19:A:DG:H1'  | 1:19:A:DG:H5'' | 8        | 0.2           |
| (1,407) | 1:20:A:DG:H1'  | 1:19:A:DG:H5'  | 7        | 0.2           |
| (1,402) | 1:20:A:DG:H1'  | 1:21:A:DA:H5'' | 10       | 0.2           |
| (1,393) | 1:22:A:DA:H2'  | 1:22:A:DA:H2'' | 7        | 0.2           |
| (1,368) | 1:20:A:DG:H1'  | 1:21:A:DA:H8   | 6        | 0.2           |
| (1,320) | 1:31:A:DG:H8   | 1:31:A:DG:H3'  | 3        | 0.2           |
| (1,312) | 1:32:A:DG:H1'  | 1:32:A:DG:H4'  | 1        | 0.2           |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 6        | 0.2           |
| (1,280) | 1:1:A:DA:H8    | 1:1:A:DA:H5'   | 8        | 0.2           |
| (1,279) | 1:1:A:DA:H8    | 1:1:A:DA:H3'   | 7        | 0.2           |
| (1,276) | 1:23:A:DG:H1'  | 1:23:A:DG:H2'' | 2        | 0.2           |
| (1,259) | 1:13:A:DG:H8   | 1:12:A:DG:H3'  | 7        | 0.2           |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 1        | 0.2           |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 2        | 0.2           |
| (1,227) | 1:9:A:DG:H8    | 1:9:A:DG:H4'   | 8        | 0.2           |
| (1,225) | 1:9:A:DG:H3'   | 1:9:A:DG:H2''  | 2        | 0.2           |
| (1,225) | 1:9:A:DG:H3'   | 1:9:A:DG:H2''  | 6        | 0.2           |
| (1,215) | 1:7:A:DG:H2'   | 1:7:A:DG:H8    | 3        | 0.2           |
| (1,189) | 1:5:A:DC:H5    | 1:5:A:DC:H3'   | 2        | 0.2           |
| (1,156) | 1:8:A:DT:H6    | 1:8:A:DT:H2'   | 1        | 0.2           |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 6        | 0.2           |
| (1,124) | 1:4:A:DG:H8    | 1:3:A:DG:H2'   | 2        | 0.2           |
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 9        | 0.2           |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 10       | 0.2           |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 3        | 0.2           |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,95)  | 1:28:A:DG:H1'  | 1:28:A:DG:H2'' | 8        | 0.2           |
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 1        | 0.2           |
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 5        | 0.2           |
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 9        | 0.2           |
| (1,84)  | 1:26:A:DG:H1'  | 1:26:A:DG:H2'' | 10       | 0.2           |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 4        | 0.2           |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 10       | 0.2           |
| (1,46)  | 1:3:A:DG:H8    | 1:2:A:DG:H1'   | 5        | 0.2           |
| (1,46)  | 1:3:A:DG:H8    | 1:2:A:DG:H1'   | 8        | 0.2           |
| (1,42)  | 1:3:A:DG:H8    | 1:2:A:DG:H3'   | 9        | 0.2           |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 7        | 0.2           |
| (1,25)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'' | 4        | 0.2           |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'  | 10       | 0.2           |
| (1,15)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'' | 10       | 0.2           |
| (1,7)   | 1:7:A:DG:H1    | 1:11:A:DG:H1   | 9        | 0.2           |
| (1,552) | 1:8:A:DT:H2'   | 1:8:A:DT:H2''  | 6        | 0.19          |
| (1,549) | 1:30:A:DA:H2'  | 1:30:A:DA:H5'  | 4        | 0.19          |
| (1,526) | 1:32:A:DG:H5'  | 1:31:A:DG:H5'  | 4        | 0.19          |
| (1,515) | 1:18:A:DG:H3'  | 1:18:A:DG:H2'  | 7        | 0.19          |
| (1,506) | 1:12:A:DG:H1'  | 1:12:A:DG:H4'  | 9        | 0.19          |
| (1,497) | 1:1:A:DA:H2    | 1:2:A:DG:H5''  | 6        | 0.19          |
| (1,482) | 1:30:A:DA:H8   | 1:30:A:DA:H5'' | 8        | 0.19          |
| (1,456) | 1:9:A:DG:H8    | 1:9:A:DG:H3'   | 2        | 0.19          |
| (1,449) | 1:15:A:DA:H1'  | 1:15:A:DA:H2'' | 7        | 0.19          |
| (1,436) | 1:16:A:DG:H8   | 1:16:A:DG:H2'  | 2        | 0.19          |
| (1,423) | 1:5:A:DC:H6    | 1:5:A:DC:H4'   | 1        | 0.19          |
| (1,423) | 1:5:A:DC:H6    | 1:5:A:DC:H4'   | 3        | 0.19          |
| (1,423) | 1:5:A:DC:H6    | 1:5:A:DC:H4'   | 8        | 0.19          |
| (1,412) | 1:19:A:DG:H8   | 1:19:A:DG:H2'  | 8        | 0.19          |
| (1,411) | 1:19:A:DG:H8   | 1:19:A:DG:H2'' | 6        | 0.19          |
| (1,408) | 1:19:A:DG:H1'  | 1:19:A:DG:H5'' | 7        | 0.19          |
| (1,390) | 1:22:A:DA:H8   | 1:22:A:DA:H2'' | 3        | 0.19          |
| (1,388) | 1:22:A:DA:H8   | 1:22:A:DA:H3'  | 9        | 0.19          |
| (1,388) | 1:22:A:DA:H8   | 1:22:A:DA:H3'  | 10       | 0.19          |
| (1,370) | 1:17:A:DA:H1'  | 1:18:A:DG:H8   | 7        | 0.19          |
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 3        | 0.19          |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 2        | 0.19          |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 3        | 0.19          |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 3        | 0.19          |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 9        | 0.19          |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 7        | 0.19          |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 6        | 0.19          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,279) | 1:1:A:DA:H8    | 1:1:A:DA:H3'   | 3        | 0.19          |
