



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 03:36 AM UTC

PDB ID : 2LO5 / pdb\_00002lo5  
BMRB ID : 18199  
Title : Structural Basis for Bifunctional Zn(II) Macrocyclic Complex Recognition of Thymine Bulges in DNA, Structure of a Thymine bulge  
Authors : Morrow, J.R.; Fountain, M.A.; del Mundo, I.A.; Siter, K.E.  
Deposited on : 2012-01-17

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>.

---

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

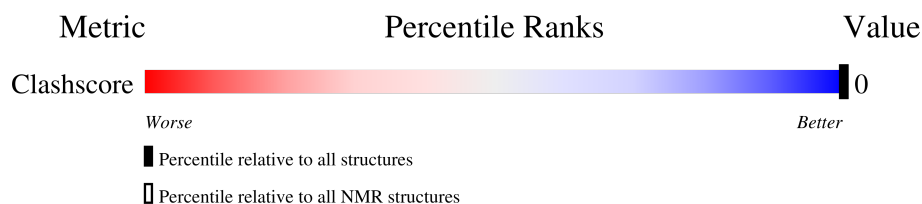
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 32%.

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     | 12     |  |

## 2 Ensemble composition and analysis ⓘ

This entry contains 18 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 [i](#)

There is only 1 type of molecule in this entry. The entry contains 378 atoms, of which 135 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3').

| Mol | Chain | Residues | Atoms |     |     |    |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|-------|
|     |       |          | Total | C   | H   | N  | O  | P  |       |
| 1   | A     | 12       | 378   | 115 | 135 | 47 | 70 | 11 | 0     |

## 4 Residue-property plots

### 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: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')

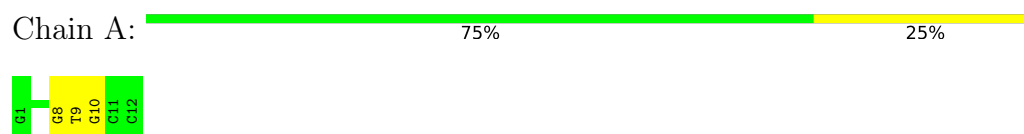


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



#### 4.2.2 Score per residue for model 2

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



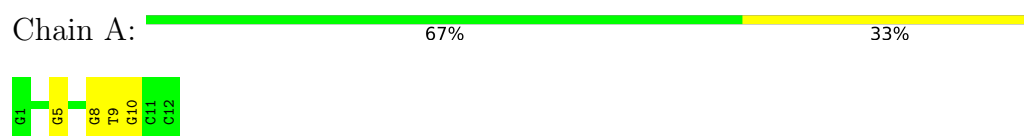
### 4.2.3 Score per residue for model 3

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



### 4.2.4 Score per residue for model 4

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



### 4.2.5 Score per residue for model 5

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



### 4.2.6 Score per residue for model 6

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



### 4.2.7 Score per residue for model 7

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



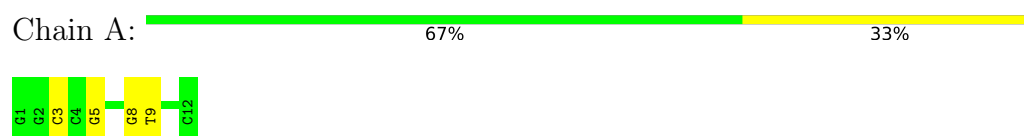
#### 4.2.8 Score per residue for model 8

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



#### 4.2.9 Score per residue for model 9

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



#### 4.2.10 Score per residue for model 10

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



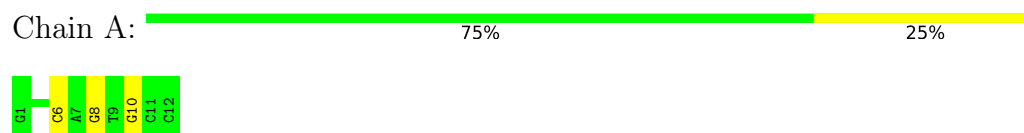
#### 4.2.11 Score per residue for model 11

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



#### 4.2.12 Score per residue for model 12

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



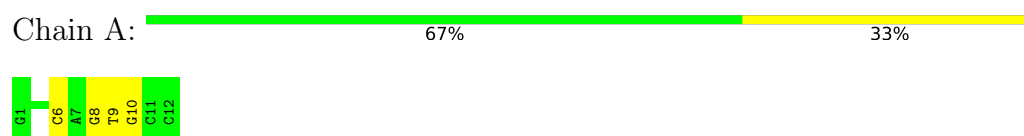
#### 4.2.13 Score per residue for model 13

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



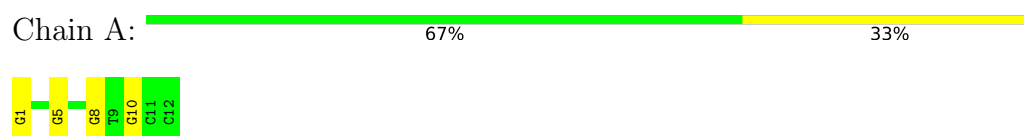
#### 4.2.14 Score per residue for model 14

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



#### 4.2.15 Score per residue for model 15

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



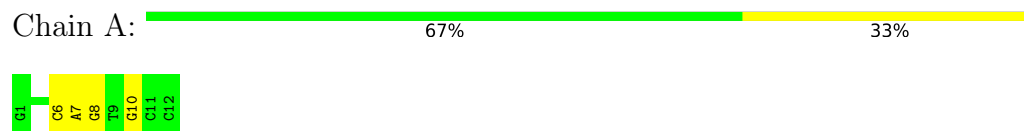
#### 4.2.16 Score per residue for model 16

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



#### 4.2.17 Score per residue for model 17

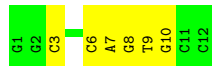
- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')



#### 4.2.18 Score per residue for model 18

- Molecule 1: DNA (5'-D(\*GP\*GP\*CP\*CP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*C)-3')

Chain A: 



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 1000 calculated structures, 18 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CYANA         | geometry optimization | 2.1     |
| CYANA         | refinement            | 2.1     |

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                       | 81             |
| Number of shifts mapped to atoms             | 81             |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 32%            |

## 6 Model quality i

### 6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (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     | 0.84±0.01    | 1±0/272 ( 0.2± 0.2%) | 1.57±0.04   | 6±1/418 ( 1.3± 0.3%) |
| All | All   | 0.84         | 11/4896 ( 0.2%)      | 1.57        | 100/7524 ( 1.3%)     |

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     | 5   | DG   | C4'-O4' | -5.62 | 1.34        | 1.45     | 9      | 10    |
| 1   | A     | 8   | DG   | C4'-O4' | -5.39 | 1.34        | 1.45     | 18     | 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     | 1   | DG   | O4'-C4'-C3' | -8.68 | 92.38       | 105.40   | 8      | 4     |
| 1   | A     | 3   | DC   | O4'-C4'-C3' | -7.84 | 93.64       | 105.40   | 3      | 6     |
| 1   | A     | 2   | DG   | O4'-C4'-C3' | -7.22 | 94.56       | 105.40   | 11     | 3     |
| 1   | A     | 7   | DA   | O4'-C4'-C3' | -7.02 | 94.87       | 105.40   | 17     | 1     |
| 1   | A     | 6   | DC   | C5'-C4'-O4' | 6.88  | 119.71      | 109.40   | 3      | 13    |
| 1   | A     | 8   | DG   | C5'-C4'-O4' | -6.78 | 99.22       | 109.40   | 14     | 2     |
| 1   | A     | 10  | DG   | O4'-C4'-C3' | -6.51 | 95.64       | 105.40   | 17     | 11    |
| 1   | A     | 8   | DG   | C1'-O4'-C4' | 5.90  | 118.55      | 109.70   | 18     | 17    |
| 1   | A     | 9   | DT   | O4'-C4'-C3' | -5.89 | 96.56       | 105.40   | 18     | 9     |
| 1   | A     | 8   | DG   | O4'-C4'-C3' | -5.86 | 96.61       | 105.40   | 14     | 1     |
| 1   | A     | 10  | DG   | C1'-O4'-C4' | 5.67  | 118.21      | 109.70   | 18     | 12    |
| 1   | A     | 9   | DT   | C1'-O4'-C4' | 5.44  | 117.86      | 109.70   | 3      | 13    |
| 1   | A     | 1   | DG   | C1'-O4'-C4' | 5.27  | 117.61      | 109.70   | 11     | 2     |
| 1   | A     | 7   | DA   | C5'-C4'-O4' | 5.17  | 117.16      | 109.40   | 18     | 1     |
| 1   | A     | 2   | DG   | C1'-O4'-C4' | 5.12  | 117.38      | 109.70   | 2      | 2     |
| 1   | A     | 5   | DG   | O4'-C4'-C3' | -5.11 | 97.73       | 105.40   | 6      | 1     |
| 1   | A     | 6   | DC   | O4'-C4'-C3' | -5.09 | 97.77       | 105.40   | 6      | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
|     |       |     |      |             |      |             |          | Worst  | Total |
| 1   | A     | 7   | DA   | C1'-O4'-C4' | 5.08 | 117.32      | 109.70   | 17     | 1     |

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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 |
|-----|-------|-------|----------|----------|---------|
| All | All   | 4374  | 2430     | 2430     | -       |

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 -.

There are no clashes.

## 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](#)

There are no ligands in this entry.

## 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

The completeness of assignment taking into account all chemical shift lists is 32% for the well-defined parts and 32% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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                  | 81 |
| Number of shifts mapped to atoms        | 81 |
| Number of unparsed shifts               | 0  |
| Number of shifts with mapping errors    | 0  |
| Number of shifts with mapping warnings  | 0  |
| Number of shift outliers (ShiftChecker) | 1  |

#### 7.1.2 Chemical shift referencing

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

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 32%, i.e. 78 atoms were assigned a chemical shift out of a possible 243. 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   | 61/144 (42%) | 61/84 (73%)    | 0/60 (0%)       | 0/0 (—%)        |
| Base    | 17/99 (17%)  | 17/63 (27%)    | 0/19 (0%)       | 0/17 (0%)       |
| Overall | 78/243 (32%) | 78/147 (53%)   | 0/79 (0%)       | 0/17 (0%)       |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 78 atoms were assigned a chemical shift out of a possible 243. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|         | <b>Total</b> | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|---------|--------------|----------------------|-----------------------|-----------------------|
| Sugar   | 61/144 (42%) | 61/84 (73%)          | 0/60 (0%)             | 0/0 (—%)              |
| Base    | 17/99 (17%)  | 17/63 (27%)          | 0/19 (0%)             | 0/17 (0%)             |
| Overall | 78/243 (32%) | 78/147 (53%)         | 0/79 (0%)             | 0/17 (0%)             |

#### 7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, <i>ppm</i> | Expected range, <i>ppm</i> | Z-score |
|---------|-------|-----|------|------|-------------------|----------------------------|---------|
| 1       | A     | 6   | DC   | H4'  | 1.32              | 2.84 – 5.45                | -10.8   |

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

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                                | 274   |
| Intra-residue ( $ i-j =0$ )                              | 105   |
| Sequential ( $ i-j =1$ )                                 | 74    |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 11    |
| Long range ( $ i-j \geq 5$ )                             | 14    |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 70    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 42    |
| Number of unmapped restraints                            | 1     |
| Number of restraints per residue                         | 26.3  |
| Number of long range restraints per residue <sup>1</sup> | 4.9   |

<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)  | 9.2                                    | 0.2     |
| 0.2-0.5 (Medium) | 13.4                                   | 0.5     |
| >0.5 (Large)     | 69.2                                   | 8.27    |

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

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 2.9                                    | 4.19    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

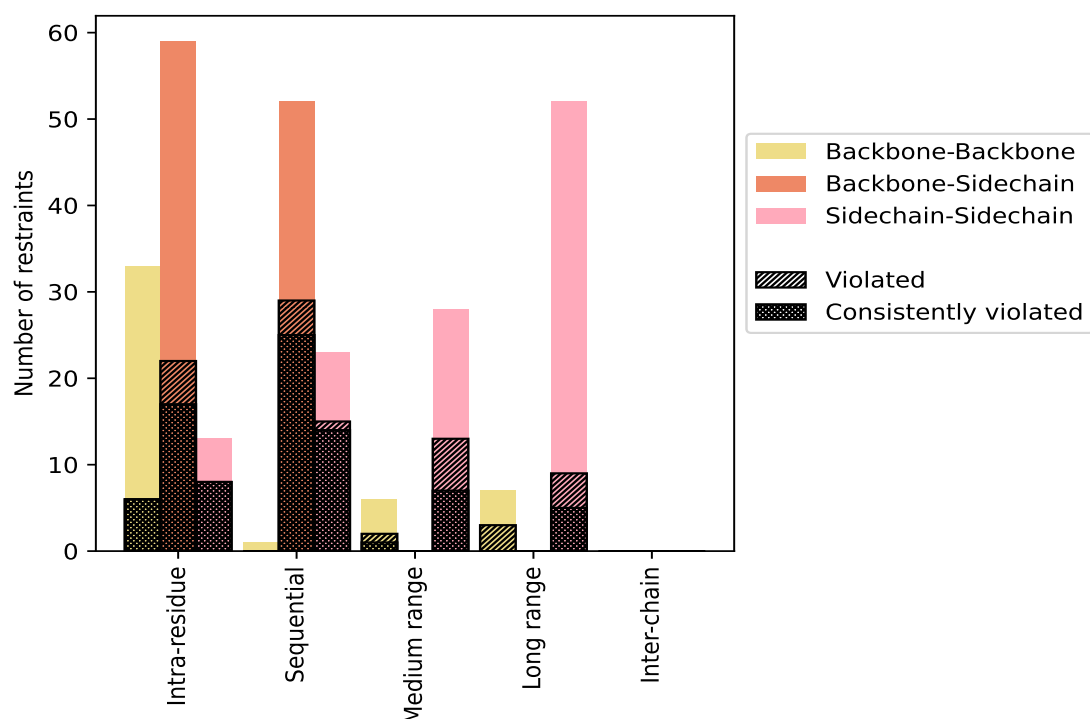
### 9.1 Summary of distance violations ⓘ

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="#">105</a> | <a href="#">38.3</a>  | <a href="#">36</a>    | <a href="#">34.3</a> | <a href="#">13.1</a> | <a href="#">31</a>                 | <a href="#">29.5</a> | <a href="#">11.3</a> |
| Backbone-Backbone                                          | 33                  | 12.0                  | 6                     | 18.2                 | 2.2                  | 6                                  | 18.2                 | 2.2                  |
| Backbone-Sidechain                                         | 59                  | 21.5                  | 22                    | 37.3                 | 8.0                  | 17                                 | 28.8                 | 6.2                  |
| Sidechain-Sidechain                                        | 13                  | 4.7                   | 8                     | 61.5                 | 2.9                  | 8                                  | 61.5                 | 2.9                  |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">74</a>  | <a href="#">27.0</a>  | <a href="#">44</a>    | <a href="#">59.5</a> | <a href="#">16.1</a> | <a href="#">39</a>                 | <a href="#">52.7</a> | <a href="#">14.2</a> |
| Backbone-Backbone                                          | 1                   | 0.4                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Backbone-Sidechain                                         | 52                  | 19.0                  | 29                    | 55.8                 | 10.6                 | 25                                 | 48.1                 | 9.1                  |
| Sidechain-Sidechain                                        | 21                  | 7.7                   | 15                    | 71.4                 | 5.5                  | 14                                 | 66.7                 | 5.1                  |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">11</a>  | <a href="#">4.0</a>   | <a href="#">4</a>     | <a href="#">36.4</a> | <a href="#">1.5</a>  | <a href="#">3</a>                  | <a href="#">27.3</a> | <a href="#">1.1</a>  |
| Backbone-Backbone                                          | 6                   | 2.2                   | 2                     | 33.3                 | 0.7                  | 1                                  | 16.7                 | 0.4                  |
| Backbone-Sidechain                                         | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Sidechain-Sidechain                                        | 5                   | 1.8                   | 2                     | 40.0                 | 0.7                  | 2                                  | 40.0                 | 0.7                  |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">14</a>  | <a href="#">5.1</a>   | <a href="#">3</a>     | <a href="#">21.4</a> | <a href="#">1.1</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| Backbone-Backbone                                          | 7                   | 2.6                   | 3                     | 42.9                 | 1.1                  | 0                                  | 0.0                  | 0.0                  |
| Backbone-Sidechain                                         | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Sidechain-Sidechain                                        | 7                   | 2.6                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| <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="#">70</a>  | <a href="#">25.5</a>  | <a href="#">20</a>    | <a href="#">28.6</a> | <a href="#">7.3</a>  | <a href="#">10</a>                 | <a href="#">14.3</a> | <a href="#">3.6</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="#">274</a> | <a href="#">100.0</a> | <a href="#">107</a>   | <a href="#">39.1</a> | <a href="#">39.1</a> | <a href="#">83</a>                 | <a href="#">30.3</a> | <a href="#">30.3</a> |
| Backbone-Backbone                                          | 47                  | 17.2                  | 11                    | 23.4                 | 4.0                  | 7                                  | 14.9                 | 2.6                  |
| Backbone-Sidechain                                         | 111                 | 40.5                  | 51                    | 45.9                 | 18.6                 | 42                                 | 37.8                 | 15.3                 |
| Sidechain-Sidechain                                        | 116                 | 42.3                  | 45                    | 38.8                 | 16.4                 | 34                                 | 29.3                 | 12.4                 |

<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        | 32                   | 40              | 8               | 11              | 0               | 91    | 1.49     | 6.16    | 1.25                | 1.21       |
| 2        | 33                   | 42              | 8               | 12              | 0               | 95    | 1.53     | 8.27    | 1.35                | 1.12       |
| 3        | 31                   | 40              | 8               | 10              | 0               | 89    | 1.57     | 7.15    | 1.33                | 1.15       |
| 4        | 32                   | 41              | 8               | 11              | 0               | 92    | 1.51     | 6.36    | 1.31                | 1.17       |
| 5        | 33                   | 41              | 8               | 11              | 0               | 93    | 1.53     | 8.1     | 1.34                | 1.11       |
| 6        | 32                   | 42              | 9               | 10              | 0               | 93    | 1.46     | 6.67    | 1.32                | 1.11       |
| 7        | 31                   | 42              | 12              | 10              | 0               | 95    | 1.45     | 7.22    | 1.29                | 1.11       |
| 8        | 34                   | 39              | 8               | 9               | 0               | 90    | 1.47     | 7.03    | 1.3                 | 1.11       |
| 9        | 33                   | 42              | 10              | 10              | 0               | 95    | 1.46     | 7.26    | 1.33                | 1.09       |
| 10       | 33                   | 42              | 14              | 10              | 0               | 99    | 1.41     | 7.14    | 1.32                | 1.01       |

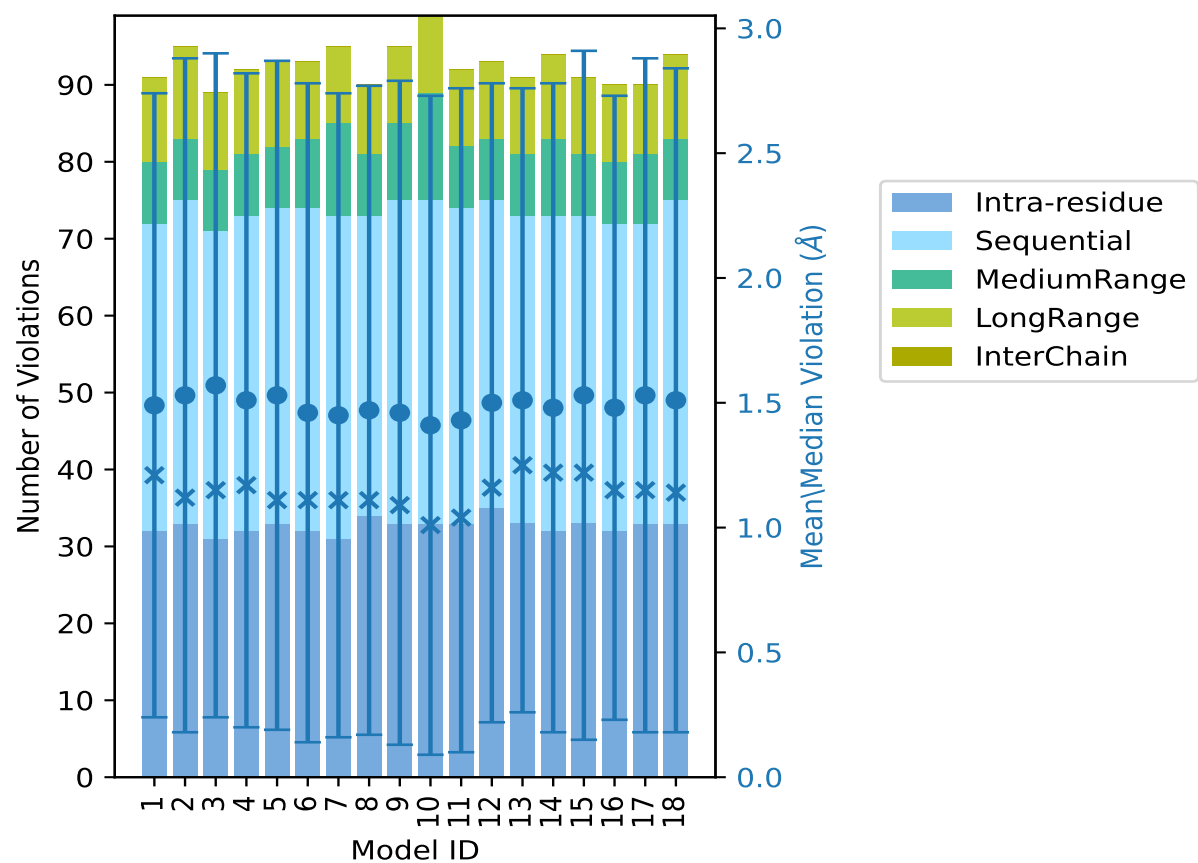
*Continued on next page...*

Continued from previous page...

| 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 |          |         |                     |            |
| 11       | 33                   | 41              | 8               | 10              | 0               | 92    | 1.43     | 8.1     | 1.33                | 1.04       |
| 12       | 35                   | 40              | 8               | 10              | 0               | 93    | 1.5      | 6.66    | 1.28                | 1.16       |
| 13       | 33                   | 40              | 8               | 10              | 0               | 91    | 1.51     | 6.44    | 1.25                | 1.25       |
| 14       | 32                   | 41              | 10              | 11              | 0               | 94    | 1.48     | 7.3     | 1.3                 | 1.22       |
| 15       | 33                   | 40              | 8               | 10              | 0               | 91    | 1.53     | 7.44    | 1.38                | 1.22       |
| 16       | 32                   | 40              | 8               | 10              | 0               | 90    | 1.48     | 6.46    | 1.25                | 1.15       |
| 17       | 33                   | 39              | 9               | 9               | 0               | 90    | 1.53     | 8.07    | 1.35                | 1.15       |
| 18       | 33                   | 42              | 8               | 11              | 0               | 94    | 1.51     | 7.98    | 1.33                | 1.14       |

<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 ⓘ



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

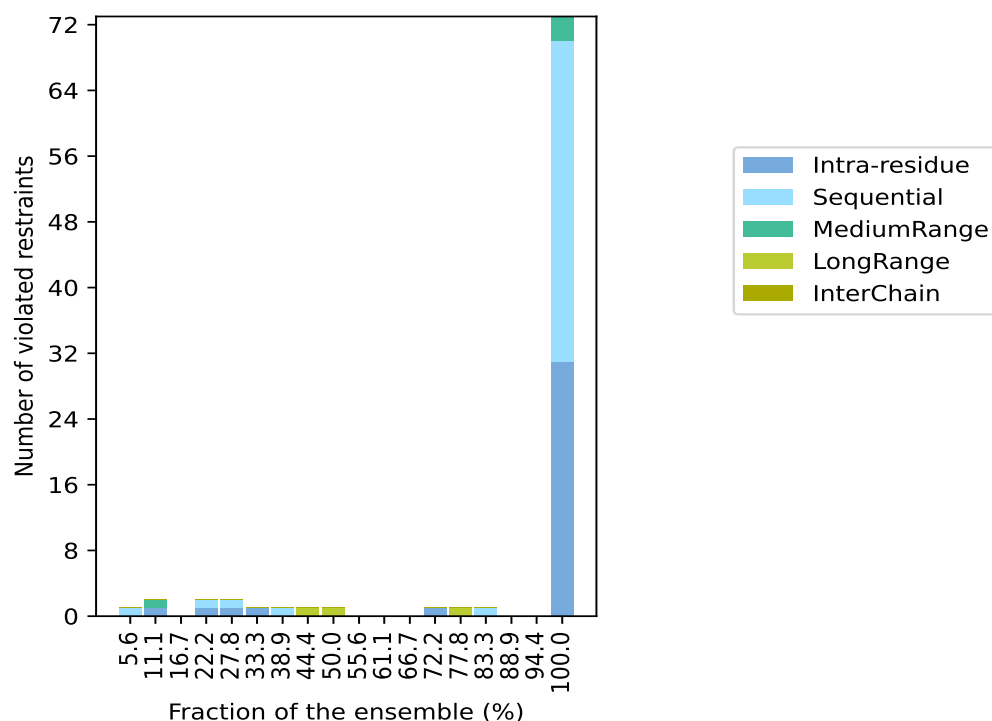
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 117(IR:69, SQ:30, MR:7, LR:11, IC:0) restraints are not violated 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>       | %     |
| 0                             | 1               | 0               | 0               | 0               | 1     | 1                        | 5.6   |
| 1                             | 0               | 1               | 0               | 0               | 2     | 2                        | 11.1  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 3                        | 16.7  |
| 1                             | 1               | 0               | 0               | 0               | 2     | 4                        | 22.2  |
| 1                             | 1               | 0               | 0               | 0               | 2     | 5                        | 27.8  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 6                        | 33.3  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 7                        | 38.9  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 8                        | 44.4  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 9                        | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 10                       | 55.6  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 61.1  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 66.7  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 13                       | 72.2  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 14                       | 77.8  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 15                       | 83.3  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 88.9  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 94.4  |
| 31                            | 39              | 3               | 0               | 0               | 73    | 18                       | 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

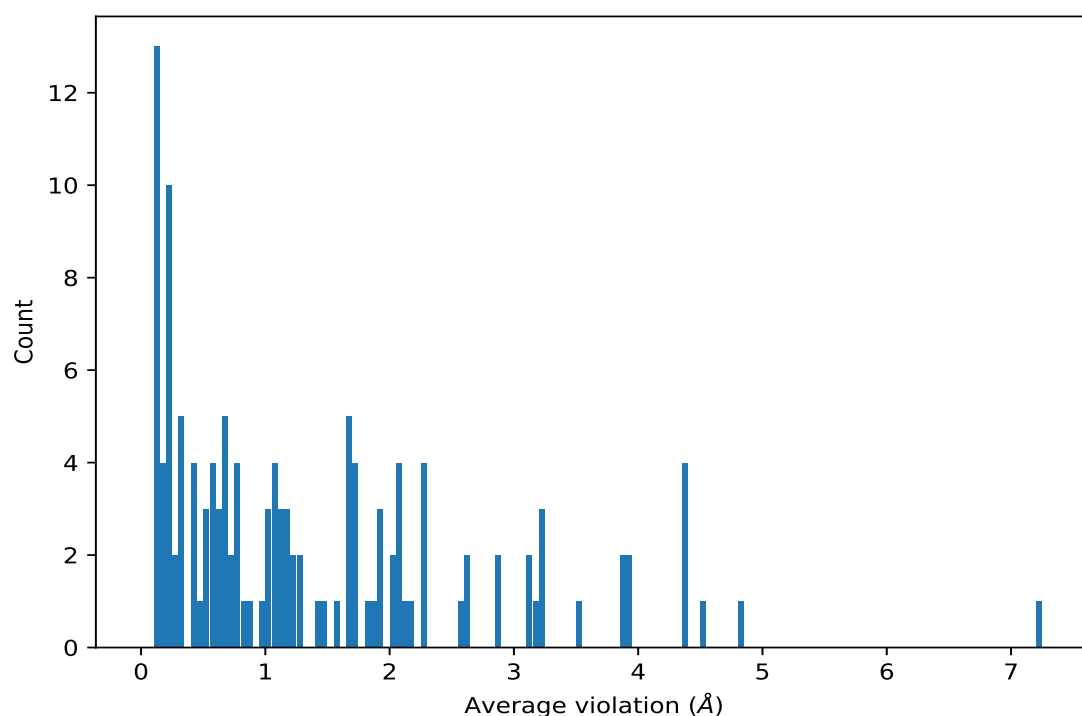
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,145) | 1:9:A:DT:H6   | 1:7:A:DA:H2   | 18                  | 7.21     | 0.65                | 7.18       |
| (1,147) | 1:9:A:DT:H6   | 1:10:A:DG:H3' | 18                  | 4.8      | 0.74                | 5.22       |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8   | 18                  | 4.51     | 0.0                 | 4.51       |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8  | 18                  | 4.39     | 0.0                 | 4.39       |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8  | 18                  | 4.39     | 0.0                 | 4.39       |
| (1,115) | 1:2:A:DG:H21  | 1:3:A:DC:H6   | 18                  | 4.38     | 0.68                | 4.72       |
| (1,115) | 1:2:A:DG:H22  | 1:3:A:DC:H6   | 18                  | 4.38     | 0.68                | 4.72       |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H21  | 18                  | 3.91     | 0.0                 | 3.91       |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H22  | 18                  | 3.91     | 0.0                 | 3.91       |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H21 | 18                  | 3.89     | 0.41                | 3.76       |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H22 | 18                  | 3.89     | 0.41                | 3.76       |
| (3,20)  | 1:9:A:DT:H6   | 1:10:A:DG:H1' | 18                  | 3.51     | 0.27                | 3.5        |
| (3,25)  | 1:9:A:DT:H6   | 1:10:A:DG:H4' | 18                  | 3.23     | 0.39                | 3.19       |
| (1,136) | 1:6:A:DC:H6   | 1:7:A:DA:H2'  | 18                  | 3.21     | 0.42                | 3.0        |
| (1,136) | 1:6:A:DC:H6   | 1:7:A:DA:H2'' | 18                  | 3.21     | 0.42                | 3.0        |
| (1,142) | 1:8:A:DG:H1'  | 1:9:A:DT:H6   | 18                  | 3.15     | 0.11                | 3.14       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (3,22)  | 1:9:A:DT:H6   | 1:8:A:DG:H21  | 18                  | 3.13     | 0.46                | 3.26       |
| (3,22)  | 1:9:A:DT:H6   | 1:8:A:DG:H22  | 18                  | 3.13     | 0.46                | 3.26       |
| (1,133) | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 18                  | 2.87     | 0.27                | 2.73       |
| (1,133) | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 18                  | 2.87     | 0.27                | 2.73       |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 18                  | 2.63     | 0.0                 | 2.63       |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 18                  | 2.63     | 0.0                 | 2.63       |
| (3,21)  | 1:9:A:DT:H6   | 1:10:A:DG:H2' | 18                  | 2.58     | 0.66                | 2.26       |
| (1,129) | 1:5:A:DG:H21  | 1:6:A:DC:H5   | 18                  | 2.29     | 0.17                | 2.28       |
| (1,129) | 1:5:A:DG:H22  | 1:6:A:DC:H5   | 18                  | 2.29     | 0.17                | 2.28       |
| (1,15)  | 1:2:A:DG:H21  | 1:3:A:DC:H6   | 18                  | 2.29     | 0.68                | 2.63       |
| (1,15)  | 1:2:A:DG:H22  | 1:3:A:DC:H6   | 18                  | 2.29     | 0.68                | 2.63       |
| (1,78)  | 1:8:A:DG:H1'  | 1:9:A:DT:H6   | 18                  | 2.15     | 0.11                | 2.14       |
| (1,66)  | 1:7:A:DA:H2   | 1:7:A:DA:H8   | 18                  | 2.11     | 0.0                 | 2.11       |
| (1,117) | 1:2:A:DG:H3'  | 1:2:A:DG:H8   | 18                  | 2.09     | 0.2                 | 2.15       |
| (1,138) | 1:7:A:DA:H1'  | 1:8:A:DG:H8   | 18                  | 2.08     | 0.04                | 2.08       |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 18                  | 2.08     | 0.63                | 2.41       |
| (1,152) | 1:9:A:DT:H6   | 1:10:A:DG:H8  | 18                  | 2.07     | 0.29                | 2.14       |
| (1,124) | 1:4:A:DC:H1'  | 1:5:A:DG:H8   | 18                  | 2.04     | 0.02                | 2.04       |
| (1,127) | 1:5:A:DG:H1'  | 1:6:A:DC:H5   | 18                  | 2.02     | 0.01                | 2.02       |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 18                  | 1.93     | 0.01                | 1.93       |
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4'  | 18                  | 1.92     | 0.17                | 1.92       |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 18                  | 1.92     | 0.03                | 1.9        |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5  | 18                  | 1.86     | 0.6                 | 1.82       |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6   | 18                  | 1.81     | 0.34                | 1.9        |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6   | 18                  | 1.74     | 0.58                | 1.84       |
| (1,9)   | 1:2:A:DG:H21  | 1:2:A:DG:H8   | 18                  | 1.72     | 0.0                 | 1.72       |
| (1,9)   | 1:2:A:DG:H22  | 1:2:A:DG:H8   | 18                  | 1.72     | 0.0                 | 1.72       |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6  | 18                  | 1.7      | 0.65                | 1.23       |
| (3,26)  | 1:9:A:DT:H6   | 1:8:A:DG:H5'  | 18                  | 1.69     | 0.33                | 1.71       |
| (1,149) | 1:9:A:DT:H3'  | 1:9:A:DT:H6   | 18                  | 1.68     | 0.06                | 1.67       |
| (1,118) | 1:3:A:DC:H3'  | 1:3:A:DC:H1'  | 18                  | 1.68     | 0.02                | 1.68       |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5   | 18                  | 1.65     | 0.68                | 1.9        |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5   | 18                  | 1.65     | 0.68                | 1.9        |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6  | 18                  | 1.57     | 0.02                | 1.56       |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6   | 18                  | 1.48     | 0.49                | 1.4        |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1'  | 18                  | 1.41     | 0.0                 | 1.41       |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6   | 18                  | 1.28     | 0.5                 | 1.42       |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6  | 18                  | 1.27     | 0.0                 | 1.27       |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8   | 18                  | 1.22     | 0.0                 | 1.22       |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8   | 18                  | 1.22     | 0.0                 | 1.22       |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6   | 18                  | 1.19     | 0.48                | 1.52       |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8   | 18                  | 1.17     | 0.52                | 1.0        |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1'  | 18                  | 1.15     | 0.11                | 1.14       |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6  | 18                  | 1.12     | 0.0                 | 1.12       |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6  | 18                  | 1.11     | 0.28                | 1.08       |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5   | 18                  | 1.11     | 0.45                | 1.14       |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5   | 18                  | 1.09     | 0.13                | 1.06       |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1'  | 18                  | 1.09     | 0.32                | 0.93       |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2   | 18                  | 1.09     | 0.07                | 1.11       |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1'  | 18                  | 1.07     | 0.01                | 1.06       |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5   | 18                  | 1.04     | 0.12                | 1.01       |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1'  | 18                  | 1.01     | 0.03                | 1.0        |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6   | 18                  | 0.98     | 0.01                | 0.98       |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 18                  | 0.87     | 0.18                | 0.79       |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 18                  | 0.81     | 0.04                | 0.8        |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 18                  | 0.76     | 0.03                | 0.75       |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8   | 18                  | 0.75     | 0.13                | 0.72       |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8   | 18                  | 0.75     | 0.13                | 0.72       |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8   | 18                  | 0.75     | 0.13                | 0.72       |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 18                  | 0.73     | 0.03                | 0.73       |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8  | 18                  | 0.72     | 0.32                | 0.5        |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6   | 18                  | 0.68     | 0.03                | 0.67       |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6   | 18                  | 0.68     | 0.03                | 0.67       |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6   | 18                  | 0.68     | 0.03                | 0.67       |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 18                  | 0.67     | 0.27                | 0.53       |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 18                  | 0.67     | 0.27                | 0.53       |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1'  | 18                  | 0.6      | 0.08                | 0.58       |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1'  | 18                  | 0.6      | 0.08                | 0.58       |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8  | 18                  | 0.6      | 0.0                 | 0.6        |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7   | 18                  | 0.58     | 0.04                | 0.59       |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71  | 18                  | 0.58     | 0.34                | 0.58       |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72  | 18                  | 0.58     | 0.34                | 0.58       |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73  | 18                  | 0.58     | 0.34                | 0.58       |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1'  | 18                  | 0.53     | 0.19                | 0.47       |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2'  | 18                  | 0.53     | 0.04                | 0.51       |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6   | 18                  | 0.48     | 0.09                | 0.52       |
| (1,72)  | 1:8:A:DG:H21  | 1:8:A:DG:H8   | 18                  | 0.4      | 0.0                 | 0.4        |
| (1,72)  | 1:8:A:DG:H22  | 1:8:A:DG:H8   | 18                  | 0.4      | 0.0                 | 0.4        |
| (1,88)  | 1:10:A:DG:H21 | 1:10:A:DG:H8  | 18                  | 0.4      | 0.0                 | 0.4        |
| (1,88)  | 1:10:A:DG:H22 | 1:10:A:DG:H8  | 18                  | 0.4      | 0.0                 | 0.4        |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1'  | 18                  | 0.34     | 0.0                 | 0.34       |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1'  | 18                  | 0.34     | 0.0                 | 0.34       |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2  | 18                  | 0.28     | 0.05                | 0.28       |
| (2,62)  | 1:4:A:DC:O2   | 1:8:A:DG:N2   | 18                  | 0.27     | 0.05                | 0.26       |

*Continued on next page...*

Continued from previous page...