| (1,250) | 1:11:A:DG:H1'  | 1:11:A:DG:H2'' | 9        | 0.19          |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 2        | 0.19          |
| (1,227) | 1:9:A:DG:H8    | 1:9:A:DG:H4'   | 2        | 0.19          |
| (1,210) | 1:7:A:DG:H2''  | 1:7:A:DG:H1'   | 9        | 0.19          |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 2        | 0.19          |
| (1,195) | 1:4:A:DG:H2''  | 1:4:A:DG:H2'   | 8        | 0.19          |
| (1,171) | 1:7:A:DG:H1    | 1:13:A:DG:H8   | 1        | 0.19          |
| (1,105) | 1:29:A:DG:H8   | 1:29:A:DG:H3'  | 8        | 0.19          |
| (1,103) | 1:28:A:DG:H8   | 1:28:A:DG:H3'  | 3        | 0.19          |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 8        | 0.19          |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 10       | 0.19          |
| (1,65)  | 1:24:A:DA:H8   | 1:24:A:DA:H2'  | 4        | 0.19          |
| (1,51)  | 1:3:A:DG:H8    | 1:2:A:DG:H2''  | 5        | 0.19          |
| (1,51)  | 1:3:A:DG:H8    | 1:2:A:DG:H2''  | 6        | 0.19          |
| (1,46)  | 1:3:A:DG:H8    | 1:2:A:DG:H1'   | 2        | 0.19          |
| (1,35)  | 1:28:A:DG:H1   | 1:3:A:DG:H8    | 2        | 0.19          |
| (1,28)  | 1:26:A:DG:H8   | 1:26:A:DG:H2'' | 4        | 0.19          |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 10       | 0.19          |
| (1,25)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'' | 6        | 0.19          |
| (1,25)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'' | 7        | 0.19          |
| (1,552) | 1:8:A:DT:H2'   | 1:8:A:DT:H2''  | 3        | 0.18          |
| (1,544) | 1:22:A:DA:H2'' | 1:21:A:DA:H5'' | 10       | 0.18          |
| (1,524) | 1:16:A:DG:H4'  | 1:16:A:DG:H5'  | 5        | 0.18          |
| (1,514) | 1:16:A:DG:H2'  | 1:16:A:DG:H3'  | 4        | 0.18          |
| (1,509) | 1:12:A:DG:H1'  | 1:12:A:DG:H5'  | 5        | 0.18          |
| (1,508) | 1:12:A:DG:H8   | 1:12:A:DG:H5'  | 6        | 0.18          |
| (1,497) | 1:1:A:DA:H2    | 1:2:A:DG:H5''  | 9        | 0.18          |
| (1,491) | 1:13:A:DG:H5'  | 1:31:A:DG:H8   | 4        | 0.18          |
| (1,487) | 1:30:A:DA:H8   | 1:30:A:DA:H4'  | 1        | 0.18          |
| (1,487) | 1:30:A:DA:H8   | 1:30:A:DA:H4'  | 5        | 0.18          |
| (1,486) | 1:30:A:DA:H1'  | 1:30:A:DA:H5'  | 3        | 0.18          |
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 3        | 0.18          |
| (1,459) | 1:3:A:DG:H1    | 1:5:A:DC:H1'   | 4        | 0.18          |
| (1,451) | 1:14:A:DA:H1'  | 1:14:A:DA:H2'  | 4        | 0.18          |
| (1,448) | 1:15:A:DA:H8   | 1:15:A:DA:H2'' | 1        | 0.18          |
| (1,423) | 1:5:A:DC:H6    | 1:5:A:DC:H4'   | 5        | 0.18          |
| (1,412) | 1:19:A:DG:H8   | 1:19:A:DG:H2'  | 1        | 0.18          |
| (1,405) | 1:19:A:DG:H1'  | 1:19:A:DG:H4'  | 3        | 0.18          |
| (1,384) | 1:28:A:DG:H1   | 1:27:A:DG:H8   | 3        | 0.18          |
| (1,368) | 1:20:A:DG:H1'  | 1:21:A:DA:H8   | 9        | 0.18          |
| (1,336) | 1:2:A:DG:H1    | 1:3:A:DG:H1'   | 9        | 0.18          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,333) | 1:26:A:DG:H8   | 1:27:A:DG:H8   | 5        | 0.18          |
| (1,324) | 1:32:A:DG:H8   | 1:31:A:DG:H2'' | 6        | 0.18          |
| (1,313) | 1:32:A:DG:H8   | 1:32:A:DG:H4'  | 5        | 0.18          |
| (1,311) | 1:32:A:DG:H1'  | 1:32:A:DG:H5'  | 4        | 0.18          |
| (1,311) | 1:32:A:DG:H1'  | 1:32:A:DG:H5'  | 7        | 0.18          |
| (1,301) | 1:30:A:DA:H8   | 1:30:A:DA:H2'' | 3        | 0.18          |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 10       | 0.18          |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 6        | 0.18          |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 2        | 0.18          |
| (1,276) | 1:23:A:DG:H1'  | 1:23:A:DG:H2'' | 8        | 0.18          |
| (1,251) | 1:11:A:DG:H2'' | 1:11:A:DG:H3'  | 8        | 0.18          |
| (1,244) | 1:11:A:DG:H8   | 1:11:A:DG:H2'' | 6        | 0.18          |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 7        | 0.18          |
| (1,156) | 1:8:A:DT:H6    | 1:8:A:DT:H2'   | 3        | 0.18          |
| (1,155) | 1:8:A:DT:H6    | 1:8:A:DT:H2''  | 5        | 0.18          |
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 4        | 0.18          |
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 7        | 0.18          |
| (1,129) | 1:10:A:DT:H6   | 1:10:A:DT:H2'  | 6        | 0.18          |
| (1,119) | 1:2:A:DG:H3'   | 1:2:A:DG:H2''  | 2        | 0.18          |
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 8        | 0.18          |
| (1,108) | 1:28:A:DG:H2'' | 1:28:A:DG:H2'  | 2        | 0.18          |
| (1,105) | 1:29:A:DG:H8   | 1:29:A:DG:H3'  | 1        | 0.18          |
| (1,101) | 1:29:A:DG:H1'  | 1:29:A:DG:H2'' | 5        | 0.18          |
| (1,90)  | 1:7:A:DG:H2'   | 1:7:A:DG:H2''  | 8        | 0.18          |
| (1,80)  | 1:25:A:DT:H1'  | 1:25:A:DT:H5'  | 2        | 0.18          |
| (1,78)  | 1:25:A:DT:H1'  | 1:25:A:DT:H2'' | 9        | 0.18          |