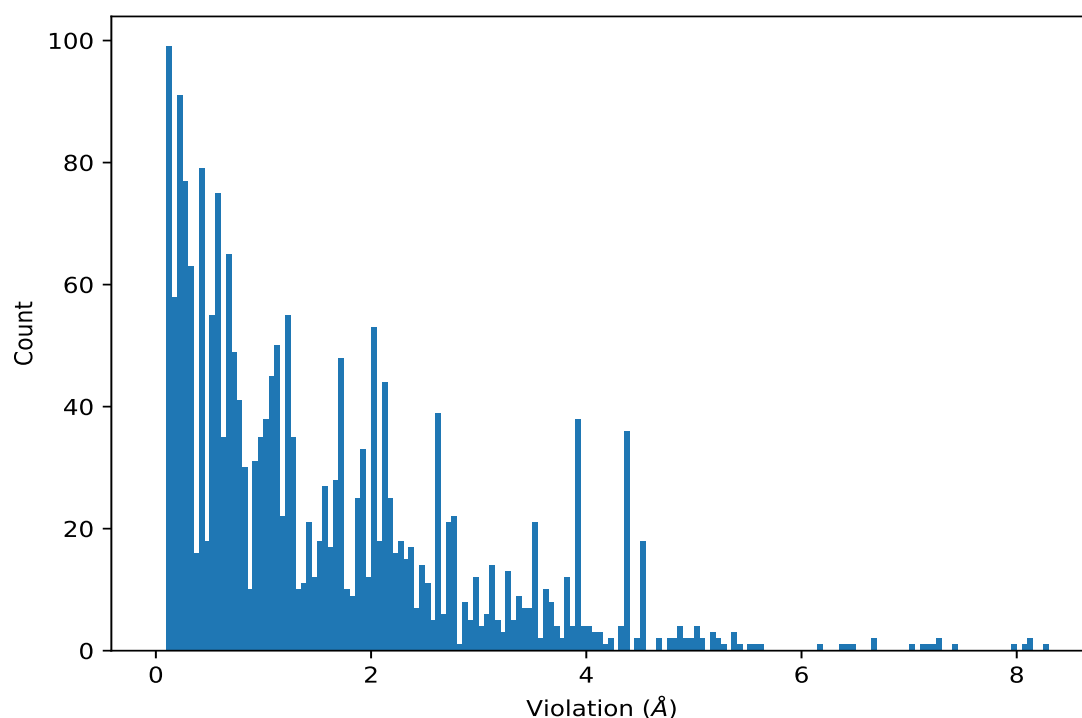
| Key     | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2  | 18                  | 0.24     | 0.07                | 0.23       |
| (2,61)  | 1:4:A:DC:N4   | 1:8:A:DG:O6   | 18                  | 0.21     | 0.06                | 0.24       |
| (2,60)  | 1:4:A:DC:N3   | 1:8:A:DG:N1   | 18                  | 0.21     | 0.06                | 0.22       |
| (2,57)  | 1:3:A:DC:N3   | 1:10:A:DG:N1  | 18                  | 0.21     | 0.02                | 0.2        |
| (1,119) | 1:3:A:DC:H1'  | 1:3:A:DC:H6   | 18                  | 0.21     | 0.0                 | 0.21       |
| (2,51)  | 1:1:A:DG:N1   | 1:12:A:DC:N3  | 18                  | 0.2      | 0.03                | 0.2        |
| (2,54)  | 1:2:A:DG:N1   | 1:11:A:DC:N3  | 18                  | 0.19     | 0.01                | 0.19       |
| (2,56)  | 1:2:A:DG:O6   | 1:11:A:DC:N4  | 17                  | 0.23     | 0.07                | 0.26       |
| (2,55)  | 1:2:A:DG:N2   | 1:11:A:DC:O2  | 17                  | 0.23     | 0.06                | 0.24       |
| (2,53)  | 1:1:A:DG:O6   | 1:12:A:DC:N4  | 17                  | 0.2      | 0.06                | 0.18       |
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8   | 15                  | 1.01     | 0.57                | 0.74       |
| (3,29)  | 1:3:A:DC:C1'  | 1:10:A:DG:C1' | 14                  | 0.16     | 0.05                | 0.15       |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8   | 13                  | 0.54     | 0.33                | 0.6        |
| (2,58)  | 1:3:A:DC:N4   | 1:10:A:DG:O6  | 13                  | 0.2      | 0.06                | 0.23       |
| (3,28)  | 1:2:A:DG:C1'  | 1:11:A:DC:C1' | 9                   | 0.15     | 0.04                | 0.14       |
| (3,27)  | 1:1:A:DG:C1'  | 1:12:A:DC:C1' | 8                   | 0.18     | 0.05                | 0.16       |
| (1,68)  | 1:7:A:DA:H1'  | 1:8:A:DG:H8   | 7                   | 0.13     | 0.02                | 0.13       |
| (1,41)  | 1:5:A:DG:H3'  | 1:5:A:DG:H8   | 6                   | 0.1      | 0.0                 | 0.1        |
| (1,79)  | 1:8:A:DG:H2'  | 1:9:A:DT:H6   | 5                   | 0.14     | 0.03                | 0.13       |
| (1,11)  | 1:2:A:DG:H3'  | 1:2:A:DG:H8   | 5                   | 0.12     | 0.02                | 0.11       |
| (1,121) | 1:3:A:DC:H2'  | 1:3:A:DC:H6   | 4                   | 0.31     | 0.01                | 0.31       |
| (1,121) | 1:3:A:DC:H2'  | 1:3:A:DC:H6   | 4                   | 0.31     | 0.01                | 0.31       |
| (1,121) | 1:3:A:DC:H2'' | 1:3:A:DC:H6   | 4                   | 0.31     | 0.01                | 0.31       |
| (2,25)  | 1:5:A:DG:N2   | 1:7:A:DA:N7   | 4                   | 0.13     | 0.02                | 0.14       |
| (2,49)  | 1:5:A:DG:N2   | 1:7:A:DA:N7   | 4                   | 0.13     | 0.02                | 0.14       |
| (1,42)  | 1:5:A:DG:H1'  | 1:6:A:DC:H5   | 4                   | 0.11     | 0.01                | 0.11       |
| (3,30)  | 1:4:A:DC:C1'  | 1:8:A:DG:C1'  | 2                   | 0.14     | 0.0                 | 0.14       |
| (2,19)  | 1:4:A:DC:H41  | 1:8:A:DG:O6   | 2                   | 0.14     | 0.01                | 0.14       |
| (2,43)  | 1:4:A:DC:H41  | 1:8:A:DG:O6   | 2                   | 0.14     | 0.01                | 0.14       |
| (4,2)   | 1:4:A:DC:H2'  | 1:4:A:DC:H6   | 2                   | 0.12     | 0.02                | 0.12       |
| (4,2)   | 1:4:A:DC:H2'  | 1:4:A:DC:H6   | 2                   | 0.12     | 0.02                | 0.12       |
| (4,2)   | 1:4:A:DC:H2'' | 1:4:A:DC:H6   | 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) |
|---------|-------------|-------------|----------|---------------|
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 2        | 8.27          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 5        | 8.1           |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 11       | 8.1           |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 17       | 8.07          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 18       | 7.98          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 15       | 7.44          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 14       | 7.3           |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 9        | 7.26          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 7        | 7.22          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 3        | 7.15          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 10       | 7.14          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 8        | 7.03          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 6        | 6.67          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 12       | 6.66          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 16       | 6.46          |
| (1,145) | 1:9:A:DT:H6 | 1:7:A:DA:H2 | 13       | 6.44          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,145) | 1:9:A:DT:H6  | 1:7:A:DA:H2   | 4        | 6.36          |
| (1,145) | 1:9:A:DT:H6  | 1:7:A:DA:H2   | 1        | 6.16          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 12       | 5.64          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 6        | 5.58          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 4        | 5.51          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 17       | 5.44          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 15       | 5.38          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 11       | 5.37          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 13       | 5.37          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 16       | 5.25          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 8        | 5.24          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 1        | 5.21          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 14       | 5.18          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 3        | 5.18          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 3        | 5.18          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 14       | 5.08          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 14       | 5.08          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 4        | 5.05          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 4        | 5.05          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 15       | 5.02          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 15       | 5.02          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 9        | 4.97          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 9        | 4.97          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 1        | 4.94          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 1        | 4.94          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 10       | 4.87          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 10       | 4.87          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 5        | 4.86          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 5        | 4.86          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 2        | 4.85          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 2        | 4.85          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 16       | 4.78          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 16       | 4.78          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 7        | 4.66          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 7        | 4.66          |
| (1,140) | 1:7:A:DA:H2  | 1:7:A:DA:H8   | 1        | 4.51          |
| (1,140) | 1:7:A:DA:H2  | 1:7:A:DA:H8   | 2        | 4.51          |
| (1,140) | 1:7:A:DA:H2  | 1:7:A:DA:H8   | 3        | 4.51          |
| (1,140) | 1:7:A:DA:H2  | 1:7:A:DA:H8   | 4        | 4.51          |
| (1,140) | 1:7:A:DA:H2  | 1:7:A:DA:H8   | 5        | 4.51          |
| (1,140) | 1:7:A:DA:H2  | 1:7:A:DA:H8   | 6        | 4.51          |
| (1,140) | 1:7:A:DA:H2  | 1:7:A:DA:H8   | 7        | 4.51          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 8        | 4.51          |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 9        | 4.51          |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 10       | 4.51          |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 11       | 4.51          |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 12       | 4.51          |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 13       | 4.51          |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 14       | 4.51          |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 15       | 4.51          |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 16       | 4.51          |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 17       | 4.51          |
| (1,140) | 1:7:A:DA:H2   | 1:7:A:DA:H8  | 18       | 4.51          |
| (1,115) | 1:2:A:DG:H21  | 1:3:A:DC:H6  | 18       | 4.48          |
| (1,115) | 1:2:A:DG:H22  | 1:3:A:DC:H6  | 18       | 4.48          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 1        | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 1        | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 2        | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 2        | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 3        | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 3        | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 4        | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 4        | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 5        | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 5        | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 6        | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 6        | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 7        | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 7        | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 8        | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 8        | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 9        | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 9        | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 10       | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 10       | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 11       | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 11       | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 12       | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 12       | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 13       | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 13       | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 14       | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 14       | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 15       | 4.39          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8  | 15       | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8  | 16       | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8  | 16       | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8  | 17       | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8  | 17       | 4.39          |
| (1,156) | 1:10:A:DG:H21 | 1:10:A:DG:H8  | 18       | 4.39          |
| (1,156) | 1:10:A:DG:H22 | 1:10:A:DG:H8  | 18       | 4.39          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H21 | 4        | 4.34          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H22 | 4        | 4.34          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H21 | 12       | 4.34          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H22 | 12       | 4.34          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H21 | 6        | 4.2           |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H22 | 6        | 4.2           |
| (3,25)  | 1:9:A:DT:H6   | 1:10:A:DG:H4' | 6        | 4.18          |
| (1,147) | 1:9:A:DT:H6   | 1:10:A:DG:H3' | 2        | 4.14          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H21 | 17       | 4.13          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H22 | 17       | 4.13          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H21 | 11       | 4.07          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H22 | 11       | 4.07          |
| (3,20)  | 1:9:A:DT:H6   | 1:10:A:DG:H1' | 15       | 4.06          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H21 | 8        | 4.04          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H22 | 8        | 4.04          |
| (1,147) | 1:9:A:DT:H6   | 1:10:A:DG:H3' | 10       | 4.04          |
| (1,147) | 1:9:A:DT:H6   | 1:10:A:DG:H3' | 5        | 4.03          |
| (1,115) | 1:2:A:DG:H21  | 1:3:A:DC:H6   | 13       | 3.97          |
| (1,115) | 1:2:A:DG:H22  | 1:3:A:DC:H6   | 13       | 3.97          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H21 | 13       | 3.96          |
| (3,23)  | 1:9:A:DT:H6   | 1:10:A:DG:H22 | 13       | 3.96          |
| (3,20)  | 1:9:A:DT:H6   | 1:10:A:DG:H1' | 12       | 3.94          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H21  | 10       | 3.92          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H22  | 10       | 3.92          |
| (3,20)  | 1:9:A:DT:H6   | 1:10:A:DG:H1' | 6        | 3.91          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H21  | 1        | 3.91          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H22  | 1        | 3.91          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H21  | 2        | 3.91          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H22  | 2        | 3.91          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H21  | 3        | 3.91          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H22  | 3        | 3.91          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H21  | 4        | 3.91          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H22  | 4        | 3.91          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H21  | 5        | 3.91          |
| (1,40)  | 1:5:A:DG:H3'  | 1:5:A:DG:H22  | 5        | 3.91          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 6        | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 6        | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 7        | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 7        | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 8        | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 8        | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 9        | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 9        | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 11       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 11       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 12       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 12       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 13       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 13       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 14       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 14       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 15       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 15       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 16       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 16       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 17       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 17       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H21  | 18       | 3.91          |
| (1,40)  | 1:5:A:DG:H3' | 1:5:A:DG:H22  | 18       | 3.91          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 3        | 3.85          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 9        | 3.85          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 15       | 3.85          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 15       | 3.85          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 18       | 3.83          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 8        | 3.83          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 8        | 3.83          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 17       | 3.83          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 17       | 3.83          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 15       | 3.82          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 15       | 3.82          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 18       | 3.81          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 18       | 3.81          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 18       | 3.81          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 3        | 3.81          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 3        | 3.81          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 4        | 3.77          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 12       | 3.76          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 15       | 3.73          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 15       | 3.73          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 14       | 3.72          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 14       | 3.72          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 2        | 3.68          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 2        | 3.68          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 6        | 3.68          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 6        | 3.68          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 1        | 3.66          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 1        | 3.66          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 16       | 3.66          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 16       | 3.66          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 7        | 3.65          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 7        | 3.65          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 2        | 3.64          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 18       | 3.64          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 2        | 3.63          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 17       | 3.61          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 12       | 3.61          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 12       | 3.61          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 3        | 3.6           |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 3        | 3.6           |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 9        | 3.57          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 9        | 3.57          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 9        | 3.55          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 9        | 3.55          |
| (1,147) | 1:9:A:DT:H6  | 1:10:A:DG:H3' | 7        | 3.55          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 7        | 3.55          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 7        | 3.55          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 10       | 3.55          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 10       | 3.55          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 11       | 3.54          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 9        | 3.53          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 9        | 3.53          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 18       | 3.51          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 18       | 3.51          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 13       | 3.51          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 7        | 3.5           |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 7        | 3.5           |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 17       | 3.5           |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 17       | 3.5           |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 13       | 3.5           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 13       | 3.5           |
| (1,133) | 1:5:A:DG:H21 | 1:6:A:DC:H6   | 6        | 3.5           |
| (1,133) | 1:5:A:DG:H22 | 1:6:A:DC:H6   | 6        | 3.5           |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 5        | 3.49          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 10       | 3.48          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 3        | 3.47          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 3        | 3.47          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 5        | 3.46          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 5        | 3.45          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 5        | 3.45          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 2        | 3.43          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 2        | 3.43          |
| (1,133) | 1:5:A:DG:H21 | 1:6:A:DC:H6   | 15       | 3.43          |
| (1,133) | 1:5:A:DG:H22 | 1:6:A:DC:H6   | 15       | 3.43          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 8        | 3.42          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 8        | 3.42          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 8        | 3.41          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 2        | 3.4           |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 15       | 3.4           |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 9        | 3.4           |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 6        | 3.39          |
| (1,133) | 1:5:A:DG:H21 | 1:6:A:DC:H6   | 8        | 3.39          |
| (1,133) | 1:5:A:DG:H22 | 1:6:A:DC:H6   | 8        | 3.39          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 5        | 3.38          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 3        | 3.37          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 10       | 3.36          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H21 | 10       | 3.34          |
| (3,23)  | 1:9:A:DT:H6  | 1:10:A:DG:H22 | 10       | 3.34          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 4        | 3.33          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 13       | 3.33          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 18       | 3.31          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 4        | 3.3           |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 9        | 3.28          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 15       | 3.28          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 10       | 3.27          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 10       | 3.27          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 3        | 3.27          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 5        | 3.26          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 5        | 3.26          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 8        | 3.26          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 8        | 3.26          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 11       | 3.26          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 11       | 3.26          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 16       | 3.25          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 10       | 3.22          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 1        | 3.2           |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 14       | 3.2           |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 14       | 3.17          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 3        | 3.17          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 16       | 3.16          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 7        | 3.16          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 12       | 3.16          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 11       | 3.15          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 11       | 3.15          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 18       | 3.15          |
| (3,20)  | 1:9:A:DT:H6  | 1:10:A:DG:H1' | 7        | 3.15          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 1        | 3.15          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 16       | 3.14          |
| (1,133) | 1:5:A:DG:H21 | 1:6:A:DC:H6   | 3        | 3.14          |
| (1,133) | 1:5:A:DG:H22 | 1:6:A:DC:H6   | 3        | 3.14          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 17       | 3.13          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 9        | 3.12          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 13       | 3.12          |
| (1,115) | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 6        | 3.12          |
| (1,115) | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 6        | 3.12          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 7        | 3.1           |
| (1,15)  | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 3        | 3.09          |
| (1,15)  | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 3        | 3.09          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 6        | 3.08          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 6        | 3.08          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 2        | 3.08          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 8        | 3.08          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 1        | 3.05          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 5        | 3.03          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 1        | 3.0           |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 1        | 3.0           |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 4        | 2.99          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 4        | 2.99          |
| (1,15)  | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 14       | 2.99          |
| (1,15)  | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 14       | 2.99          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 9        | 2.98          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 10       | 2.98          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 17       | 2.98          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 17       | 2.98          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 3        | 2.97          |
| (1,142) | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 11       | 2.97          |
| (1,15)  | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 4        | 2.96          |
| (1,15)  | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 4        | 2.96          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 17       | 2.94          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 12       | 2.92          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 12       | 2.92          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 18       | 2.91          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 18       | 2.91          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 7        | 2.89          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 4        | 2.89          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 4        | 2.89          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 11       | 2.88          |
| (1,15)  | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 9        | 2.88          |
| (1,15)  | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 9        | 2.88          |
| (1,15)  | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 1        | 2.85          |
| (1,15)  | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 1        | 2.85          |
| (3,25)  | 1:9:A:DT:H6  | 1:10:A:DG:H4' | 14       | 2.83          |
| (1,133) | 1:5:A:DG:H21 | 1:6:A:DC:H6   | 13       | 2.8           |
| (1,133) | 1:5:A:DG:H22 | 1:6:A:DC:H6   | 13       | 2.8           |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H21  | 14       | 2.79          |
| (3,22)  | 1:9:A:DT:H6  | 1:8:A:DG:H22  | 14       | 2.79          |
| (1,133) | 1:5:A:DG:H21 | 1:6:A:DC:H6   | 4        | 2.79          |
| (1,133) | 1:5:A:DG:H22 | 1:6:A:DC:H6   | 4        | 2.79          |
| (1,133) | 1:5:A:DG:H21 | 1:6:A:DC:H6   | 16       | 2.79          |
| (1,133) | 1:5:A:DG:H22 | 1:6:A:DC:H6   | 16       | 2.79          |
| (1,133) | 1:5:A:DG:H21 | 1:6:A:DC:H6   | 1        | 2.78          |
| (1,133) | 1:5:A:DG:H22 | 1:6:A:DC:H6   | 1        | 2.78          |
| (1,15)  | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 10       | 2.78          |
| (1,15)  | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 10       | 2.78          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 16       | 2.77          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 16       | 2.77          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 6        | 2.77          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 6        | 2.77          |
| (1,15)  | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 5        | 2.77          |
| (1,15)  | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 5        | 2.77          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'  | 5        | 2.76          |
| (1,136) | 1:6:A:DC:H6  | 1:7:A:DA:H2'' | 5        | 2.76          |
| (1,15)  | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 2        | 2.76          |
| (1,15)  | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 2        | 2.76          |
| (1,133) | 1:5:A:DG:H21 | 1:6:A:DC:H6   | 5        | 2.73          |
| (1,133) | 1:5:A:DG:H22 | 1:6:A:DC:H6   | 5        | 2.73          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,133) | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 10       | 2.73          |
| (1,133) | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 10       | 2.73          |
| (1,133) | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 11       | 2.73          |
| (1,133) | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 11       | 2.73          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6  | 9        | 2.72          |
| (1,133) | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 2        | 2.72          |
| (1,133) | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 2        | 2.72          |
| (1,133) | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 7        | 2.72          |
| (1,133) | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 7        | 2.72          |
| (1,133) | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 12       | 2.72          |
| (1,133) | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 12       | 2.72          |
| (1,136) | 1:6:A:DC:H6   | 1:7:A:DA:H2'  | 2        | 2.71          |
| (1,136) | 1:6:A:DC:H6   | 1:7:A:DA:H2'' | 2        | 2.71          |
| (1,136) | 1:6:A:DC:H6   | 1:7:A:DA:H2'  | 14       | 2.71          |
| (1,136) | 1:6:A:DC:H6   | 1:7:A:DA:H2'' | 14       | 2.71          |
| (1,133) | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 18       | 2.71          |
| (1,133) | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 18       | 2.71          |
| (1,136) | 1:6:A:DC:H6   | 1:7:A:DA:H2'  | 11       | 2.7           |
| (1,136) | 1:6:A:DC:H6   | 1:7:A:DA:H2'' | 11       | 2.7           |
| (1,133) | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 14       | 2.69          |
| (1,133) | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 14       | 2.69          |
| (1,133) | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 17       | 2.69          |