| (1,58)  | 1:2:A:DG:H2''  | 1:2:A:DG:H2'   | 5        | 0.18          |
| (1,49)  | 1:2:A:DG:H8    | 1:2:A:DG:H2'   | 3        | 0.18          |
| (1,47)  | 1:3:A:DG:H8    | 1:3:A:DG:H3'   | 3        | 0.18          |
| (1,41)  | 1:2:A:DG:H8    | 1:2:A:DG:H3'   | 2        | 0.18          |
| (1,535) | 1:29:A:DG:H2'' | 1:29:A:DG:H4'  | 7        | 0.17          |
| (1,524) | 1:16:A:DG:H4'  | 1:16:A:DG:H5'  | 4        | 0.17          |
| (1,514) | 1:16:A:DG:H2'  | 1:16:A:DG:H3'  | 3        | 0.17          |
| (1,497) | 1:1:A:DA:H2    | 1:2:A:DG:H5''  | 1        | 0.17          |
| (1,497) | 1:1:A:DA:H2    | 1:2:A:DG:H5''  | 8        | 0.17          |
| (1,479) | 1:30:A:DA:H8   | 1:30:A:DA:H3'  | 2        | 0.17          |
| (1,479) | 1:30:A:DA:H8   | 1:30:A:DA:H3'  | 4        | 0.17          |
| (1,431) | 1:3:A:DG:H1'   | 1:4:A:DG:H3'   | 3        | 0.17          |
| (1,419) | 1:17:A:DA:H8   | 1:17:A:DA:H3'  | 2        | 0.17          |
| (1,412) | 1:19:A:DG:H8   | 1:19:A:DG:H2'  | 5        | 0.17          |
| (1,385) | 1:28:A:DG:H1   | 1:30:A:DA:H8   | 4        | 0.17          |
| (1,377) | 1:10:A:DT:H6   | 1:9:A:DG:H8    | 8        | 0.17          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,372) | 1:19:A:DG:H8   | 1:19:A:DG:H1'  | 4        | 0.17          |
| (1,354) | 1:10:A:DT:H5'  | 1:7:A:DG:H3'   | 10       | 0.17          |
| (1,354) | 1:10:A:DT:H5'' | 1:7:A:DG:H3'   | 10       | 0.17          |
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 9        | 0.17          |
| (1,314) | 1:32:A:DG:H8   | 1:32:A:DG:H5'  | 3        | 0.17          |
| (1,314) | 1:32:A:DG:H8   | 1:32:A:DG:H5'  | 8        | 0.17          |
| (1,311) | 1:32:A:DG:H1'  | 1:32:A:DG:H5'  | 5        | 0.17          |
| (1,301) | 1:30:A:DA:H8   | 1:30:A:DA:H2'' | 4        | 0.17          |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 2        | 0.17          |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 8        | 0.17          |
| (1,259) | 1:13:A:DG:H8   | 1:12:A:DG:H3'  | 1        | 0.17          |
| (1,241) | 1:6:A:DG:H8    | 1:6:A:DG:H2''  | 6        | 0.17          |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 8        | 0.17          |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 10       | 0.17          |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 5        | 0.17          |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 8        | 0.17          |
| (1,210) | 1:7:A:DG:H2''  | 1:7:A:DG:H1'   | 2        | 0.17          |
| (1,173) | 1:3:A:DG:H1    | 1:4:A:DG:H8    | 4        | 0.17          |
| (1,171) | 1:7:A:DG:H1    | 1:13:A:DG:H8   | 6        | 0.17          |
| (1,145) | 1:5:A:DC:H2''  | 1:5:A:DC:H2'   | 4        | 0.17          |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 1        | 0.17          |
| (1,129) | 1:10:A:DT:H6   | 1:10:A:DT:H2'  | 4        | 0.17          |
| (1,123) | 1:4:A:DG:H8    | 1:3:A:DG:H2''  | 3        | 0.17          |
| (1,101) | 1:29:A:DG:H1'  | 1:29:A:DG:H2'' | 8        | 0.17          |
| (1,99)  | 1:28:A:DG:H8   | 1:28:A:DG:H2'' | 8        | 0.17          |
| (1,69)  | 1:27:A:DG:H8   | 1:27:A:DG:H3'  | 1        | 0.17          |
| (1,68)  | 1:27:A:DG:H8   | 1:26:A:DG:H3'  | 3        | 0.17          |
| (1,64)  | 1:8:A:DT:H5'   | 1:8:A:DT:H1'   | 4        | 0.17          |
| (1,64)  | 1:8:A:DT:H5''  | 1:8:A:DT:H1'   | 4        | 0.17          |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 4        | 0.17          |
| (1,48)  | 1:2:A:DG:H8    | 1:2:A:DG:H2''  | 1        | 0.17          |
| (1,46)  | 1:3:A:DG:H8    | 1:2:A:DG:H1'   | 6        | 0.17          |
| (1,26)  | 1:25:A:DT:H6   | 1:25:A:DT:H2'  | 5        | 0.17          |
| (1,552) | 1:8:A:DT:H2'   | 1:8:A:DT:H2''  | 1        | 0.16          |
| (1,520) | 1:17:A:DA:H4'  | 1:17:A:DA:H5'  | 2        | 0.16          |
| (1,492) | 1:14:A:DA:H8   | 1:14:A:DA:H5'  | 3        | 0.16          |
| (1,486) | 1:30:A:DA:H1'  | 1:30:A:DA:H5'  | 4        | 0.16          |
| (1,481) | 1:2:A:DG:H8    | 1:1:A:DA:H3'   | 5        | 0.16          |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 6        | 0.16          |
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 7        | 0.16          |
| (1,440) | 1:15:A:DA:H8   | 1:15:A:DA:H3'  | 10       | 0.16          |
| (1,425) | 1:17:A:DA:H8   | 1:17:A:DA:H4'  | 6        | 0.16          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,423) | 1:5:A:DC:H6    | 1:5:A:DC:H4'   | 2        | 0.16          |
| (1,423) | 1:5:A:DC:H6    | 1:5:A:DC:H4'   | 4        | 0.16          |
| (1,418) | 1:18:A:DG:H8   | 1:18:A:DG:H2'  | 7        | 0.16          |
| (1,412) | 1:19:A:DG:H8   | 1:19:A:DG:H2'  | 2        | 0.16          |
| (1,386) | 1:13:A:DG:H1'  | 1:14:A:DA:H8   | 4        | 0.16          |
| (1,385) | 1:28:A:DG:H1   | 1:30:A:DA:H8   | 1        | 0.16          |
| (1,372) | 1:19:A:DG:H8   | 1:19:A:DG:H1'  | 5        | 0.16          |
| (1,354) | 1:10:A:DT:H5'  | 1:7:A:DG:H3'   | 9        | 0.16          |
| (1,354) | 1:10:A:DT:H5'' | 1:7:A:DG:H3'   | 9        | 0.16          |
| (1,337) | 1:26:A:DG:H1   | 1:27:A:DG:H1'  | 3        | 0.16          |
| (1,337) | 1:26:A:DG:H1   | 1:27:A:DG:H1'  | 5        | 0.16          |
| (1,336) | 1:2:A:DG:H1    | 1:3:A:DG:H1'   | 4        | 0.16          |
| (1,308) | 1:32:A:DG:H8   | 1:32:A:DG:H2'  | 3        | 0.16          |
| (1,288) | 1:1:A:DA:H1'   | 1:1:A:DA:H4'   | 7        | 0.16          |
| (1,281) | 1:2:A:DG:H8    | 1:1:A:DA:H5'   | 4        | 0.16          |
| (1,265) | 1:13:A:DG:H1'  | 1:13:A:DG:H2'' | 4        | 0.16          |
| (1,240) | 1:11:A:DG:H8   | 1:11:A:DG:H3'  | 5        | 0.16          |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 1        | 0.16          |
| (1,224) | 1:9:A:DG:H1'   | 1:9:A:DG:H2''  | 1        | 0.16          |
| (1,224) | 1:9:A:DG:H1'   | 1:9:A:DG:H2''  | 6        | 0.16          |
| (1,155) | 1:8:A:DT:H6    | 1:8:A:DT:H2''  | 1        | 0.16          |
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 1        | 0.16          |
| (1,131) | 1:10:A:DT:H1'  | 1:10:A:DT:H2'' | 5        | 0.16          |
| (1,124) | 1:4:A:DG:H8    | 1:3:A:DG:H2'   | 4        | 0.16          |
| (1,119) | 1:2:A:DG:H3'   | 1:2:A:DG:H2''  | 1        | 0.16          |
| (1,106) | 1:28:A:DG:H2'' | 1:28:A:DG:H3'  | 4        | 0.16          |
| (1,103) | 1:28:A:DG:H8   | 1:28:A:DG:H3'  | 4        | 0.16          |
| (1,91)  | 1:27:A:DG:H8   | 1:27:A:DG:H2'' | 6        | 0.16          |
| (1,80)  | 1:25:A:DT:H1'  | 1:25:A:DT:H5'  | 5        | 0.16          |
| (1,48)  | 1:2:A:DG:H8    | 1:2:A:DG:H2''  | 6        | 0.16          |
| (1,32)  | 1:25:A:DT:H6   | 1:26:A:DG:H8   | 5        | 0.16          |
| (1,30)  | 1:25:A:DT:H5'  | 1:24:A:DA:H8   | 1        | 0.16          |
| (1,30)  | 1:25:A:DT:H5'' | 1:24:A:DA:H8   | 1        | 0.16          |
| (1,7)   | 1:7:A:DG:H1    | 1:11:A:DG:H1   | 2        | 0.16          |
| (1,7)   | 1:7:A:DG:H1    | 1:11:A:DG:H1   | 4        | 0.16          |
| (1,548) | 1:32:A:DG:H2'  | 1:32:A:DG:H5'  | 6        | 0.15          |
| (1,527) | 1:21:A:DA:H5'  | 1:17:A:DA:H5'  | 8        | 0.15          |
| (1,513) | 1:21:A:DA:H1'  | 1:20:A:DG:H5'  | 6        | 0.15          |
| (1,507) | 1:3:A:DG:H4'   | 1:1:A:DA:H2    | 7        | 0.15          |
| (1,491) | 1:13:A:DG:H5'  | 1:31:A:DG:H8   | 9        | 0.15          |
| (1,487) | 1:30:A:DA:H8   | 1:30:A:DA:H4'  | 9        | 0.15          |
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 5        | 0.15          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,451) | 1:14:A:DA:H1'  | 1:14:A:DA:H2'  | 10       | 0.15          |
| (1,448) | 1:15:A:DA:H8   | 1:15:A:DA:H2'' | 8        | 0.15          |
| (1,419) | 1:17:A:DA:H8   | 1:17:A:DA:H3'  | 3        | 0.15          |
| (1,411) | 1:19:A:DG:H8   | 1:19:A:DG:H2'' | 8        | 0.15          |
| (1,386) | 1:13:A:DG:H1'  | 1:14:A:DA:H8   | 9        | 0.15          |
| (1,384) | 1:28:A:DG:H1   | 1:27:A:DG:H8   | 7        | 0.15          |
| (1,384) | 1:28:A:DG:H1   | 1:27:A:DG:H8   | 8        | 0.15          |
| (1,365) | 1:16:A:DG:H1'  | 1:17:A:DA:H8   | 4        | 0.15          |
| (1,363) | 1:11:A:DG:H8   | 1:12:A:DG:H8   | 8        | 0.15          |
| (1,359) | 1:25:A:DT:H5'  | 1:24:A:DA:H2'  | 3        | 0.15          |
| (1,359) | 1:25:A:DT:H5'' | 1:24:A:DA:H2'  | 3        | 0.15          |
| (1,340) | 1:13:A:DG:H1   | 1:8:A:DT:H6    | 7        | 0.15          |
| (1,314) | 1:32:A:DG:H8   | 1:32:A:DG:H5'  | 6        | 0.15          |
| (1,311) | 1:32:A:DG:H1'  | 1:32:A:DG:H5'  | 1        | 0.15          |
| (1,302) | 1:30:A:DA:H8   | 1:30:A:DA:H2'  | 3        | 0.15          |
| (1,298) | 1:8:A:DT:H6    | 1:30:A:DA:H8   | 3        | 0.15          |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 8        | 0.15          |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 9        | 0.15          |
| (1,244) | 1:11:A:DG:H8   | 1:11:A:DG:H2'' | 4        | 0.15          |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 6        | 0.15          |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 9        | 0.15          |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 4        | 0.15          |
| (1,231) | 1:9:A:DG:H1'   | 1:9:A:DG:H4'   | 9        | 0.15          |
| (1,226) | 1:9:A:DG:H3'   | 1:9:A:DG:H2'   | 5        | 0.15          |
| (1,224) | 1:9:A:DG:H1'   | 1:9:A:DG:H2''  | 7        | 0.15          |
| (1,220) | 1:7:A:DG:H2''  | 1:9:A:DG:H8    | 5        | 0.15          |
| (1,219) | 1:7:A:DG:H2'   | 1:9:A:DG:H8    | 4        | 0.15          |
| (1,215) | 1:7:A:DG:H2'   | 1:7:A:DG:H8    | 2        | 0.15          |
| (1,215) | 1:7:A:DG:H2'   | 1:7:A:DG:H8    | 6        | 0.15          |
| (1,210) | 1:7:A:DG:H2''  | 1:7:A:DG:H1'   | 8        | 0.15          |
| (1,204) | 1:6:A:DG:H3'   | 1:6:A:DG:H5'   | 5        | 0.15          |
| (1,193) | 1:3:A:DG:H1'   | 1:3:A:DG:H4'   | 3        | 0.15          |
| (1,193) | 1:3:A:DG:H1'   | 1:3:A:DG:H4'   | 7        | 0.15          |
| (1,141) | 1:5:A:DC:H5    | 1:5:A:DC:H2''  | 2        | 0.15          |
| (1,123) | 1:4:A:DG:H8    | 1:3:A:DG:H2''  | 6        | 0.15          |
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 4        | 0.15          |
| (1,79)  | 1:25:A:DT:H6   | 1:25:A:DT:H5'  | 1        | 0.15          |