| (1,133) | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 17       | 2.69          |
| (1,15)  | 1:2:A:DG:H21  | 1:3:A:DC:H6   | 16       | 2.69          |
| (1,15)  | 1:2:A:DG:H22  | 1:3:A:DC:H6   | 16       | 2.69          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6  | 10       | 2.65          |
| (1,133) | 1:5:A:DG:H21  | 1:6:A:DC:H6   | 9        | 2.65          |
| (1,133) | 1:5:A:DG:H22  | 1:6:A:DC:H6   | 9        | 2.65          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 1        | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 1        | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 2        | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 2        | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 3        | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 3        | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 4        | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 4        | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 5        | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 5        | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 6        | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 6        | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 7        | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 7        | 2.63          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 8        | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 8        | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 9        | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 9        | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 10       | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 10       | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 11       | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 11       | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 12       | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 12       | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 13       | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 13       | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 14       | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 14       | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 15       | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 15       | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 16       | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 16       | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 17       | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 17       | 2.63          |
| (1,37)  | 1:5:A:DG:H21  | 1:5:A:DG:H8   | 18       | 2.63          |
| (1,37)  | 1:5:A:DG:H22  | 1:5:A:DG:H8   | 18       | 2.63          |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5   | 4        | 2.58          |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5   | 4        | 2.58          |
| (3,25)  | 1:9:A:DT:H6   | 1:10:A:DG:H4' | 8        | 2.57          |
| (1,15)  | 1:2:A:DG:H21  | 1:3:A:DC:H6   | 7        | 2.57          |
| (1,15)  | 1:2:A:DG:H22  | 1:3:A:DC:H6   | 7        | 2.57          |
| (1,129) | 1:5:A:DG:H21  | 1:6:A:DC:H5   | 8        | 2.53          |
| (1,129) | 1:5:A:DG:H22  | 1:6:A:DC:H5   | 8        | 2.53          |
| (1,129) | 1:5:A:DG:H21  | 1:6:A:DC:H5   | 15       | 2.53          |
| (1,129) | 1:5:A:DG:H22  | 1:6:A:DC:H5   | 15       | 2.53          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5  | 2        | 2.5           |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5  | 5        | 2.5           |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5  | 7        | 2.5           |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5  | 9        | 2.5           |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5  | 10       | 2.5           |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5  | 12       | 2.5           |
| (1,152) | 1:9:A:DT:H6   | 1:10:A:DG:H8  | 2        | 2.5           |
| (3,22)  | 1:9:A:DT:H6   | 1:8:A:DG:H21  | 1        | 2.49          |
| (3,22)  | 1:9:A:DT:H6   | 1:8:A:DG:H22  | 1        | 2.49          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6  | 3        | 2.49          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 3        | 2.49          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6  | 18       | 2.48          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 13       | 2.48          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 15       | 2.48          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5  | 18       | 2.47          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 8        | 2.47          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 12       | 2.46          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 17       | 2.46          |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5   | 14       | 2.46          |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5   | 14       | 2.46          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 2        | 2.45          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5  | 17       | 2.43          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6  | 2        | 2.43          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 5        | 2.42          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6  | 5        | 2.41          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 7        | 2.41          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 11       | 2.41          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 18       | 2.41          |
| (3,22)  | 1:9:A:DT:H6   | 1:8:A:DG:H21  | 12       | 2.4           |
| (3,22)  | 1:9:A:DT:H6   | 1:8:A:DG:H22  | 12       | 2.4           |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6  | 7        | 2.4           |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5   | 3        | 2.4           |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5   | 3        | 2.4           |
| (3,22)  | 1:9:A:DT:H6   | 1:8:A:DG:H21  | 16       | 2.39          |
| (3,22)  | 1:9:A:DT:H6   | 1:8:A:DG:H22  | 16       | 2.39          |
| (1,152) | 1:9:A:DT:H6   | 1:10:A:DG:H8  | 10       | 2.39          |
| (1,78)  | 1:8:A:DG:H1'  | 1:9:A:DT:H6   | 6        | 2.39          |
| (1,15)  | 1:2:A:DG:H21  | 1:3:A:DC:H6   | 18       | 2.39          |
| (1,15)  | 1:2:A:DG:H22  | 1:3:A:DC:H6   | 18       | 2.39          |
| (1,152) | 1:9:A:DT:H6   | 1:10:A:DG:H8  | 5        | 2.38          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6   | 6        | 2.37          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 9        | 2.37          |
| (3,21)  | 1:9:A:DT:H6   | 1:10:A:DG:H2' | 17       | 2.35          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6   | 11       | 2.35          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6   | 16       | 2.35          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6   | 3        | 2.34          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8   | 10       | 2.34          |
| (1,129) | 1:5:A:DG:H21  | 1:6:A:DC:H5   | 5        | 2.33          |
| (1,129) | 1:5:A:DG:H22  | 1:6:A:DC:H5   | 5        | 2.33          |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5   | 1        | 2.33          |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5   | 1        | 2.33          |
| (3,22)  | 1:9:A:DT:H6   | 1:8:A:DG:H21  | 13       | 2.32          |
| (3,22)  | 1:9:A:DT:H6   | 1:8:A:DG:H22  | 13       | 2.32          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,152) | 1:9:A:DT:H6  | 1:10:A:DG:H8  | 6        | 2.32          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 3        | 2.31          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 3        | 2.31          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 17       | 2.31          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 17       | 2.31          |
| (1,116) | 1:2:A:DG:H3' | 1:3:A:DC:H6   | 13       | 2.31          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 18       | 2.31          |
| (3,26)  | 1:9:A:DT:H6  | 1:8:A:DG:H5'  | 12       | 2.3           |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 2        | 2.3           |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 2        | 2.3           |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 11       | 2.3           |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 11       | 2.3           |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 4        | 2.3           |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 16       | 2.29          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 16       | 2.29          |
| (1,113) | 1:2:A:DG:H1' | 1:3:A:DC:H6   | 4        | 2.29          |
| (1,113) | 1:2:A:DG:H1' | 1:3:A:DC:H6   | 14       | 2.29          |
| (1,152) | 1:9:A:DT:H6  | 1:10:A:DG:H8  | 9        | 2.28          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 15       | 2.28          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 11       | 2.27          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 12       | 2.27          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 12       | 2.27          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 8        | 2.26          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 18       | 2.26          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 18       | 2.26          |
| (1,152) | 1:9:A:DT:H6  | 1:10:A:DG:H8  | 3        | 2.24          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 4        | 2.23          |
| (1,152) | 1:9:A:DT:H6  | 1:10:A:DG:H8  | 15       | 2.23          |
| (1,152) | 1:9:A:DT:H6  | 1:10:A:DG:H8  | 18       | 2.23          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 14       | 2.23          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 14       | 2.23          |
| (3,26)  | 1:9:A:DT:H6  | 1:8:A:DG:H5'  | 14       | 2.22          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 12       | 2.22          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8   | 8        | 2.22          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 1        | 2.21          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 1        | 2.21          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 4        | 2.21          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 4        | 2.21          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 15       | 2.2           |
| (1,152) | 1:9:A:DT:H6  | 1:10:A:DG:H8  | 12       | 2.2           |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6   | 14       | 2.2           |
| (1,113) | 1:2:A:DG:H1' | 1:3:A:DC:H6   | 1        | 2.19          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (3,24)  | 1:9:A:DT:H6  | 1:8:A:DG:H4' | 2        | 2.18          |
| (3,24)  | 1:9:A:DT:H6  | 1:8:A:DG:H4' | 5        | 2.18          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 9        | 2.18          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 10       | 2.18          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 12       | 2.18          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 17       | 2.18          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 3        | 2.17          |
| (1,120) | 1:3:A:DC:H1' | 1:4:A:DC:H6  | 3        | 2.16          |
| (1,120) | 1:3:A:DC:H1' | 1:4:A:DC:H6  | 18       | 2.16          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 5        | 2.16          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 7        | 2.16          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 18       | 2.16          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 7        | 2.16          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 12       | 2.16          |
| (3,24)  | 1:9:A:DT:H6  | 1:8:A:DG:H4' | 10       | 2.15          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 7        | 2.15          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 18       | 2.15          |
| (1,120) | 1:3:A:DC:H1' | 1:4:A:DC:H6  | 7        | 2.15          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 1        | 2.15          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 2        | 2.15          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 4        | 2.15          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 14       | 2.15          |
| (1,116) | 1:2:A:DG:H3' | 1:3:A:DC:H6  | 17       | 2.15          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 1        | 2.15          |
| (1,120) | 1:3:A:DC:H1' | 1:4:A:DC:H6  | 5        | 2.14          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 3        | 2.14          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 13       | 2.14          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 15       | 2.14          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 16       | 2.14          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 5        | 2.13          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 9        | 2.13          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 10       | 2.13          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 17       | 2.13          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5  | 9        | 2.12          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5  | 9        | 2.12          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 9        | 2.12          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 13       | 2.12          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 2        | 2.11          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 11       | 2.11          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5  | 7        | 2.11          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5  | 7        | 2.11          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5  | 10       | 2.11          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5  | 10       | 2.11          |
| (1,112) | 1:2:A:DG:H8  | 1:3:A:DC:H5  | 11       | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 1        | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 2        | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 3        | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 4        | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 5        | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 6        | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 7        | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 8        | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 9        | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 10       | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 11       | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 12       | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 13       | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 14       | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 15       | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 16       | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 17       | 2.11          |
| (1,66)  | 1:7:A:DA:H2  | 1:7:A:DA:H8  | 18       | 2.11          |
| (1,14)  | 1:2:A:DG:H21 | 1:3:A:DC:H5  | 2        | 2.11          |
| (1,14)  | 1:2:A:DG:H22 | 1:3:A:DC:H5  | 2        | 2.11          |
| (1,14)  | 1:2:A:DG:H21 | 1:3:A:DC:H5  | 5        | 2.11          |
| (1,14)  | 1:2:A:DG:H22 | 1:3:A:DC:H5  | 5        | 2.11          |
| (1,113) | 1:2:A:DG:H1' | 1:3:A:DC:H6  | 9        | 2.1           |
| (1,110) | 1:1:A:DG:H1' | 1:2:A:DG:H8  | 6        | 2.1           |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 15       | 2.09          |
| (1,113) | 1:2:A:DG:H1' | 1:3:A:DC:H6  | 10       | 2.09          |
| (3,24)  | 1:9:A:DT:H6  | 1:8:A:DG:H4' | 11       | 2.08          |
| (1,152) | 1:9:A:DT:H6  | 1:10:A:DG:H8 | 17       | 2.08          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 3        | 2.08          |
| (1,129) | 1:5:A:DG:H21 | 1:6:A:DC:H5  | 13       | 2.08          |
| (1,129) | 1:5:A:DG:H22 | 1:6:A:DC:H5  | 13       | 2.08          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 14       | 2.08          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8  | 6        | 2.08          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 2        | 2.08          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 8        | 2.08          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 8        | 2.07          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 16       | 2.07          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 5        | 2.07          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 6        | 2.06          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 2        | 2.06          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 9        | 2.06          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 11       | 2.06          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 12       | 2.05          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 14       | 2.05          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 9        | 2.05          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 3        | 2.05          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 15       | 2.05          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 16       | 2.05          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 17       | 2.05          |
| (1,116) | 1:2:A:DG:H3' | 1:3:A:DC:H6  | 18       | 2.05          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 17       | 2.04          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 7        | 2.04          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 10       | 2.04          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 6        | 2.04          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 7        | 2.04          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 8        | 2.04          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 10       | 2.04          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 18       | 2.04          |
| (3,26)  | 1:9:A:DT:H6  | 1:8:A:DG:H5' | 10       | 2.03          |
| (1,152) | 1:9:A:DT:H6  | 1:10:A:DG:H8 | 4        | 2.03          |
| (1,150) | 1:9:A:DT:H1' | 1:8:A:DG:H8  | 16       | 2.03          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 4        | 2.03          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 6        | 2.03          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 12       | 2.03          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 14       | 2.03          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 18       | 2.03          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 12       | 2.03          |
| (1,78)  | 1:8:A:DG:H1' | 1:9:A:DT:H6  | 5        | 2.03          |
| (1,14)  | 1:2:A:DG:H21 | 1:3:A:DC:H5  | 16       | 2.03          |
| (1,14)  | 1:2:A:DG:H22 | 1:3:A:DC:H5  | 16       | 2.03          |
| (1,138) | 1:7:A:DA:H1' | 1:8:A:DG:H8  | 1        | 2.02          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 1        | 2.02          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 2        | 2.02          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 3        | 2.02          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 4        | 2.02          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 5        | 2.02          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 8        | 2.02          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 11       | 2.02          |
| (1,127) | 1:5:A:DG:H1' | 1:6:A:DC:H5  | 17       | 2.02          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 4        | 2.02          |
| (1,124) | 1:4:A:DC:H1' | 1:5:A:DG:H8  | 13       | 2.02          |
| (1,116) | 1:2:A:DG:H3' | 1:3:A:DC:H6  | 12       | 2.02          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4'  | 12       | 2.01          |
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4'  | 17       | 2.01          |
| (1,138) | 1:7:A:DA:H1'  | 1:8:A:DG:H8   | 13       | 2.01          |
| (1,127) | 1:5:A:DG:H1'  | 1:6:A:DC:H5   | 13       | 2.01          |
| (1,127) | 1:5:A:DG:H1'  | 1:6:A:DC:H5   | 15       | 2.01          |
| (1,127) | 1:5:A:DG:H1'  | 1:6:A:DC:H5   | 16       | 2.01          |
| (1,124) | 1:4:A:DC:H1'  | 1:5:A:DG:H8   | 1        | 2.01          |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6   | 10       | 2.01          |
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4'  | 13       | 2.0           |
| (1,152) | 1:9:A:DT:H6   | 1:10:A:DG:H8  | 7        | 2.0           |
| (1,152) | 1:9:A:DT:H6   | 1:10:A:DG:H8  | 11       | 2.0           |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5   | 9        | 2.0           |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5   | 9        | 2.0           |
| (3,26)  | 1:9:A:DT:H6   | 1:8:A:DG:H5'  | 16       | 1.99          |
| (1,152) | 1:9:A:DT:H6   | 1:10:A:DG:H8  | 8        | 1.99          |
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8   | 1        | 1.99          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 8        | 1.99          |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6   | 8        | 1.99          |
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4'  | 14       | 1.98          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 3        | 1.98          |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6   | 9        | 1.98          |
| (1,78)  | 1:8:A:DG:H1'  | 1:9:A:DT:H6   | 10       | 1.98          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 13       | 1.97          |
| (1,78)  | 1:8:A:DG:H1'  | 1:9:A:DT:H6   | 11       | 1.97          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8   | 12       | 1.96          |
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4'  | 8        | 1.95          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 17       | 1.95          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6   | 9        | 1.95          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6   | 10       | 1.95          |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6   | 3        | 1.95          |
| (3,21)  | 1:9:A:DT:H6   | 1:10:A:DG:H2' | 13       | 1.94          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 2        | 1.94          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 6        | 1.94          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 8        | 1.94          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 9        | 1.94          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 10       | 1.94          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 12       | 1.94          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 17       | 1.94          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 1        | 1.93          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 3        | 1.93          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 4        | 1.93          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 5        | 1.93          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 7        | 1.93          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 11       | 1.93          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 14       | 1.93          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 15       | 1.93          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 16       | 1.93          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 18       | 1.93          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 7        | 1.93          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 10       | 1.93          |
| (3,21)  | 1:9:A:DT:H6   | 1:10:A:DG:H2' | 6        | 1.92          |
| (1,163) | 1:12:A:DC:H3' | 1:12:A:DC:H6  | 13       | 1.92          |
| (3,26)  | 1:9:A:DT:H6   | 1:8:A:DG:H5'  | 15       | 1.91          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 9        | 1.91          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 11       | 1.91          |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6   | 7        | 1.91          |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5   | 7        | 1.91          |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5   | 7        | 1.91          |
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4'  | 1        | 1.9           |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5  | 1        | 1.9           |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 2        | 1.9           |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 5        | 1.9           |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 15       | 1.9           |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 16       | 1.9           |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5   | 10       | 1.9           |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5   | 10       | 1.9           |
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4'  | 16       | 1.89          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8   | 6        | 1.89          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 1        | 1.89          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 4        | 1.89          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 12       | 1.89          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 14       | 1.89          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 18       | 1.89          |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6   | 15       | 1.89          |
| (1,15)  | 1:2:A:DG:H21  | 1:3:A:DC:H6   | 13       | 1.88          |
| (1,15)  | 1:2:A:DG:H22  | 1:3:A:DC:H6   | 13       | 1.88          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8   | 13       | 1.87          |
| (1,135) | 1:6:A:DC:H3'  | 1:6:A:DC:H6   | 6        | 1.87          |
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4'  | 3        | 1.86          |
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4'  | 9        | 1.86          |
| (3,21)  | 1:9:A:DT:H6   | 1:10:A:DG:H2' | 14       | 1.86          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6   | 17       | 1.86          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8   | 4        | 1.85          |
| (1,149) | 1:9:A:DT:H3'  | 1:9:A:DT:H6   | 6        | 1.82          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,116) | 1:2:A:DG:H3' | 1:3:A:DC:H6   | 1        | 1.82          |
| (1,116) | 1:2:A:DG:H3' | 1:3:A:DC:H6   | 14       | 1.82          |
| (3,24)  | 1:9:A:DT:H6  | 1:8:A:DG:H4'  | 7        | 1.81          |
| (1,114) | 1:2:A:DG:H2' | 1:3:A:DC:H6   | 13       | 1.81          |
| (3,26)  | 1:9:A:DT:H6  | 1:8:A:DG:H5'  | 2        | 1.8           |
| (3,26)  | 1:9:A:DT:H6  | 1:8:A:DG:H5'  | 8        | 1.8           |
| (1,150) | 1:9:A:DT:H1' | 1:8:A:DG:H8   | 13       | 1.8           |
| (1,116) | 1:2:A:DG:H3' | 1:3:A:DC:H6   | 5        | 1.8           |
| (1,152) | 1:9:A:DT:H6  | 1:10:A:DG:H8  | 13       | 1.79          |
| (3,24)  | 1:9:A:DT:H6  | 1:8:A:DG:H4'  | 15       | 1.78          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 16       | 1.78          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6   | 17       | 1.78          |
| (3,26)  | 1:9:A:DT:H6  | 1:8:A:DG:H5'  | 3        | 1.77          |
| (3,24)  | 1:9:A:DT:H6  | 1:8:A:DG:H4'  | 4        | 1.77          |
| (3,21)  | 1:9:A:DT:H6  | 1:10:A:DG:H2' | 1        | 1.77          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6   | 12       | 1.76          |
| (1,15)  | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 15       | 1.76          |
| (1,15)  | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 15       | 1.76          |
| (3,26)  | 1:9:A:DT:H6  | 1:8:A:DG:H5'  | 5        | 1.74          |
| (1,151) | 1:9:A:DT:H6  | 1:8:A:DG:H8   | 16       | 1.74          |
| (1,15)  | 1:2:A:DG:H21 | 1:3:A:DC:H6   | 17       | 1.74          |
| (1,15)  | 1:2:A:DG:H22 | 1:3:A:DC:H6   | 17       | 1.74          |
| (1,158) | 1:11:A:DC:H6 | 1:12:A:DC:H5  | 14       | 1.73          |
| (1,117) | 1:2:A:DG:H3' | 1:2:A:DG:H8   | 11       | 1.73          |
| (3,24)  | 1:9:A:DT:H6  | 1:8:A:DG:H4'  | 18       | 1.72          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6   | 11       | 1.72          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6   | 15       | 1.72          |
| (1,114) | 1:2:A:DG:H2' | 1:3:A:DC:H6   | 12       | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8   | 1        | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8   | 1        | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8   | 2        | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8   | 2        | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8   | 3        | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8   | 3        | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8   | 4        | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8   | 4        | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8   | 5        | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8   | 5        | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8   | 6        | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8   | 6        | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8   | 7        | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8   | 7        | 1.72          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 8        | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 8        | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 9        | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 9        | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 10       | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 10       | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 11       | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 11       | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 12       | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 12       | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 13       | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 13       | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 14       | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 14       | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 15       | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 15       | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 16       | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 16       | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 17       | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 17       | 1.72          |
| (1,9)   | 1:2:A:DG:H21 | 1:2:A:DG:H8  | 18       | 1.72          |
| (1,9)   | 1:2:A:DG:H22 | 1:2:A:DG:H8  | 18       | 1.72          |
| (1,151) | 1:9:A:DT:H6  | 1:8:A:DG:H8  | 1        | 1.71          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6  | 4        | 1.71          |
| (1,118) | 1:3:A:DC:H3' | 1:3:A:DC:H1' | 6        | 1.7           |
| (1,118) | 1:3:A:DC:H3' | 1:3:A:DC:H1' | 11       | 1.7           |
| (1,118) | 1:3:A:DC:H3' | 1:3:A:DC:H1' | 16       | 1.7           |
| (1,116) | 1:2:A:DG:H3' | 1:3:A:DC:H6  | 4        | 1.7           |
| (1,118) | 1:3:A:DC:H3' | 1:3:A:DC:H1' | 3        | 1.69          |
| (1,118) | 1:3:A:DC:H3' | 1:3:A:DC:H1' | 5        | 1.69          |
| (1,118) | 1:3:A:DC:H3' | 1:3:A:DC:H1' | 7        | 1.69          |
| (1,118) | 1:3:A:DC:H3' | 1:3:A:DC:H1' | 9        | 1.69          |
| (1,118) | 1:3:A:DC:H3' | 1:3:A:DC:H1' | 10       | 1.69          |
| (1,118) | 1:3:A:DC:H3' | 1:3:A:DC:H1' | 18       | 1.69          |
| (3,26)  | 1:9:A:DT:H6  | 1:8:A:DG:H5' | 9        | 1.68          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6  | 2        | 1.68          |
| (3,26)  | 1:9:A:DT:H6  | 1:8:A:DG:H5' | 6        | 1.67          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6  | 5        | 1.67          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6  | 7        | 1.67          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6  | 8        | 1.67          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6  | 9        | 1.67          |