| (1,22)  | 1:25:A:DT:H6   | 1:24:A:DA:H1'  | 9        | 0.15          |
| (1,21)  | 1:8:A:DT:H6    | 1:8:A:DT:H1'   | 9        | 0.15          |
| (1,552) | 1:8:A:DT:H2'   | 1:8:A:DT:H2''  | 5        | 0.14          |
| (1,552) | 1:8:A:DT:H2'   | 1:8:A:DT:H2''  | 9        | 0.14          |
| (1,538) | 1:25:A:DT:H2'' | 1:25:A:DT:H5'  | 8        | 0.14          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,535) | 1:29:A:DG:H2'' | 1:29:A:DG:H4'  | 2        | 0.14          |
| (1,535) | 1:29:A:DG:H2'' | 1:29:A:DG:H4'  | 10       | 0.14          |
| (1,529) | 1:9:A:DG:H2'   | 1:9:A:DG:H5''  | 5        | 0.14          |
| (1,526) | 1:32:A:DG:H5'  | 1:31:A:DG:H5'  | 9        | 0.14          |
| (1,520) | 1:17:A:DA:H4'  | 1:17:A:DA:H5'  | 1        | 0.14          |
| (1,520) | 1:17:A:DA:H4'  | 1:17:A:DA:H5'  | 4        | 0.14          |
| (1,514) | 1:16:A:DG:H2'  | 1:16:A:DG:H3'  | 8        | 0.14          |
| (1,497) | 1:1:A:DA:H2    | 1:2:A:DG:H5''  | 2        | 0.14          |
| (1,484) | 1:30:A:DA:H1'  | 1:30:A:DA:H4'  | 8        | 0.14          |
| (1,481) | 1:2:A:DG:H8    | 1:1:A:DA:H3'   | 7        | 0.14          |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 4        | 0.14          |
| (1,475) | 1:25:A:DT:H2'' | 1:24:A:DA:H5'' | 3        | 0.14          |
| (1,451) | 1:14:A:DA:H1'  | 1:14:A:DA:H2'  | 5        | 0.14          |
| (1,443) | 1:15:A:DA:H1'  | 1:15:A:DA:H5'  | 8        | 0.14          |
| (1,432) | 1:16:A:DG:H1'  | 1:16:A:DG:H4'  | 2        | 0.14          |
| (1,425) | 1:17:A:DA:H8   | 1:17:A:DA:H4'  | 9        | 0.14          |
| (1,418) | 1:18:A:DG:H8   | 1:18:A:DG:H2'  | 8        | 0.14          |
| (1,413) | 1:19:A:DG:H8   | 1:19:A:DG:H3'  | 2        | 0.14          |
| (1,409) | 1:19:A:DG:H1'  | 1:19:A:DG:H2'' | 8        | 0.14          |
| (1,408) | 1:19:A:DG:H1'  | 1:19:A:DG:H5'' | 6        | 0.14          |
| (1,401) | 1:20:A:DG:H1'  | 1:21:A:DA:H5'  | 3        | 0.14          |
| (1,390) | 1:22:A:DA:H8   | 1:22:A:DA:H2'' | 8        | 0.14          |
| (1,388) | 1:22:A:DA:H8   | 1:22:A:DA:H3'  | 6        | 0.14          |
| (1,385) | 1:28:A:DG:H1   | 1:30:A:DA:H8   | 9        | 0.14          |
| (1,375) | 1:16:A:DG:H8   | 1:15:A:DA:H1'  | 1        | 0.14          |
| (1,370) | 1:17:A:DA:H1'  | 1:18:A:DG:H8   | 9        | 0.14          |
| (1,359) | 1:25:A:DT:H5'  | 1:24:A:DA:H2'  | 5        | 0.14          |
| (1,359) | 1:25:A:DT:H5'' | 1:24:A:DA:H2'  | 5        | 0.14          |
| (1,332) | 1:27:A:DG:H8   | 1:28:A:DG:H8   | 4        | 0.14          |
| (1,324) | 1:32:A:DG:H8   | 1:31:A:DG:H2'' | 5        | 0.14          |
| (1,293) | 1:2:A:DG:H8    | 1:1:A:DA:H1'   | 4        | 0.14          |
| (1,289) | 1:1:A:DA:H5'   | 1:1:A:DA:H4'   | 7        | 0.14          |
| (1,276) | 1:23:A:DG:H1'  | 1:23:A:DG:H2'' | 7        | 0.14          |
| (1,260) | 1:13:A:DG:H8   | 1:12:A:DG:H2'  | 5        | 0.14          |
| (1,260) | 1:13:A:DG:H8   | 1:12:A:DG:H2'  | 7        | 0.14          |
| (1,237) | 1:6:A:DG:H8    | 1:6:A:DG:H5''  | 8        | 0.14          |
| (1,228) | 1:9:A:DG:H1'   | 1:7:A:DG:H3'   | 4        | 0.14          |
| (1,199) | 1:6:A:DG:H3'   | 1:6:A:DG:H2'   | 4        | 0.14          |
| (1,193) | 1:3:A:DG:H1'   | 1:3:A:DG:H4'   | 6        | 0.14          |
| (1,156) | 1:8:A:DT:H6    | 1:8:A:DT:H2'   | 2        | 0.14          |
| (1,145) | 1:5:A:DC:H2''  | 1:5:A:DC:H2'   | 8        | 0.14          |
| (1,124) | 1:4:A:DG:H8    | 1:3:A:DG:H2'   | 3        | 0.14          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 4        | 0.14          |
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 7        | 0.14          |
| (1,113) | 1:29:A:DG:H2'' | 1:29:A:DG:H2'  | 4        | 0.14          |
| (1,113) | 1:29:A:DG:H2'' | 1:29:A:DG:H2'  | 9        | 0.14          |
| (1,109) | 1:29:A:DG:H8   | 1:28:A:DG:H2'  | 9        | 0.14          |
| (1,105) | 1:29:A:DG:H8   | 1:29:A:DG:H3'  | 3        | 0.14          |
| (1,101) | 1:29:A:DG:H1'  | 1:29:A:DG:H2'' | 3        | 0.14          |
| (1,101) | 1:29:A:DG:H1'  | 1:29:A:DG:H2'' | 6        | 0.14          |
| (1,95)  | 1:28:A:DG:H1'  | 1:28:A:DG:H2'' | 6        | 0.14          |
| (1,90)  | 1:7:A:DG:H2'   | 1:7:A:DG:H2''  | 6        | 0.14          |
| (1,87)  | 1:26:A:DG:H2'  | 1:26:A:DG:H3'  | 7        | 0.14          |
| (1,81)  | 1:25:A:DT:H2'' | 1:25:A:DT:H2'  | 9        | 0.14          |
| (1,80)  | 1:25:A:DT:H1'  | 1:25:A:DT:H5'  | 6        | 0.14          |
| (1,78)  | 1:25:A:DT:H1'  | 1:25:A:DT:H2'' | 4        | 0.14          |
| (1,78)  | 1:25:A:DT:H1'  | 1:25:A:DT:H2'' | 7        | 0.14          |
| (1,74)  | 1:28:A:DG:H1'  | 1:29:A:DG:H8   | 10       | 0.14          |
| (1,47)  | 1:3:A:DG:H8    | 1:3:A:DG:H3'   | 4        | 0.14          |
| (1,28)  | 1:26:A:DG:H8   | 1:26:A:DG:H2'' | 1        | 0.14          |
| (1,28)  | 1:26:A:DG:H8   | 1:26:A:DG:H2'' | 3        | 0.14          |
| (1,24)  | 1:24:A:DA:H8   | 1:23:A:DG:H1'  | 8        | 0.14          |
| (1,22)  | 1:25:A:DT:H6   | 1:24:A:DA:H1'  | 5        | 0.14          |
| (1,7)   | 1:7:A:DG:H1    | 1:11:A:DG:H1   | 3        | 0.14          |
| (1,7)   | 1:7:A:DG:H1    | 1:11:A:DG:H1   | 6        | 0.14          |
| (1,549) | 1:30:A:DA:H2'  | 1:30:A:DA:H5'  | 5        | 0.13          |
| (1,548) | 1:32:A:DG:H2'  | 1:32:A:DG:H5'  | 3        | 0.13          |
| (1,547) | 1:32:A:DG:H2'' | 1:32:A:DG:H5'  | 1        | 0.13          |
| (1,520) | 1:17:A:DA:H4'  | 1:17:A:DA:H5'  | 8        | 0.13          |
| (1,511) | 1:25:A:DT:H6   | 1:12:A:DG:H8   | 6        | 0.13          |
| (1,508) | 1:12:A:DG:H8   | 1:12:A:DG:H5'  | 10       | 0.13          |
| (1,504) | 1:11:A:DG:H1'  | 1:11:A:DG:H5'  | 4        | 0.13          |
| (1,499) | 1:19:A:DG:H8   | 1:19:A:DG:H5'' | 1        | 0.13          |
| (1,496) | 1:3:A:DG:H1'   | 1:3:A:DG:H5''  | 6        | 0.13          |
| (1,482) | 1:30:A:DA:H8   | 1:30:A:DA:H5'' | 10       | 0.13          |
| (1,481) | 1:2:A:DG:H8    | 1:1:A:DA:H3'   | 4        | 0.13          |
| (1,480) | 1:13:A:DG:H5'  | 1:14:A:DA:H2   | 8        | 0.13          |
| (1,479) | 1:30:A:DA:H8   | 1:30:A:DA:H3'  | 10       | 0.13          |
| (1,475) | 1:25:A:DT:H2'' | 1:24:A:DA:H5'' | 7        | 0.13          |
| (1,451) | 1:14:A:DA:H1'  | 1:14:A:DA:H2'  | 6        | 0.13          |
| (1,449) | 1:15:A:DA:H1'  | 1:15:A:DA:H2'' | 6        | 0.13          |
| (1,447) | 1:15:A:DA:H8   | 1:15:A:DA:H2'  | 2        | 0.13          |
| (1,422) | 1:5:A:DC:H1'   | 1:5:A:DC:H5'   | 6        | 0.13          |
| (1,414) | 1:18:A:DG:H8   | 1:18:A:DG:H3'  | 3        | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,389) | 1:22:A:DA:H8   | 1:22:A:DA:H2'  | 5        | 0.13          |
| (1,385) | 1:28:A:DG:H1   | 1:30:A:DA:H8   | 10       | 0.13          |
| (1,372) | 1:19:A:DG:H8   | 1:19:A:DG:H1'  | 10       | 0.13          |
| (1,351) | 1:25:A:DT:H5'  | 1:24:A:DA:H1'  | 3        | 0.13          |
| (1,351) | 1:25:A:DT:H5'' | 1:24:A:DA:H1'  | 3        | 0.13          |
| (1,311) | 1:32:A:DG:H1'  | 1:32:A:DG:H5'  | 3        | 0.13          |
| (1,301) | 1:30:A:DA:H8   | 1:30:A:DA:H2'' | 7        | 0.13          |
| (1,286) | 1:1:A:DA:H1'   | 1:1:A:DA:H2'   | 2        | 0.13          |
| (1,284) | 1:1:A:DA:H8    | 1:1:A:DA:H2''  | 7        | 0.13          |
| (1,280) | 1:1:A:DA:H8    | 1:1:A:DA:H5'   | 6        | 0.13          |
| (1,279) | 1:1:A:DA:H8    | 1:1:A:DA:H3'   | 8        | 0.13          |
| (1,274) | 1:23:A:DG:H8   | 1:23:A:DG:H2'' | 3        | 0.13          |
| (1,273) | 1:23:A:DG:H8   | 1:23:A:DG:H2'  | 8        | 0.13          |
| (1,251) | 1:11:A:DG:H2'' | 1:11:A:DG:H3'  | 10       | 0.13          |
| (1,244) | 1:11:A:DG:H8   | 1:11:A:DG:H2'' | 9        | 0.13          |
| (1,241) | 1:6:A:DG:H8    | 1:6:A:DG:H2''  | 10       | 0.13          |
| (1,239) | 1:11:A:DG:H2'  | 1:11:A:DG:H2'' | 3        | 0.13          |
| (1,238) | 1:10:A:DT:H6   | 1:10:A:DT:H4'  | 3        | 0.13          |
| (1,216) | 1:7:A:DG:H2''  | 1:7:A:DG:H8    | 3        | 0.13          |
| (1,193) | 1:3:A:DG:H1'   | 1:3:A:DG:H4'   | 9        | 0.13          |
| (1,180) | 1:9:A:DG:H8    | 1:7:A:DG:H1'   | 10       | 0.13          |
| (1,162) | 1:7:A:DG:H1    | 1:12:A:DG:H8   | 2        | 0.13          |
| (1,155) | 1:8:A:DT:H6    | 1:8:A:DT:H2''  | 10       | 0.13          |
| (1,145) | 1:5:A:DC:H2''  | 1:5:A:DC:H2'   | 9        | 0.13          |
| (1,139) | 1:5:A:DC:H6    | 1:5:A:DC:H2'   | 1        | 0.13          |
| (1,139) | 1:5:A:DC:H6    | 1:5:A:DC:H2'   | 3        | 0.13          |
| (1,139) | 1:5:A:DC:H6    | 1:5:A:DC:H2'   | 5        | 0.13          |
| (1,119) | 1:2:A:DG:H3'   | 1:2:A:DG:H2''  | 9        | 0.13          |
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 1        | 0.13          |
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 5        | 0.13          |
| (1,101) | 1:29:A:DG:H1'  | 1:29:A:DG:H2'' | 4        | 0.13          |
| (1,101) | 1:29:A:DG:H1'  | 1:29:A:DG:H2'' | 9        | 0.13          |
| (1,90)  | 1:7:A:DG:H2'   | 1:7:A:DG:H2''  | 1        | 0.13          |
| (1,90)  | 1:7:A:DG:H2'   | 1:7:A:DG:H2''  | 2        | 0.13          |
| (1,84)  | 1:26:A:DG:H1'  | 1:26:A:DG:H2'' | 1        | 0.13          |
| (1,78)  | 1:25:A:DT:H1'  | 1:25:A:DT:H2'' | 1        | 0.13          |
| (1,74)  | 1:28:A:DG:H1'  | 1:29:A:DG:H8   | 4        | 0.13          |
| (1,64)  | 1:8:A:DT:H5'   | 1:8:A:DT:H1'   | 2        | 0.13          |
| (1,64)  | 1:8:A:DT:H5''  | 1:8:A:DT:H1'   | 2        | 0.13          |
| (1,63)  | 1:8:A:DT:H1'   | 1:8:A:DT:H2''  | 3        | 0.13          |
| (1,51)  | 1:3:A:DG:H8    | 1:2:A:DG:H2''  | 4        | 0.13          |
| (1,48)  | 1:2:A:DG:H8    | 1:2:A:DG:H2''  | 7        | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,41)  | 1:2:A:DG:H8    | 1:2:A:DG:H3'   | 8        | 0.13          |
| (1,27)  | 1:26:A:DG:H8   | 1:25:A:DT:H2'' | 1        | 0.13          |
| (1,22)  | 1:25:A:DT:H6   | 1:24:A:DA:H1'  | 1        | 0.13          |
| (1,22)  | 1:25:A:DT:H6   | 1:24:A:DA:H1'  | 4        | 0.13          |
| (1,6)   | 1:11:A:DG:H1   | 1:26:A:DG:H1   | 8        | 0.13          |
| (1,548) | 1:32:A:DG:H2'  | 1:32:A:DG:H5'  | 10       | 0.12          |
| (1,539) | 1:21:A:DA:H2'  | 1:21:A:DA:H5'' | 6        | 0.12          |
| (1,509) | 1:12:A:DG:H1'  | 1:12:A:DG:H5'  | 3        | 0.12          |