| (1,149) | 1:9:A:DT:H3' | 1:9:A:DT:H6  | 10       | 1.67          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,118) | 1:3:A:DC:H3'  | 1:3:A:DC:H1' | 8        | 1.67          |
| (1,118) | 1:3:A:DC:H3'  | 1:3:A:DC:H1' | 12       | 1.67          |
| (1,118) | 1:3:A:DC:H3'  | 1:3:A:DC:H1' | 13       | 1.67          |
| (1,118) | 1:3:A:DC:H3'  | 1:3:A:DC:H1' | 14       | 1.67          |
| (1,118) | 1:3:A:DC:H3'  | 1:3:A:DC:H1' | 15       | 1.67          |
| (1,149) | 1:9:A:DT:H3'  | 1:9:A:DT:H6  | 3        | 1.66          |
| (1,118) | 1:3:A:DC:H3'  | 1:3:A:DC:H1' | 1        | 1.66          |
| (1,118) | 1:3:A:DC:H3'  | 1:3:A:DC:H1' | 2        | 1.66          |
| (1,118) | 1:3:A:DC:H3'  | 1:3:A:DC:H1' | 17       | 1.66          |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6  | 2        | 1.66          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5 | 4        | 1.65          |
| (1,118) | 1:3:A:DC:H3'  | 1:3:A:DC:H1' | 4        | 1.65          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 8        | 1.65          |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5  | 18       | 1.64          |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5  | 18       | 1.64          |
| (1,149) | 1:9:A:DT:H3'  | 1:9:A:DT:H6  | 13       | 1.63          |
| (1,149) | 1:9:A:DT:H3'  | 1:9:A:DT:H6  | 14       | 1.63          |
| (1,149) | 1:9:A:DT:H3'  | 1:9:A:DT:H6  | 18       | 1.63          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 9        | 1.62          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 10       | 1.62          |
| (1,149) | 1:9:A:DT:H3'  | 1:9:A:DT:H6  | 1        | 1.62          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 14       | 1.62          |
| (1,149) | 1:9:A:DT:H3'  | 1:9:A:DT:H6  | 16       | 1.61          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 7        | 1.6           |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 18       | 1.6           |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 1        | 1.6           |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 8        | 1.6           |
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8  | 14       | 1.59          |
| (1,152) | 1:9:A:DT:H6   | 1:10:A:DG:H8 | 16       | 1.58          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 15       | 1.58          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6  | 5        | 1.58          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 2        | 1.58          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 2        | 1.57          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 3        | 1.57          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 5        | 1.57          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 11       | 1.57          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 12       | 1.57          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 6        | 1.57          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 11       | 1.57          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 4        | 1.56          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 6        | 1.56          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 14       | 1.56          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 16       | 1.56          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 17       | 1.56          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 2        | 1.56          |
| (3,26)  | 1:9:A:DT:H6   | 1:8:A:DG:H5' | 7        | 1.55          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 1        | 1.55          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 8        | 1.55          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 15       | 1.55          |
| (1,152) | 1:9:A:DT:H6   | 1:10:A:DG:H8 | 14       | 1.55          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 13       | 1.55          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 16       | 1.55          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 15       | 1.55          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 5        | 1.55          |
| (1,161) | 1:11:A:DC:H3' | 1:11:A:DC:H6 | 13       | 1.54          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5 | 16       | 1.54          |
| (1,152) | 1:9:A:DT:H6   | 1:10:A:DG:H8 | 1        | 1.54          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 11       | 1.54          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 12       | 1.54          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 8        | 1.53          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 17       | 1.53          |
| (3,26)  | 1:9:A:DT:H6   | 1:8:A:DG:H5' | 13       | 1.52          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 14       | 1.52          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 14       | 1.52          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 4        | 1.52          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 13       | 1.52          |
| (1,15)  | 1:2:A:DG:H21  | 1:3:A:DC:H6  | 12       | 1.52          |
| (1,15)  | 1:2:A:DG:H22  | 1:3:A:DC:H6  | 12       | 1.52          |
| (3,26)  | 1:9:A:DT:H6   | 1:8:A:DG:H5' | 17       | 1.51          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 1        | 1.51          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6  | 13       | 1.51          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 14       | 1.5           |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 2        | 1.49          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 4        | 1.49          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 14       | 1.49          |
| (3,24)  | 1:9:A:DT:H6   | 1:8:A:DG:H4' | 6        | 1.48          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 2        | 1.48          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 17       | 1.48          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 18       | 1.48          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 17       | 1.48          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 4        | 1.47          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6  | 7        | 1.47          |
| (3,26)  | 1:9:A:DT:H6   | 1:8:A:DG:H5' | 11       | 1.46          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6  | 2        | 1.46          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8  | 14       | 1.43          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 5        | 1.43          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 1        | 1.42          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 16       | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 1        | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 2        | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 3        | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 4        | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 5        | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 6        | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 7        | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 8        | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 9        | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 10       | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 11       | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 12       | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 13       | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 14       | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 15       | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 16       | 1.41          |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 18       | 1.41          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 12       | 1.4           |
| (1,126) | 1:5:A:DG:H3'  | 1:5:A:DG:H1' | 17       | 1.4           |
| (1,117) | 1:2:A:DG:H3'  | 1:2:A:DG:H8  | 16       | 1.4           |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5  | 13       | 1.4           |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5  | 13       | 1.4           |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 6        | 1.39          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 4        | 1.39          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 7        | 1.39          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6  | 18       | 1.38          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 6        | 1.37          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 18       | 1.35          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 15       | 1.34          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5 | 15       | 1.33          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 13       | 1.33          |
| (1,15)  | 1:2:A:DG:H21  | 1:3:A:DC:H6  | 8        | 1.33          |
| (1,15)  | 1:2:A:DG:H22  | 1:3:A:DC:H6  | 8        | 1.33          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 13       | 1.32          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 18       | 1.31          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 4        | 1.3           |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 6        | 1.3           |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 6        | 1.3           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 12       | 1.29          |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6  | 11       | 1.29          |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6  | 16       | 1.29          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 15       | 1.28          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 2        | 1.28          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 3        | 1.28          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 5        | 1.28          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 7        | 1.28          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 9        | 1.28          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 10       | 1.28          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 18       | 1.28          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 3        | 1.28          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6  | 15       | 1.28          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 1        | 1.27          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 4        | 1.27          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 6        | 1.27          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 8        | 1.27          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 11       | 1.27          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 12       | 1.27          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 13       | 1.27          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 14       | 1.27          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 15       | 1.27          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 16       | 1.27          |
| (1,159) | 1:11:A:DC:H1' | 1:11:A:DC:H6 | 17       | 1.27          |
| (3,26)  | 1:9:A:DT:H6   | 1:8:A:DG:H5' | 1        | 1.26          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6  | 6        | 1.26          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6  | 15       | 1.26          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 7        | 1.26          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 10       | 1.26          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 12       | 1.26          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 17       | 1.25          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 15       | 1.25          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 13       | 1.25          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 1        | 1.25          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 8        | 1.25          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 4        | 1.23          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 13       | 1.23          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71 | 12       | 1.23          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72 | 12       | 1.23          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73 | 12       | 1.23          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 3        | 1.23          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 15       | 1.23          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 15       | 1.23          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 18       | 1.22          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5 | 13       | 1.22          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 14       | 1.22          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 9        | 1.22          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 10       | 1.22          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 14       | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 1        | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 1        | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 2        | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 2        | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 3        | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 3        | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 4        | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 4        | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 5        | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 5        | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 6        | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 6        | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 7        | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 7        | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 8        | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 8        | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 9        | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 9        | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 10       | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 10       | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 11       | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 11       | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 12       | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 12       | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 13       | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 13       | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 14       | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 14       | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 15       | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 15       | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 16       | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 16       | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 17       | 1.22          |
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 17       | 1.22          |
| (1,3)   | 1:1:A:DG:H21  | 1:1:A:DG:H8  | 18       | 1.22          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,3)   | 1:1:A:DG:H22  | 1:1:A:DG:H8  | 18       | 1.22          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 1        | 1.21          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71 | 6        | 1.21          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72 | 6        | 1.21          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73 | 6        | 1.21          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 7        | 1.21          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 12       | 1.2           |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 14       | 1.2           |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 17       | 1.2           |
| (3,26)  | 1:9:A:DT:H6   | 1:8:A:DG:H5' | 4        | 1.19          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 16       | 1.19          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 8        | 1.19          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 8        | 1.19          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 18       | 1.18          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6  | 8        | 1.18          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 17       | 1.18          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 3        | 1.17          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 2        | 1.17          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 1        | 1.17          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 16       | 1.17          |
| (1,15)  | 1:2:A:DG:H21  | 1:3:A:DC:H6  | 11       | 1.17          |
| (1,15)  | 1:2:A:DG:H22  | 1:3:A:DC:H6  | 11       | 1.17          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 8        | 1.16          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 7        | 1.16          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 12       | 1.16          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 6        | 1.16          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 12       | 1.16          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8  | 18       | 1.16          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 1        | 1.15          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5 | 11       | 1.15          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 3        | 1.15          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 5        | 1.15          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 4        | 1.15          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 6        | 1.14          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 16       | 1.14          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 16       | 1.14          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 10       | 1.14          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 13       | 1.13          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 17       | 1.13          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 1        | 1.13          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 4        | 1.13          |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5  | 15       | 1.13          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5  | 15       | 1.13          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 2        | 1.12          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 9        | 1.12          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 13       | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 2        | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 3        | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 4        | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 5        | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 6        | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 7        | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 8        | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 9        | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 10       | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 11       | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 12       | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 13       | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 14       | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 15       | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 16       | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 17       | 1.12          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 18       | 1.12          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 9        | 1.12          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 2        | 1.12          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 3        | 1.11          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 5        | 1.11          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 11       | 1.11          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 14       | 1.11          |
| (1,162) | 1:12:A:DC:H1' | 1:12:A:DC:H6 | 1        | 1.11          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5 | 3        | 1.11          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5 | 6        | 1.11          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 7        | 1.11          |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5  | 17       | 1.11          |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5  | 17       | 1.11          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 8        | 1.1           |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 14       | 1.1           |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 3        | 1.1           |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 15       | 1.09          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 2        | 1.09          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 9        | 1.09          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 6        | 1.09          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 1        | 1.09          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 9        | 1.09          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 16       | 1.09          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 2        | 1.08          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 8        | 1.08          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 7        | 1.08          |
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8  | 12       | 1.08          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 16       | 1.08          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 18       | 1.08          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 4        | 1.08          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 15       | 1.08          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 12       | 1.08          |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5  | 12       | 1.08          |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5  | 12       | 1.08          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 10       | 1.07          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 1        | 1.07          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 2        | 1.07          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 4        | 1.07          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 12       | 1.07          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 13       | 1.07          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 5        | 1.06          |
| (1,153) | 1:10:A:DG:H1' | 1:11:A:DC:H6 | 11       | 1.06          |
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8  | 18       | 1.06          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 3        | 1.06          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 5        | 1.06          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 7        | 1.06          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 8        | 1.06          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 9        | 1.06          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 10       | 1.06          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 11       | 1.06          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 15       | 1.06          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 17       | 1.06          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 8        | 1.06          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 18       | 1.06          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 16       | 1.06          |
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8  | 4        | 1.05          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 12       | 1.05          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 2        | 1.05          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 5        | 1.05          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 7        | 1.05          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 18       | 1.05          |
| (1,141) | 1:8:A:DG:H3'  | 1:8:A:DG:H1' | 14       | 1.04          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 9        | 1.04          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 10       | 1.04          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 12       | 1.04          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 17       | 1.04          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 4        | 1.03          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 17       | 1.03          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 5        | 1.03          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8  | 2        | 1.03          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6  | 3        | 1.03          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 15       | 1.03          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 16       | 1.03          |
| (1,15)  | 1:2:A:DG:H21  | 1:3:A:DC:H6  | 6        | 1.03          |
| (1,15)  | 1:2:A:DG:H22  | 1:3:A:DC:H6  | 6        | 1.03          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 1        | 1.02          |
| (3,26)  | 1:9:A:DT:H6   | 1:8:A:DG:H5' | 18       | 1.02          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 18       | 1.02          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 2        | 1.02          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 14       | 1.02          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 7        | 1.01          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 10       | 1.01          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71 | 4        | 1.01          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72 | 4        | 1.01          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73 | 4        | 1.01          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 11       | 1.01          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 11       | 1.01          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 9        | 1.01          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 10       | 1.01          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 8        | 1.01          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 13       | 1.0           |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 17       | 1.0           |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 2        | 1.0           |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 11       | 1.0           |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 12       | 1.0           |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 18       | 1.0           |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 6        | 1.0           |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 11       | 1.0           |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 16       | 1.0           |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 5        | 0.99          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 1        | 0.99          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 4        | 0.99          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 6        | 0.99          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 12       | 0.99          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 16       | 0.99          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 18       | 0.99          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 10       | 0.98          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5  | 5        | 0.98          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 2        | 0.98          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 3        | 0.98          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 5        | 0.98          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 7        | 0.98          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 8        | 0.98          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 10       | 0.98          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 13       | 0.98          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 14       | 0.98          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 17       | 0.98          |
| (3,19)  | 1:9:A:DT:H6   | 1:8:A:DG:H1' | 11       | 0.97          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8  | 15       | 0.97          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 9        | 0.97          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 11       | 0.97          |
| (1,123) | 1:4:A:DC:H1'  | 1:4:A:DC:H6  | 15       | 0.97          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 1        | 0.97          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 3        | 0.97          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 4        | 0.97          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 13       | 0.97          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 14       | 0.97          |
| (1,111) | 1:2:A:DG:H3'  | 1:2:A:DG:H1' | 15       | 0.97          |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8  | 2        | 0.96          |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8  | 11       | 0.96          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 17       | 0.96          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 2        | 0.96          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 2        | 0.96          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 2        | 0.96          |
| (3,31)  | 1:5:A:DG:N1   | 1:7:A:DA:C2  | 9        | 0.95          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 15       | 0.95          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71 | 13       | 0.94          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72 | 13       | 0.94          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73 | 13       | 0.94          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 11       | 0.94          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 11       | 0.94          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 11       | 0.94          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 17       | 0.94          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 17       | 0.94          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 17       | 0.94          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8  | 16       | 0.94          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 3        | 0.94          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 3        | 0.94          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1' | 17       | 0.93          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5  | 8        | 0.93          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 1        | 0.93          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 4        | 0.93          |
| (1,158) | 1:11:A:DC:H6  | 1:12:A:DC:H5 | 8        | 0.92          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8  | 5        | 0.92          |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8  | 5        | 0.92          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5  | 5        | 0.92          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8  | 1        | 0.92          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 12       | 0.91          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 12       | 0.91          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 12       | 0.91          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8  | 14       | 0.91          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 5        | 0.9           |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 5        | 0.9           |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 5        | 0.9           |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 6        | 0.9           |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 18       | 0.89          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 18       | 0.89          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 18       | 0.89          |
| (1,116) | 1:2:A:DG:H3'  | 1:3:A:DC:H6  | 6        | 0.89          |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8  | 14       | 0.88          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6  | 17       | 0.88          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 15       | 0.86          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1' | 2        | 0.86          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1' | 5        | 0.86          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 13       | 0.86          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 17       | 0.85          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1' | 11       | 0.85          |
| (1,110) | 1:1:A:DG:H1'  | 1:2:A:DG:H8  | 4        | 0.85          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 12       | 0.84          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 18       | 0.83          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1' | 9        | 0.83          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1' | 7        | 0.82          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1' | 10       | 0.82          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1' | 14       | 0.82          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6  | 1        | 0.82          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6  | 4        | 0.82          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 7        | 0.82          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 10       | 0.82          |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5  | 8        | 0.82          |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5  | 8        | 0.82          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1'  | 6        | 0.81          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 2        | 0.81          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 5        | 0.81          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 6        | 0.81          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 12       | 0.81          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1'  | 6        | 0.81          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1'  | 6        | 0.81          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 3        | 0.8           |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 7        | 0.8           |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 13       | 0.8           |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 15       | 0.8           |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 9        | 0.8           |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6   | 8        | 0.8           |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5   | 18       | 0.8           |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1'  | 9        | 0.8           |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6  | 8        | 0.79          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 18       | 0.79          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71  | 1        | 0.79          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72  | 1        | 0.79          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73  | 1        | 0.79          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 3        | 0.79          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 8        | 0.79          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 15       | 0.79          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 18       | 0.79          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 14       | 0.79          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 18       | 0.79          |
| (1,130) | 1:5:A:DG:H8   | 1:6:A:DC:H5   | 6        | 0.79          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5   | 3        | 0.79          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6  | 3        | 0.78          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 9        | 0.78          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 10       | 0.78          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8   | 17       | 0.78          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 12       | 0.78          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 10       | 0.78          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 10       | 0.78          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 1        | 0.77          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 4        | 0.77          |
| (1,137) | 1:7:A:DA:H3'  | 1:7:A:DA:H1'  | 16       | 0.77          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 7        | 0.77          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 7        | 0.77          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 13       | 0.77          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 13       | 0.76          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 2        | 0.76          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 11       | 0.76          |
| (1,112) | 1:2:A:DG:H8   | 1:3:A:DC:H5   | 7        | 0.76          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 1        | 0.75          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 4        | 0.75          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 6        | 0.75          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 14       | 0.75          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 16       | 0.75          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 17       | 0.75          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6   | 6        | 0.75          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6   | 6        | 0.75          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6   | 6        | 0.75          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 5        | 0.75          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 16       | 0.75          |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6  | 6        | 0.74          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 8        | 0.74          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 11       | 0.74          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 12       | 0.74          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 13       | 0.74          |
| (1,157) | 1:11:A:DC:H3' | 1:11:A:DC:H1' | 15       | 0.74          |
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8   | 9        | 0.74          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 2        | 0.74          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 5        | 0.74          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8   | 6        | 0.74          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8   | 6        | 0.74          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8   | 6        | 0.74          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8   | 13       | 0.74          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8   | 13       | 0.74          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8   | 13       | 0.74          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6   | 8        | 0.73          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6   | 8        | 0.73          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6   | 8        | 0.73          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 1        | 0.73          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 3        | 0.73          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 4        | 0.73          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6   | 11       | 0.73          |
| (1,131) | 1:5:A:DG:H1'  | 1:6:A:DC:H6   | 17       | 0.73          |
| (1,128) | 1:5:A:DG:H2'  | 1:6:A:DC:H5   | 6        | 0.73          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8   | 15       | 0.73          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8   | 15       | 0.73          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8   | 15       | 0.73          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1'  | 3        | 0.73          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8  | 10       | 0.72          |
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8  | 3        | 0.72          |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8  | 18       | 0.72          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 3        | 0.72          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 3        | 0.72          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 3        | 0.72          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 15       | 0.72          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 15       | 0.72          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 15       | 0.72          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6  | 12       | 0.72          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6  | 14       | 0.72          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6  | 16       | 0.72          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6  | 18       | 0.72          |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 15       | 0.72          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 13       | 0.71          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 13       | 0.71          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 13       | 0.71          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6  | 6        | 0.71          |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6  | 9        | 0.71          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 11       | 0.71          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 11       | 0.71          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 13       | 0.7           |
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8  | 5        | 0.7           |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71 | 16       | 0.7           |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72 | 16       | 0.7           |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73 | 16       | 0.7           |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6  | 8        | 0.7           |
| (1,132) | 1:5:A:DG:H2'  | 1:6:A:DC:H6  | 17       | 0.7           |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 3        | 0.7           |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 3        | 0.7           |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 3        | 0.7           |
| (1,65)  | 1:7:A:DA:H2   | 1:7:A:DA:H1' | 8        | 0.7           |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8  | 3        | 0.69          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 17       | 0.69          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 17       | 0.69          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 17       | 0.69          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 14       | 0.69          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 14       | 0.69          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 14       | 0.69          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 16       | 0.69          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 16       | 0.69          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 16       | 0.69          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8  | 7        | 0.68          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 2        | 0.67          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 2        | 0.67          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 2        | 0.67          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 5        | 0.67          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 5        | 0.67          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 5        | 0.67          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 7        | 0.67          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 7        | 0.67          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 7        | 0.67          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 10       | 0.67          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 10       | 0.67          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 10       | 0.67          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 11       | 0.67          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 11       | 0.67          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 11       | 0.67          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 6        | 0.67          |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 10       | 0.66          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 14       | 0.66          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 14       | 0.66          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 14       | 0.66          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 8        | 0.66          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 8        | 0.66          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 8        | 0.66          |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 7        | 0.65          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8  | 11       | 0.65          |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 6        | 0.65          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 1        | 0.65          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 1        | 0.65          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 1        | 0.65          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 9        | 0.65          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 9        | 0.65          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 9        | 0.65          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 12       | 0.65          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 12       | 0.65          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 12       | 0.65          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 16       | 0.65          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 16       | 0.65          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 16       | 0.65          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 18       | 0.65          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 18       | 0.65          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 18       | 0.65          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 18       | 0.65          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 18       | 0.65          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8  | 8        | 0.64          |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8  | 17       | 0.64          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 4        | 0.64          |
| (1,134) | 1:6:A:DC:H2'  | 1:6:A:DC:H6  | 4        | 0.64          |
| (1,134) | 1:6:A:DC:H2'' | 1:6:A:DC:H6  | 4        | 0.64          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 2        | 0.64          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 2        | 0.64          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 5        | 0.64          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 5        | 0.64          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 7        | 0.64          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 7        | 0.64          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 12       | 0.64          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 12       | 0.64          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 17       | 0.64          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 17       | 0.64          |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 9        | 0.62          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71 | 2        | 0.62          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72 | 2        | 0.62          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73 | 2        | 0.62          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 1        | 0.62          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 1        | 0.62          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 1        | 0.62          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 4        | 0.62          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 4        | 0.62          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 4        | 0.62          |
| (1,120) | 1:3:A:DC:H1'  | 1:4:A:DC:H6  | 16       | 0.62          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71 | 18       | 0.61          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72 | 18       | 0.61          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73 | 18       | 0.61          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 7        | 0.61          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 7        | 0.61          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 7        | 0.61          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 10       | 0.61          |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 10       | 0.61          |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 10       | 0.61          |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 5        | 0.6           |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 12       | 0.6           |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 14       | 0.6           |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 18       | 0.6           |
| (1,160) | 1:11:A:DC:H1' | 1:12:A:DC:H6 | 11       | 0.6           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 1        | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 2        | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 3        | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 4        | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 5        | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 6        | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 7        | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 8        | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 9        | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 10       | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 12       | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 13       | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 14       | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 15       | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 16       | 0.6           |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 18       | 0.6           |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8  | 12       | 0.6           |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 9        | 0.6           |
| (1,125) | 1:4:A:DC:H2'  | 1:5:A:DG:H8  | 9        | 0.6           |
| (1,125) | 1:4:A:DC:H2'' | 1:5:A:DG:H8  | 9        | 0.6           |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 10       | 0.6           |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 13       | 0.6           |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 13       | 0.6           |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 2        | 0.59          |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 1        | 0.59          |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 4        | 0.59          |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 11       | 0.59          |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 11       | 0.59          |
| (1,154) | 1:10:A:DG:H1' | 1:10:A:DG:H8 | 17       | 0.59          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71 | 15       | 0.59          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72 | 15       | 0.59          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73 | 15       | 0.59          |
| (1,113) | 1:2:A:DG:H1'  | 1:3:A:DC:H6  | 12       | 0.59          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 4        | 0.59          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 4        | 0.59          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 16       | 0.59          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 16       | 0.59          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 9        | 0.59          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 9        | 0.59          |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 5        | 0.58          |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 2        | 0.58          |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 16       | 0.58          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (1,151) | 1:9:A:DT:H6  | 1:8:A:DG:H8  | 7        | 0.58          |
| (1,150) | 1:9:A:DT:H1' | 1:8:A:DG:H8  | 10       | 0.58          |
| (1,146) | 1:9:A:DT:H6  | 1:8:A:DG:H2' | 4        | 0.58          |
| (1,146) | 1:9:A:DT:H6  | 1:8:A:DG:H2' | 18       | 0.58          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H71 | 14       | 0.58          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H72 | 14       | 0.58          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H73 | 14       | 0.58          |
| (1,47)  | 1:5:A:DG:H21 | 1:6:A:DC:H6  | 1        | 0.58          |
| (1,47)  | 1:5:A:DG:H22 | 1:6:A:DC:H6  | 1        | 0.58          |
| (1,8)   | 1:2:A:DG:H21 | 1:2:A:DG:H1' | 10       | 0.58          |
| (1,8)   | 1:2:A:DG:H22 | 1:2:A:DG:H1' | 10       | 0.58          |
| (2,64)  | 1:5:A:DG:N3  | 1:7:A:DA:N6  | 11       | 0.57          |
| (2,63)  | 1:5:A:DG:N2  | 1:7:A:DA:N7  | 13       | 0.57          |
| (1,8)   | 1:2:A:DG:H21 | 1:2:A:DG:H1' | 8        | 0.57          |
| (1,8)   | 1:2:A:DG:H22 | 1:2:A:DG:H1' | 8        | 0.57          |
| (2,64)  | 1:5:A:DG:N3  | 1:7:A:DA:N6  | 6        | 0.56          |
| (2,64)  | 1:5:A:DG:N3  | 1:7:A:DA:N6  | 16       | 0.56          |
| (1,146) | 1:9:A:DT:H6  | 1:8:A:DG:H2' | 2        | 0.56          |
| (1,146) | 1:9:A:DT:H6  | 1:8:A:DG:H2' | 15       | 0.56          |
| (1,122) | 1:3:A:DC:H3' | 1:3:A:DC:H6  | 9        | 0.56          |
| (1,8)   | 1:2:A:DG:H21 | 1:2:A:DG:H1' | 13       | 0.56          |
| (1,8)   | 1:2:A:DG:H22 | 1:2:A:DG:H1' | 13       | 0.56          |
| (2,64)  | 1:5:A:DG:N3  | 1:7:A:DA:N6  | 14       | 0.55          |
| (2,64)  | 1:5:A:DG:N3  | 1:7:A:DA:N6  | 17       | 0.55          |
| (2,63)  | 1:5:A:DG:N2  | 1:7:A:DA:N7  | 3        | 0.55          |
| (2,63)  | 1:5:A:DG:N2  | 1:7:A:DA:N7  | 15       | 0.55          |
| (1,8)   | 1:2:A:DG:H21 | 1:2:A:DG:H1' | 3        | 0.55          |
| (1,8)   | 1:2:A:DG:H22 | 1:2:A:DG:H1' | 3        | 0.55          |
| (3,32)  | 1:5:A:DG:C1' | 1:7:A:DA:C1' | 2        | 0.54          |
| (3,32)  | 1:5:A:DG:C1' | 1:7:A:DA:C1' | 5        | 0.54          |
| (2,63)  | 1:5:A:DG:N2  | 1:7:A:DA:N7  | 8        | 0.54          |
| (2,63)  | 1:5:A:DG:N2  | 1:7:A:DA:N7  | 17       | 0.54          |
| (1,146) | 1:9:A:DT:H6  | 1:8:A:DG:H2' | 12       | 0.54          |
| (3,32)  | 1:5:A:DG:C1' | 1:7:A:DA:C1' | 11       | 0.53          |
| (2,64)  | 1:5:A:DG:N3  | 1:7:A:DA:N6  | 8        | 0.53          |
| (2,64)  | 1:5:A:DG:N3  | 1:7:A:DA:N6  | 12       | 0.53          |
| (1,150) | 1:9:A:DT:H1' | 1:8:A:DG:H8  | 2        | 0.53          |
| (1,146) | 1:9:A:DT:H6  | 1:8:A:DG:H2' | 5        | 0.53          |
| (1,122) | 1:3:A:DC:H3' | 1:3:A:DC:H6  | 7        | 0.53          |
| (1,47)  | 1:5:A:DG:H21 | 1:6:A:DC:H6  | 5        | 0.53          |
| (1,47)  | 1:5:A:DG:H22 | 1:6:A:DC:H6  | 5        | 0.53          |
| (1,47)  | 1:5:A:DG:H21 | 1:6:A:DC:H6  | 10       | 0.53          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 10       | 0.53          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 11       | 0.53          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 11       | 0.53          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 1        | 0.53          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 1        | 0.53          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 14       | 0.53          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 14       | 0.53          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 15       | 0.53          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 15       | 0.53          |
| (2,63)  | 1:5:A:DG:N2   | 1:7:A:DA:N7  | 6        | 0.52          |
| (1,151) | 1:9:A:DT:H6   | 1:8:A:DG:H8  | 9        | 0.52          |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 13       | 0.52          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 2        | 0.52          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 2        | 0.52          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 7        | 0.52          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 7        | 0.52          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 12       | 0.52          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 12       | 0.52          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 4        | 0.52          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 4        | 0.52          |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 18       | 0.51          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 12       | 0.51          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 13       | 0.51          |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 1        | 0.51          |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 3        | 0.51          |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 14       | 0.51          |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 16       | 0.51          |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 17       | 0.51          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 5        | 0.51          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 18       | 0.51          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 18       | 0.51          |
| (1,8)   | 1:2:A:DG:H21  | 1:2:A:DG:H1' | 16       | 0.51          |
| (1,8)   | 1:2:A:DG:H22  | 1:2:A:DG:H1' | 16       | 0.51          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 4        | 0.5           |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 6        | 0.5           |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 7        | 0.5           |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 10       | 0.5           |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71 | 5        | 0.5           |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72 | 5        | 0.5           |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73 | 5        | 0.5           |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8  | 16       | 0.5           |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 1        | 0.49          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 14       | 0.49          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 15       | 0.49          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 16       | 0.49          |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 9        | 0.49          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 14       | 0.49          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 14       | 0.49          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 17       | 0.49          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 17       | 0.49          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 16       | 0.48          |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 8        | 0.48          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 18       | 0.47          |
| (1,14)  | 1:2:A:DG:H21  | 1:3:A:DC:H5  | 11       | 0.47          |
| (1,14)  | 1:2:A:DG:H22  | 1:3:A:DC:H5  | 11       | 0.47          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 3        | 0.46          |
| (1,146) | 1:9:A:DT:H6   | 1:8:A:DG:H2' | 11       | 0.46          |
| (1,47)  | 1:5:A:DG:H21  | 1:6:A:DC:H6  | 9        | 0.45          |
| (1,47)  | 1:5:A:DG:H22  | 1:6:A:DC:H6  | 9        | 0.45          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 14       | 0.43          |
| (1,122) | 1:3:A:DC:H3'  | 1:3:A:DC:H6  | 3        | 0.41          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 1        | 0.4           |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 4        | 0.4           |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 15       | 0.4           |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 15       | 0.4           |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 11       | 0.4           |
| (1,88)  | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 1        | 0.4           |
| (1,88)  | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 1        | 0.4           |
| (1,88)  | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 2        | 0.4           |
| (1,88)  | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 2        | 0.4           |
| (1,88)  | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 3        | 0.4           |
| (1,88)  | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 3        | 0.4           |
| (1,88)  | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 4        | 0.4           |
| (1,88)  | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 4        | 0.4           |
| (1,88)  | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 5        | 0.4           |
| (1,88)  | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 5        | 0.4           |
| (1,88)  | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 6        | 0.4           |
| (1,88)  | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 6        | 0.4           |
| (1,88)  | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 7        | 0.4           |
| (1,88)  | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 7        | 0.4           |
| (1,88)  | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 8        | 0.4           |
| (1,88)  | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 8        | 0.4           |
| (1,88)  | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 9        | 0.4           |
| (1,88)  | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 9        | 0.4           |