| (1,475) | 1:25:A:DT:H2'' | 1:24:A:DA:H5'' | 9        | 0.12          |
| (1,451) | 1:14:A:DA:H1'  | 1:14:A:DA:H2'  | 1        | 0.12          |
| (1,447) | 1:15:A:DA:H8   | 1:15:A:DA:H2'  | 9        | 0.12          |
| (1,443) | 1:15:A:DA:H1'  | 1:15:A:DA:H5'  | 6        | 0.12          |
| (1,440) | 1:15:A:DA:H8   | 1:15:A:DA:H3'  | 9        | 0.12          |
| (1,425) | 1:17:A:DA:H8   | 1:17:A:DA:H4'  | 3        | 0.12          |
| (1,390) | 1:22:A:DA:H8   | 1:22:A:DA:H2'' | 1        | 0.12          |
| (1,384) | 1:28:A:DG:H1   | 1:27:A:DG:H8   | 2        | 0.12          |
| (1,372) | 1:19:A:DG:H8   | 1:19:A:DG:H1'  | 2        | 0.12          |
| (1,370) | 1:17:A:DA:H1'  | 1:18:A:DG:H8   | 6        | 0.12          |
| (1,351) | 1:25:A:DT:H5'  | 1:24:A:DA:H1'  | 6        | 0.12          |
| (1,351) | 1:25:A:DT:H5'' | 1:24:A:DA:H1'  | 6        | 0.12          |
| (1,336) | 1:2:A:DG:H1    | 1:3:A:DG:H1'   | 6        | 0.12          |
| (1,332) | 1:27:A:DG:H8   | 1:28:A:DG:H8   | 2        | 0.12          |
| (1,331) | 1:14:A:DA:H8   | 1:14:A:DA:H1'  | 4        | 0.12          |
| (1,331) | 1:14:A:DA:H8   | 1:14:A:DA:H1'  | 10       | 0.12          |
| (1,314) | 1:32:A:DG:H8   | 1:32:A:DG:H5'  | 5        | 0.12          |
| (1,285) | 1:1:A:DA:H1'   | 1:1:A:DA:H2''  | 9        | 0.12          |
| (1,282) | 1:1:A:DA:H5'   | 1:1:A:DA:H2    | 7        | 0.12          |
| (1,251) | 1:11:A:DG:H2'' | 1:11:A:DG:H3'  | 2        | 0.12          |
| (1,251) | 1:11:A:DG:H2'' | 1:11:A:DG:H3'  | 6        | 0.12          |
| (1,227) | 1:9:A:DG:H8    | 1:9:A:DG:H4'   | 6        | 0.12          |
| (1,224) | 1:9:A:DG:H1'   | 1:9:A:DG:H2''  | 4        | 0.12          |
| (1,216) | 1:7:A:DG:H2''  | 1:7:A:DG:H8    | 5        | 0.12          |
| (1,215) | 1:7:A:DG:H2'   | 1:7:A:DG:H8    | 5        | 0.12          |
| (1,199) | 1:6:A:DG:H3'   | 1:6:A:DG:H2'   | 6        | 0.12          |
| (1,194) | 1:3:A:DG:H1'   | 1:3:A:DG:H5'   | 6        | 0.12          |
| (1,147) | 1:24:A:DA:H8   | 1:24:A:DA:H4'  | 7        | 0.12          |
| (1,130) | 1:10:A:DT:H6   | 1:10:A:DT:H2'' | 9        | 0.12          |
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 3        | 0.12          |
| (1,116) | 1:29:A:DG:H1'  | 1:29:A:DG:H5'  | 6        | 0.12          |
| (1,110) | 1:29:A:DG:H8   | 1:28:A:DG:H2'' | 2        | 0.12          |
| (1,105) | 1:29:A:DG:H8   | 1:29:A:DG:H3'  | 7        | 0.12          |
| (1,103) | 1:28:A:DG:H8   | 1:28:A:DG:H3'  | 9        | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,90)  | 1:7:A:DG:H2'   | 1:7:A:DG:H2''  | 3        | 0.12          |
| (1,90)  | 1:7:A:DG:H2'   | 1:7:A:DG:H2''  | 10       | 0.12          |
| (1,84)  | 1:26:A:DG:H1'  | 1:26:A:DG:H2'' | 3        | 0.12          |
| (1,84)  | 1:26:A:DG:H1'  | 1:26:A:DG:H2'' | 9        | 0.12          |
| (1,68)  | 1:27:A:DG:H8   | 1:26:A:DG:H3'  | 6        | 0.12          |
| (1,64)  | 1:8:A:DT:H5'   | 1:8:A:DT:H1'   | 7        | 0.12          |
| (1,64)  | 1:8:A:DT:H5''  | 1:8:A:DT:H1'   | 7        | 0.12          |
| (1,59)  | 1:3:A:DG:H2'   | 1:3:A:DG:H2''  | 8        | 0.12          |
| (1,49)  | 1:2:A:DG:H8    | 1:2:A:DG:H2'   | 8        | 0.12          |
| (1,7)   | 1:7:A:DG:H1    | 1:11:A:DG:H1   | 8        | 0.12          |
| (1,6)   | 1:11:A:DG:H1   | 1:26:A:DG:H1   | 4        | 0.12          |
| (1,552) | 1:8:A:DT:H2'   | 1:8:A:DT:H2''  | 4        | 0.11          |
| (1,552) | 1:8:A:DT:H2'   | 1:8:A:DT:H2''  | 8        | 0.11          |
| (1,547) | 1:32:A:DG:H2'' | 1:32:A:DG:H5'  | 5        | 0.11          |
| (1,534) | 1:3:A:DG:H2''  | 1:2:A:DG:H5'   | 6        | 0.11          |
| (1,511) | 1:25:A:DT:H6   | 1:12:A:DG:H8   | 8        | 0.11          |
| (1,504) | 1:11:A:DG:H1'  | 1:11:A:DG:H5'  | 3        | 0.11          |
| (1,503) | 1:11:A:DG:H1'  | 1:11:A:DG:H4'  | 4        | 0.11          |
| (1,496) | 1:3:A:DG:H1'   | 1:3:A:DG:H5''  | 10       | 0.11          |
| (1,486) | 1:30:A:DA:H1'  | 1:30:A:DA:H5'  | 5        | 0.11          |
| (1,480) | 1:13:A:DG:H5'  | 1:14:A:DA:H2   | 3        | 0.11          |
| (1,479) | 1:30:A:DA:H8   | 1:30:A:DA:H3'  | 7        | 0.11          |
| (1,479) | 1:30:A:DA:H8   | 1:30:A:DA:H3'  | 8        | 0.11          |
| (1,441) | 1:7:A:DG:H1'   | 1:9:A:DG:H1'   | 3        | 0.11          |
| (1,419) | 1:17:A:DA:H8   | 1:17:A:DA:H3'  | 6        | 0.11          |
| (1,418) | 1:18:A:DG:H8   | 1:18:A:DG:H2'  | 10       | 0.11          |
| (1,414) | 1:18:A:DG:H8   | 1:18:A:DG:H3'  | 5        | 0.11          |
| (1,396) | 1:21:A:DA:H8   | 1:21:A:DA:H3'  | 10       | 0.11          |
| (1,390) | 1:22:A:DA:H8   | 1:22:A:DA:H2'' | 2        | 0.11          |
| (1,377) | 1:10:A:DT:H6   | 1:9:A:DG:H8    | 9        | 0.11          |
| (1,375) | 1:16:A:DG:H8   | 1:15:A:DA:H1'  | 8        | 0.11          |
| (1,368) | 1:20:A:DG:H1'  | 1:21:A:DA:H8   | 8        | 0.11          |
| (1,308) | 1:32:A:DG:H8   | 1:32:A:DG:H2'  | 5        | 0.11          |
| (1,301) | 1:30:A:DA:H8   | 1:30:A:DA:H2'' | 6        | 0.11          |
| (1,301) | 1:30:A:DA:H8   | 1:30:A:DA:H2'' | 8        | 0.11          |
| (1,290) | 1:1:A:DA:H5'   | 1:1:A:DA:H2'   | 2        | 0.11          |