*Continued on next page...*

*Continued from previous page...*

| Key    | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|--------|---------------|--------------|----------|---------------|
| (1,88) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 10       | 0.4           |
| (1,88) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 10       | 0.4           |
| (1,88) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 11       | 0.4           |
| (1,88) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 11       | 0.4           |
| (1,88) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 12       | 0.4           |
| (1,88) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 12       | 0.4           |
| (1,88) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 13       | 0.4           |
| (1,88) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 13       | 0.4           |
| (1,88) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 14       | 0.4           |
| (1,88) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 14       | 0.4           |
| (1,88) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 15       | 0.4           |
| (1,88) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 15       | 0.4           |
| (1,88) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 16       | 0.4           |
| (1,88) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 16       | 0.4           |
| (1,88) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 17       | 0.4           |
| (1,88) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 17       | 0.4           |
| (1,88) | 1:10:A:DG:H21 | 1:10:A:DG:H8 | 18       | 0.4           |
| (1,88) | 1:10:A:DG:H22 | 1:10:A:DG:H8 | 18       | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 1        | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 1        | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 2        | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 2        | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 3        | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 3        | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 4        | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 4        | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 5        | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 5        | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 6        | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 6        | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 7        | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 7        | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 8        | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 8        | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 9        | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 9        | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 10       | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 10       | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 11       | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 11       | 0.4           |
| (1,72) | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 12       | 0.4           |
| (1,72) | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 12       | 0.4           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,72)  | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 13       | 0.4           |
| (1,72)  | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 13       | 0.4           |
| (1,72)  | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 14       | 0.4           |
| (1,72)  | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 14       | 0.4           |
| (1,72)  | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 15       | 0.4           |
| (1,72)  | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 15       | 0.4           |
| (1,72)  | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 16       | 0.4           |
| (1,72)  | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 16       | 0.4           |
| (1,72)  | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 17       | 0.4           |
| (1,72)  | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 17       | 0.4           |
| (1,72)  | 1:8:A:DG:H21  | 1:8:A:DG:H8  | 18       | 0.4           |
| (1,72)  | 1:8:A:DG:H22  | 1:8:A:DG:H8  | 18       | 0.4           |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 9        | 0.39          |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 1        | 0.39          |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 3        | 0.39          |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 4        | 0.39          |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 13       | 0.39          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 17       | 0.39          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 16       | 0.39          |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 10       | 0.38          |
| (1,155) | 1:10:A:DG:H2' | 1:10:A:DG:H8 | 8        | 0.38          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71 | 17       | 0.38          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72 | 17       | 0.38          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73 | 17       | 0.38          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6  | 11       | 0.38          |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 7        | 0.37          |
| (2,64)  | 1:5:A:DG:N3   | 1:7:A:DA:N6  | 9        | 0.37          |
| (2,62)  | 1:4:A:DC:O2   | 1:8:A:DG:N2  | 10       | 0.36          |
| (2,62)  | 1:4:A:DC:O2   | 1:8:A:DG:N2  | 7        | 0.35          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 3        | 0.35          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 3        | 0.35          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 6        | 0.35          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 6        | 0.35          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 8        | 0.35          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 8        | 0.35          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 15       | 0.35          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 15       | 0.35          |
| (2,62)  | 1:4:A:DC:O2   | 1:8:A:DG:N2  | 3        | 0.34          |
| (1,150) | 1:9:A:DT:H1'  | 1:8:A:DG:H8  | 11       | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 1        | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 1        | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 2        | 0.34          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 2        | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 4        | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 4        | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 5        | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 5        | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 7        | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 7        | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 9        | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 9        | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 10       | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 10       | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 11       | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 11       | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 12       | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 12       | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 13       | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 13       | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 14       | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 14       | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 16       | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 16       | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 17       | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 17       | 0.34          |
| (1,36)  | 1:5:A:DG:H21  | 1:5:A:DG:H1' | 18       | 0.34          |
| (1,36)  | 1:5:A:DG:H22  | 1:5:A:DG:H1' | 18       | 0.34          |
| (2,62)  | 1:4:A:DC:O2   | 1:8:A:DG:N2  | 9        | 0.33          |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2 | 6        | 0.32          |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2 | 8        | 0.32          |
| (2,56)  | 1:2:A:DG:O6   | 1:11:A:DC:N4 | 11       | 0.32          |
| (1,121) | 1:3:A:DC:H2'  | 1:3:A:DC:H6  | 15       | 0.32          |
| (1,121) | 1:3:A:DC:H2'  | 1:3:A:DC:H6  | 15       | 0.32          |
| (1,121) | 1:3:A:DC:H2'' | 1:3:A:DC:H6  | 15       | 0.32          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 7        | 0.31          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1' | 8        | 0.31          |
| (2,61)  | 1:4:A:DC:N4   | 1:8:A:DG:O6  | 6        | 0.31          |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2 | 1        | 0.31          |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2 | 4        | 0.31          |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2 | 11       | 0.31          |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2 | 14       | 0.31          |
| (2,53)  | 1:1:A:DG:O6   | 1:12:A:DC:N4 | 3        | 0.31          |
| (2,53)  | 1:1:A:DG:O6   | 1:12:A:DC:N4 | 13       | 0.31          |
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2 | 8        | 0.31          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2  | 15       | 0.31          |
| (1,121) | 1:3:A:DC:H2'  | 1:3:A:DC:H6   | 12       | 0.31          |
| (1,121) | 1:3:A:DC:H2'  | 1:3:A:DC:H6   | 12       | 0.31          |
| (1,121) | 1:3:A:DC:H2'' | 1:3:A:DC:H6   | 12       | 0.31          |
| (1,121) | 1:3:A:DC:H2'  | 1:3:A:DC:H6   | 13       | 0.31          |
| (1,121) | 1:3:A:DC:H2'  | 1:3:A:DC:H6   | 13       | 0.31          |
| (1,121) | 1:3:A:DC:H2'' | 1:3:A:DC:H6   | 13       | 0.31          |
| (3,32)  | 1:5:A:DG:C1'  | 1:7:A:DA:C1'  | 10       | 0.3           |
| (3,27)  | 1:1:A:DG:C1'  | 1:12:A:DC:C1' | 6        | 0.3           |
| (2,61)  | 1:4:A:DC:N4   | 1:8:A:DG:O6   | 12       | 0.3           |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2  | 2        | 0.3           |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2  | 16       | 0.3           |
| (2,56)  | 1:2:A:DG:O6   | 1:11:A:DC:N4  | 8        | 0.3           |
| (2,56)  | 1:2:A:DG:O6   | 1:11:A:DC:N4  | 17       | 0.3           |
| (2,55)  | 1:2:A:DG:N2   | 1:11:A:DC:O2  | 1        | 0.3           |
| (2,55)  | 1:2:A:DG:N2   | 1:11:A:DC:O2  | 2        | 0.3           |
| (2,55)  | 1:2:A:DG:N2   | 1:11:A:DC:O2  | 3        | 0.3           |
| (2,55)  | 1:2:A:DG:N2   | 1:11:A:DC:O2  | 4        | 0.3           |
| (2,55)  | 1:2:A:DG:N2   | 1:11:A:DC:O2  | 14       | 0.3           |
| (2,53)  | 1:1:A:DG:O6   | 1:12:A:DC:N4  | 11       | 0.3           |
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2  | 6        | 0.3           |
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2  | 9        | 0.3           |
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2  | 10       | 0.3           |
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2  | 12       | 0.3           |
| (2,51)  | 1:1:A:DG:N1   | 1:12:A:DC:N3  | 6        | 0.3           |
| (1,121) | 1:3:A:DC:H2'  | 1:3:A:DC:H6   | 8        | 0.3           |
| (1,121) | 1:3:A:DC:H2'  | 1:3:A:DC:H6   | 8        | 0.3           |
| (1,121) | 1:3:A:DC:H2'' | 1:3:A:DC:H6   | 8        | 0.3           |
| (2,62)  | 1:4:A:DC:O2   | 1:8:A:DG:N2   | 5        | 0.29          |
| (2,62)  | 1:4:A:DC:O2   | 1:8:A:DG:N2   | 8        | 0.29          |
| (2,62)  | 1:4:A:DC:O2   | 1:8:A:DG:N2   | 17       | 0.29          |
| (2,60)  | 1:4:A:DC:N3   | 1:8:A:DG:N1   | 14       | 0.29          |
| (2,56)  | 1:2:A:DG:O6   | 1:11:A:DC:N4  | 12       | 0.29          |
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2  | 2        | 0.29          |
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2  | 17       | 0.29          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H71  | 10       | 0.29          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H72  | 10       | 0.29          |
| (1,144) | 1:8:A:DG:H8   | 1:9:A:DT:H73  | 10       | 0.29          |
| (2,62)  | 1:4:A:DC:O2   | 1:8:A:DG:N2   | 15       | 0.28          |
| (2,61)  | 1:4:A:DC:N4   | 1:8:A:DG:O6   | 13       | 0.28          |
| (2,60)  | 1:4:A:DC:N3   | 1:8:A:DG:N1   | 6        | 0.28          |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2  | 3        | 0.28          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (2,59)  | 1:3:A:DC:O2  | 1:10:A:DG:N2  | 5        | 0.28          |
| (2,59)  | 1:3:A:DC:O2  | 1:10:A:DG:N2  | 10       | 0.28          |
| (2,59)  | 1:3:A:DC:O2  | 1:10:A:DG:N2  | 18       | 0.28          |
| (2,56)  | 1:2:A:DG:O6  | 1:11:A:DC:N4  | 7        | 0.28          |
| (2,56)  | 1:2:A:DG:O6  | 1:11:A:DC:N4  | 10       | 0.28          |
| (2,56)  | 1:2:A:DG:O6  | 1:11:A:DC:N4  | 15       | 0.28          |
| (3,29)  | 1:3:A:DC:C1' | 1:10:A:DG:C1' | 2        | 0.27          |
| (2,62)  | 1:4:A:DC:O2  | 1:8:A:DG:N2   | 14       | 0.27          |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6   | 14       | 0.27          |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6   | 17       | 0.27          |
| (2,59)  | 1:3:A:DC:O2  | 1:10:A:DG:N2  | 12       | 0.27          |
| (2,59)  | 1:3:A:DC:O2  | 1:10:A:DG:N2  | 17       | 0.27          |
| (2,58)  | 1:3:A:DC:N4  | 1:10:A:DG:O6  | 3        | 0.27          |
| (2,58)  | 1:3:A:DC:N4  | 1:10:A:DG:O6  | 7        | 0.27          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 3        | 0.27          |
| (2,56)  | 1:2:A:DG:O6  | 1:11:A:DC:N4  | 6        | 0.27          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4  | 6        | 0.27          |
| (1,46)  | 1:5:A:DG:H21 | 1:6:A:DC:H5   | 6        | 0.27          |
| (1,46)  | 1:5:A:DG:H22 | 1:6:A:DC:H5   | 6        | 0.27          |
| (2,62)  | 1:4:A:DC:O2  | 1:8:A:DG:N2   | 2        | 0.26          |
| (2,62)  | 1:4:A:DC:O2  | 1:8:A:DG:N2   | 11       | 0.26          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 4        | 0.26          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 12       | 0.26          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 16       | 0.26          |
| (2,59)  | 1:3:A:DC:O2  | 1:10:A:DG:N2  | 9        | 0.26          |
| (2,59)  | 1:3:A:DC:O2  | 1:10:A:DG:N2  | 15       | 0.26          |
| (2,58)  | 1:3:A:DC:N4  | 1:10:A:DG:O6  | 4        | 0.26          |
| (2,56)  | 1:2:A:DG:O6  | 1:11:A:DC:N4  | 5        | 0.26          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 11       | 0.26          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H71  | 3        | 0.26          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H72  | 3        | 0.26          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H73  | 3        | 0.26          |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6   | 2        | 0.25          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 1        | 0.25          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 13       | 0.25          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 17       | 0.25          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 5        | 0.25          |
| (2,56)  | 1:2:A:DG:O6  | 1:11:A:DC:N4  | 9        | 0.25          |
| (2,56)  | 1:2:A:DG:O6  | 1:11:A:DC:N4  | 13       | 0.25          |
| (2,56)  | 1:2:A:DG:O6  | 1:11:A:DC:N4  | 18       | 0.25          |
| (2,55)  | 1:2:A:DG:N2  | 1:11:A:DC:O2  | 13       | 0.25          |
| (2,55)  | 1:2:A:DG:N2  | 1:11:A:DC:O2  | 16       | 0.25          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (2,62)  | 1:4:A:DC:O2  | 1:8:A:DG:N2   | 4        | 0.24          |
| (2,62)  | 1:4:A:DC:O2  | 1:8:A:DG:N2   | 16       | 0.24          |