| (1,290) | 1:1:A:DA:H5'   | 1:1:A:DA:H2'   | 5        | 0.11          |
| (1,288) | 1:1:A:DA:H1'   | 1:1:A:DA:H4'   | 3        | 0.11          |
| (1,276) | 1:23:A:DG:H1'  | 1:23:A:DG:H2'' | 10       | 0.11          |
| (1,265) | 1:13:A:DG:H1'  | 1:13:A:DG:H2'' | 7        | 0.11          |
| (1,265) | 1:13:A:DG:H1'  | 1:13:A:DG:H2'' | 9        | 0.11          |
| (1,265) | 1:13:A:DG:H1'  | 1:13:A:DG:H2'' | 10       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,251) | 1:11:A:DG:H2'' | 1:11:A:DG:H3'  | 7        | 0.11          |
| (1,250) | 1:11:A:DG:H1'  | 1:11:A:DG:H2'' | 8        | 0.11          |
| (1,244) | 1:11:A:DG:H8   | 1:11:A:DG:H2'' | 2        | 0.11          |
| (1,240) | 1:11:A:DG:H8   | 1:11:A:DG:H3'  | 1        | 0.11          |
| (1,226) | 1:9:A:DG:H3'   | 1:9:A:DG:H2'   | 10       | 0.11          |
| (1,204) | 1:6:A:DG:H3'   | 1:6:A:DG:H5'   | 4        | 0.11          |
| (1,199) | 1:6:A:DG:H3'   | 1:6:A:DG:H2'   | 9        | 0.11          |
| (1,189) | 1:5:A:DC:H5    | 1:5:A:DC:H3'   | 9        | 0.11          |
| (1,183) | 1:13:A:DG:H8   | 1:12:A:DG:H1'  | 5        | 0.11          |
| (1,179) | 1:9:A:DG:H8    | 1:9:A:DG:H1'   | 3        | 0.11          |
| (1,150) | 1:24:A:DA:H1'  | 1:24:A:DA:H4'  | 10       | 0.11          |
| (1,127) | 1:10:A:DT:H6   | 1:10:A:DT:H5'  | 2        | 0.11          |
| (1,123) | 1:4:A:DG:H8    | 1:3:A:DG:H2''  | 9        | 0.11          |
| (1,119) | 1:2:A:DG:H3'   | 1:2:A:DG:H2''  | 7        | 0.11          |
| (1,119) | 1:2:A:DG:H3'   | 1:2:A:DG:H2''  | 8        | 0.11          |
| (1,113) | 1:29:A:DG:H2'' | 1:29:A:DG:H2'  | 5        | 0.11          |
| (1,112) | 1:29:A:DG:H8   | 1:29:A:DG:H2'  | 9        | 0.11          |
| (1,105) | 1:29:A:DG:H8   | 1:29:A:DG:H3'  | 2        | 0.11          |
| (1,103) | 1:28:A:DG:H8   | 1:28:A:DG:H3'  | 5        | 0.11          |
| (1,90)  | 1:7:A:DG:H2'   | 1:7:A:DG:H2''  | 5        | 0.11          |
| (1,90)  | 1:7:A:DG:H2'   | 1:7:A:DG:H2''  | 9        | 0.11          |
| (1,80)  | 1:25:A:DT:H1'  | 1:25:A:DT:H5'  | 4        | 0.11          |
| (1,52)  | 1:4:A:DG:H8    | 1:4:A:DG:H3'   | 6        | 0.11          |
| (1,51)  | 1:3:A:DG:H8    | 1:2:A:DG:H2''  | 8        | 0.11          |
| (1,48)  | 1:2:A:DG:H8    | 1:2:A:DG:H2''  | 5        | 0.11          |
| (1,47)  | 1:3:A:DG:H8    | 1:3:A:DG:H3'   | 1        | 0.11          |
| (1,41)  | 1:2:A:DG:H8    | 1:2:A:DG:H3'   | 3        | 0.11          |
| (1,41)  | 1:2:A:DG:H8    | 1:2:A:DG:H3'   | 4        | 0.11          |
| (1,22)  | 1:25:A:DT:H6   | 1:24:A:DA:H1'  | 2        | 0.11          |
| (1,538) | 1:25:A:DT:H2'' | 1:25:A:DT:H5'  | 4        | 0.1           |
| (1,519) | 1:15:A:DA:H4'  | 1:15:A:DA:H5'  | 3        | 0.1           |
| (1,498) | 1:1:A:DA:H2    | 1:2:A:DG:H5'   | 5        | 0.1           |
| (1,497) | 1:1:A:DA:H2    | 1:2:A:DG:H5''  | 10       | 0.1           |
| (1,478) | 1:13:A:DG:H5'  | 1:31:A:DG:H1'  | 10       | 0.1           |
| (1,465) | 1:7:A:DG:H1    | 1:7:A:DG:H2''  | 1        | 0.1           |
| (1,461) | 1:28:A:DG:H1   | 1:27:A:DG:H2'' | 9        | 0.1           |
| (1,460) | 1:4:A:DG:H1    | 1:31:A:DG:H1'  | 10       | 0.1           |
| (1,436) | 1:16:A:DG:H8   | 1:16:A:DG:H2'  | 6        | 0.1           |
| (1,407) | 1:20:A:DG:H1'  | 1:19:A:DG:H5'  | 10       | 0.1           |
| (1,401) | 1:20:A:DG:H1'  | 1:21:A:DA:H5'  | 2        | 0.1           |
| (1,389) | 1:22:A:DA:H8   | 1:22:A:DA:H2'  | 7        | 0.1           |
| (1,331) | 1:14:A:DA:H8   | 1:14:A:DA:H1'  | 7        | 0.1           |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,324) | 1:32:A:DG:H8  | 1:31:A:DG:H2'' | 3        | 0.1           |
| (1,292) | 1:1:A:DA:H2'  | 1:1:A:DA:H2''  | 4        | 0.1           |
| (1,277) | 1:23:A:DG:H8  | 1:23:A:DG:H3'  | 2        | 0.1           |
| (1,276) | 1:23:A:DG:H1' | 1:23:A:DG:H2'' | 3        | 0.1           |
| (1,265) | 1:13:A:DG:H1' | 1:13:A:DG:H2'' | 5        | 0.1           |
| (1,260) | 1:13:A:DG:H8  | 1:12:A:DG:H2'  | 2        | 0.1           |
| (1,237) | 1:6:A:DG:H8   | 1:6:A:DG:H5''  | 6        | 0.1           |
| (1,230) | 1:9:A:DG:H1'  | 1:9:A:DG:H5''  | 5        | 0.1           |
| (1,221) | 1:9:A:DG:H8   | 1:9:A:DG:H2'   | 7        | 0.1           |
| (1,220) | 1:7:A:DG:H2'' | 1:9:A:DG:H8    | 2        | 0.1           |
| (1,193) | 1:3:A:DG:H1'  | 1:3:A:DG:H4'   | 8        | 0.1           |
| (1,171) | 1:7:A:DG:H1   | 1:13:A:DG:H8   | 8        | 0.1           |
| (1,145) | 1:5:A:DC:H2'' | 1:5:A:DC:H2'   | 6        | 0.1           |
| (1,123) | 1:4:A:DG:H8   | 1:3:A:DG:H2''  | 7        | 0.1           |
| (1,76)  | 1:13:A:DG:H1  | 1:28:A:DG:H8   | 4        | 0.1           |
| (1,76)  | 1:13:A:DG:H1  | 1:28:A:DG:H8   | 9        | 0.1           |
| (1,74)  | 1:28:A:DG:H1' | 1:29:A:DG:H8   | 1        | 0.1           |
| (1,72)  | 1:26:A:DG:H1  | 1:27:A:DG:H8   | 10       | 0.1           |
| (1,68)  | 1:27:A:DG:H8  | 1:26:A:DG:H3'  | 5        | 0.1           |
| (1,32)  | 1:25:A:DT:H6  | 1:26:A:DG:H8   | 4        | 0.1           |
| (1,27)  | 1:26:A:DG:H8  | 1:25:A:DT:H2'' | 5        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found