| (2,62)  | 1:4:A:DC:O2  | 1:8:A:DG:N2   | 18       | 0.24          |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6   | 1        | 0.24          |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6   | 4        | 0.24          |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6   | 11       | 0.24          |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6   | 16       | 0.24          |
| (2,59)  | 1:3:A:DC:O2  | 1:10:A:DG:N2  | 13       | 0.24          |
| (2,58)  | 1:3:A:DC:N4  | 1:10:A:DG:O6  | 5        | 0.24          |
| (2,58)  | 1:3:A:DC:N4  | 1:10:A:DG:O6  | 6        | 0.24          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 10       | 0.24          |
| (2,55)  | 1:2:A:DG:N2  | 1:11:A:DC:O2  | 7        | 0.24          |
| (2,55)  | 1:2:A:DG:N2  | 1:11:A:DC:O2  | 15       | 0.24          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4  | 18       | 0.24          |
| (2,52)  | 1:1:A:DG:N2  | 1:12:A:DC:O2  | 5        | 0.24          |
| (1,112) | 1:2:A:DG:H8  | 1:3:A:DC:H5   | 10       | 0.24          |
| (2,62)  | 1:4:A:DC:O2  | 1:8:A:DG:N2   | 1        | 0.23          |
| (2,58)  | 1:3:A:DC:N4  | 1:10:A:DG:O6  | 2        | 0.23          |
| (2,58)  | 1:3:A:DC:N4  | 1:10:A:DG:O6  | 14       | 0.23          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 18       | 0.23          |
| (2,55)  | 1:2:A:DG:N2  | 1:11:A:DC:O2  | 5        | 0.23          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4  | 7        | 0.23          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H71  | 7        | 0.23          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H72  | 7        | 0.23          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H73  | 7        | 0.23          |
| (1,139) | 1:7:A:DA:H2' | 1:7:A:DA:H8   | 1        | 0.23          |
| (1,139) | 1:7:A:DA:H2' | 1:7:A:DA:H8   | 4        | 0.23          |
| (1,14)  | 1:2:A:DG:H21 | 1:3:A:DC:H5   | 6        | 0.23          |
| (1,14)  | 1:2:A:DG:H22 | 1:3:A:DC:H5   | 6        | 0.23          |
| (3,28)  | 1:2:A:DG:C1' | 1:11:A:DC:C1' | 2        | 0.22          |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6   | 18       | 0.22          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 2        | 0.22          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 11       | 0.22          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 9        | 0.22          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 14       | 0.22          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 13       | 0.22          |
| (2,52)  | 1:1:A:DG:N2  | 1:12:A:DC:O2  | 7        | 0.22          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 3        | 0.22          |
| (3,29)  | 1:3:A:DC:C1' | 1:10:A:DG:C1' | 16       | 0.21          |
| (3,27)  | 1:1:A:DG:C1' | 1:12:A:DC:C1' | 8        | 0.21          |
| (2,62)  | 1:4:A:DC:O2  | 1:8:A:DG:N2   | 6        | 0.21          |
| (2,62)  | 1:4:A:DC:O2  | 1:8:A:DG:N2   | 13       | 0.21          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1 | 4        | 0.21          |
| (2,55)  | 1:2:A:DG:N2  | 1:11:A:DC:O2 | 18       | 0.21          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4 | 5        | 0.21          |
| (2,52)  | 1:1:A:DG:N2  | 1:12:A:DC:O2 | 4        | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 3        | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 5        | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 6        | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 7        | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 8        | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 9        | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 10       | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 12       | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 13       | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 15       | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 17       | 0.21          |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 18       | 0.21          |
| (2,62)  | 1:4:A:DC:O2  | 1:8:A:DG:N2  | 12       | 0.2           |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6  | 5        | 0.2           |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1  | 5        | 0.2           |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1 | 2        | 0.2           |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1 | 7        | 0.2           |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1 | 12       | 0.2           |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1 | 13       | 0.2           |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1 | 17       | 0.2           |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3 | 5        | 0.2           |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3 | 6        | 0.2           |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3 | 7        | 0.2           |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3 | 9        | 0.2           |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3 | 10       | 0.2           |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3 | 14       | 0.2           |
| (2,52)  | 1:1:A:DG:N2  | 1:12:A:DC:O2 | 14       | 0.2           |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3 | 4        | 0.2           |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3 | 8        | 0.2           |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3 | 13       | 0.2           |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3 | 15       | 0.2           |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3 | 16       | 0.2           |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3 | 18       | 0.2           |
| (1,150) | 1:9:A:DT:H1' | 1:8:A:DG:H8  | 6        | 0.2           |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H71 | 11       | 0.2           |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H72 | 11       | 0.2           |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H73 | 11       | 0.2           |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6  | 1        | 0.2           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6   | 2        | 0.2           |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6   | 4        | 0.2           |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6   | 11       | 0.2           |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6   | 14       | 0.2           |
| (1,119) | 1:3:A:DC:H1' | 1:3:A:DC:H6   | 16       | 0.2           |
| (1,112) | 1:2:A:DG:H8  | 1:3:A:DC:H5   | 9        | 0.2           |
| (1,79)  | 1:8:A:DG:H2' | 1:9:A:DT:H6   | 6        | 0.2           |
| (3,29)  | 1:3:A:DC:C1' | 1:10:A:DG:C1' | 6        | 0.19          |
| (3,29)  | 1:3:A:DC:C1' | 1:10:A:DG:C1' | 14       | 0.19          |
| (3,28)  | 1:2:A:DG:C1' | 1:11:A:DC:C1' | 16       | 0.19          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 18       | 0.19          |
| (2,58)  | 1:3:A:DC:N4  | 1:10:A:DG:O6  | 10       | 0.19          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 1        | 0.19          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 6        | 0.19          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 8        | 0.19          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 15       | 0.19          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 16       | 0.19          |
| (2,55)  | 1:2:A:DG:N2  | 1:11:A:DC:O2  | 8        | 0.19          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 1        | 0.19          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 2        | 0.19          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 4        | 0.19          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 15       | 0.19          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 16       | 0.19          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 17       | 0.19          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 18       | 0.19          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4  | 16       | 0.19          |
| (2,52)  | 1:1:A:DG:N2  | 1:12:A:DC:O2  | 1        | 0.19          |
| (2,52)  | 1:1:A:DG:N2  | 1:12:A:DC:O2  | 16       | 0.19          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 1        | 0.19          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 2        | 0.19          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 5        | 0.19          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 7        | 0.19          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 9        | 0.19          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 10       | 0.19          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 12       | 0.19          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 14       | 0.19          |
| (2,51)  | 1:1:A:DG:N1  | 1:12:A:DC:N3  | 17       | 0.19          |
| (3,29)  | 1:3:A:DC:C1' | 1:10:A:DG:C1' | 11       | 0.18          |
| (3,27)  | 1:1:A:DG:C1' | 1:12:A:DC:C1' | 11       | 0.18          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 8        | 0.18          |
| (2,57)  | 1:3:A:DC:N3  | 1:10:A:DG:N1  | 11       | 0.18          |
| (2,55)  | 1:2:A:DG:N2  | 1:11:A:DC:O2  | 17       | 0.18          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 3        | 0.18          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 8        | 0.18          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 11       | 0.18          |
| (2,54)  | 1:2:A:DG:N1  | 1:11:A:DC:N3  | 12       | 0.18          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4  | 14       | 0.18          |
| (2,52)  | 1:1:A:DG:N2  | 1:12:A:DC:O2  | 11       | 0.18          |
| (2,52)  | 1:1:A:DG:N2  | 1:12:A:DC:O2  | 18       | 0.18          |
| (3,29)  | 1:3:A:DC:C1' | 1:10:A:DG:C1' | 8        | 0.17          |
| (3,27)  | 1:1:A:DG:C1' | 1:12:A:DC:C1' | 15       | 0.17          |
| (2,58)  | 1:3:A:DC:N4  | 1:10:A:DG:O6  | 9        | 0.17          |
| (2,56)  | 1:2:A:DG:O6  | 1:11:A:DC:N4  | 16       | 0.17          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4  | 2        | 0.17          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H71  | 8        | 0.17          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H72  | 8        | 0.17          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H73  | 8        | 0.17          |
| (3,28)  | 1:2:A:DG:C1' | 1:11:A:DC:C1' | 18       | 0.16          |
| (3,27)  | 1:1:A:DG:C1' | 1:12:A:DC:C1' | 9        | 0.16          |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6   | 8        | 0.16          |
| (2,60)  | 1:4:A:DC:N3  | 1:8:A:DG:N1   | 3        | 0.16          |
| (2,55)  | 1:2:A:DG:N2  | 1:11:A:DC:O2  | 9        | 0.16          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4  | 4        | 0.16          |
| (2,49)  | 1:5:A:DG:N2  | 1:7:A:DA:N7   | 10       | 0.16          |
| (2,25)  | 1:5:A:DG:N2  | 1:7:A:DA:N7   | 10       | 0.16          |
| (3,29)  | 1:3:A:DC:C1' | 1:10:A:DG:C1' | 3        | 0.15          |
| (3,29)  | 1:3:A:DC:C1' | 1:10:A:DG:C1' | 4        | 0.15          |
| (3,28)  | 1:2:A:DG:C1' | 1:11:A:DC:C1' | 5        | 0.15          |
| (3,27)  | 1:1:A:DG:C1' | 1:12:A:DC:C1' | 10       | 0.15          |
| (2,61)  | 1:4:A:DC:N4  | 1:8:A:DG:O6   | 15       | 0.15          |
| (2,58)  | 1:3:A:DC:N4  | 1:10:A:DG:O6  | 18       | 0.15          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4  | 1        | 0.15          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4  | 9        | 0.15          |
| (2,53)  | 1:1:A:DG:O6  | 1:12:A:DC:N4  | 12       | 0.15          |
| (2,49)  | 1:5:A:DG:N2  | 1:7:A:DA:N7   | 7        | 0.15          |
| (2,25)  | 1:5:A:DG:N2  | 1:7:A:DA:N7   | 7        | 0.15          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H71  | 9        | 0.15          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H72  | 9        | 0.15          |
| (1,144) | 1:8:A:DG:H8  | 1:9:A:DT:H73  | 9        | 0.15          |
| (1,68)  | 1:7:A:DA:H1' | 1:8:A:DG:H8   | 7        | 0.15          |
| (1,68)  | 1:7:A:DA:H1' | 1:8:A:DG:H8   | 18       | 0.15          |
| (1,11)  | 1:2:A:DG:H3' | 1:2:A:DG:H8   | 8        | 0.15          |
| (3,30)  | 1:4:A:DC:C1' | 1:8:A:DG:C1'  | 6        | 0.14          |
| (3,30)  | 1:4:A:DC:C1' | 1:8:A:DG:C1'  | 17       | 0.14          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (3,29)  | 1:3:A:DC:C1'  | 1:10:A:DG:C1' | 1        | 0.14          |
| (3,29)  | 1:3:A:DC:C1'  | 1:10:A:DG:C1' | 5        | 0.14          |
| (3,28)  | 1:2:A:DG:C1'  | 1:11:A:DC:C1' | 3        | 0.14          |
| (3,28)  | 1:2:A:DG:C1'  | 1:11:A:DC:C1' | 7        | 0.14          |
| (3,27)  | 1:1:A:DG:C1'  | 1:12:A:DC:C1' | 2        | 0.14          |
| (2,61)  | 1:4:A:DC:N4   | 1:8:A:DG:O6   | 9        | 0.14          |
| (2,60)  | 1:4:A:DC:N3   | 1:8:A:DG:N1   | 9        | 0.14          |
| (2,60)  | 1:4:A:DC:N3   | 1:8:A:DG:N1   | 15       | 0.14          |
| (2,55)  | 1:2:A:DG:N2   | 1:11:A:DC:O2  | 10       | 0.14          |
| (2,55)  | 1:2:A:DG:N2   | 1:11:A:DC:O2  | 11       | 0.14          |
| (2,53)  | 1:1:A:DG:O6   | 1:12:A:DC:N4  | 10       | 0.14          |
| (2,53)  | 1:1:A:DG:O6   | 1:12:A:DC:N4  | 15       | 0.14          |
| (2,43)  | 1:4:A:DC:H41  | 1:8:A:DG:O6   | 10       | 0.14          |
| (2,19)  | 1:4:A:DC:H41  | 1:8:A:DG:O6   | 10       | 0.14          |
| (4,2)   | 1:4:A:DC:H2'  | 1:4:A:DC:H6   | 15       | 0.13          |
| (4,2)   | 1:4:A:DC:H2'  | 1:4:A:DC:H6   | 15       | 0.13          |
| (4,2)   | 1:4:A:DC:H2'' | 1:4:A:DC:H6   | 15       | 0.13          |
| (3,28)  | 1:2:A:DG:C1'  | 1:11:A:DC:C1' | 1        | 0.13          |
| (3,27)  | 1:1:A:DG:C1'  | 1:12:A:DC:C1' | 12       | 0.13          |
| (2,58)  | 1:3:A:DC:N4   | 1:10:A:DG:O6  | 1        | 0.13          |
| (2,56)  | 1:2:A:DG:O6   | 1:11:A:DC:N4  | 2        | 0.13          |
| (2,43)  | 1:4:A:DC:H41  | 1:8:A:DG:O6   | 7        | 0.13          |
| (2,19)  | 1:4:A:DC:H41  | 1:8:A:DG:O6   | 7        | 0.13          |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8   | 6        | 0.13          |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8   | 13       | 0.13          |
| (1,79)  | 1:8:A:DG:H2'  | 1:9:A:DT:H6   | 4        | 0.13          |
| (1,79)  | 1:8:A:DG:H2'  | 1:9:A:DT:H6   | 18       | 0.13          |
| (1,68)  | 1:7:A:DA:H1'  | 1:8:A:DG:H8   | 5        | 0.13          |
| (1,68)  | 1:7:A:DA:H1'  | 1:8:A:DG:H8   | 9        | 0.13          |
| (1,68)  | 1:7:A:DA:H1'  | 1:8:A:DG:H8   | 10       | 0.13          |
| (2,61)  | 1:4:A:DC:N4   | 1:8:A:DG:O6   | 7        | 0.12          |
| (2,61)  | 1:4:A:DC:N4   | 1:8:A:DG:O6   | 10       | 0.12          |
| (2,60)  | 1:4:A:DC:N3   | 1:8:A:DG:N1   | 7        | 0.12          |
| (2,58)  | 1:3:A:DC:N4   | 1:10:A:DG:O6  | 13       | 0.12          |
| (2,56)  | 1:2:A:DG:O6   | 1:11:A:DC:N4  | 4        | 0.12          |
| (2,56)  | 1:2:A:DG:O6   | 1:11:A:DC:N4  | 14       | 0.12          |
| (2,55)  | 1:2:A:DG:N2   | 1:11:A:DC:O2  | 12       | 0.12          |
| (2,53)  | 1:1:A:DG:O6   | 1:12:A:DC:N4  | 17       | 0.12          |
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2  | 13       | 0.12          |
| (2,49)  | 1:5:A:DG:N2   | 1:7:A:DA:N7   | 9        | 0.12          |
| (2,47)  | 1:4:A:DC:O2   | 1:8:A:DG:H21  | 10       | 0.12          |
| (2,25)  | 1:5:A:DG:N2   | 1:7:A:DA:N7   | 9        | 0.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (2,23)  | 1:4:A:DC:O2   | 1:8:A:DG:H21  | 10       | 0.12          |
| (1,114) | 1:2:A:DG:H2'  | 1:3:A:DC:H6   | 6        | 0.12          |
| (1,42)  | 1:5:A:DG:H1'  | 1:6:A:DC:H5   | 9        | 0.12          |
| (3,29)  | 1:3:A:DC:C1'  | 1:10:A:DG:C1' | 12       | 0.11          |
| (3,29)  | 1:3:A:DC:C1'  | 1:10:A:DG:C1' | 13       | 0.11          |
| (3,29)  | 1:3:A:DC:C1'  | 1:10:A:DG:C1' | 18       | 0.11          |
| (3,28)  | 1:2:A:DG:C1'  | 1:11:A:DC:C1' | 14       | 0.11          |
| (2,61)  | 1:4:A:DC:N4   | 1:8:A:DG:O6   | 3        | 0.11          |
| (2,60)  | 1:4:A:DC:N3   | 1:8:A:DG:N1   | 10       | 0.11          |
| (2,56)  | 1:2:A:DG:O6   | 1:11:A:DC:N4  | 1        | 0.11          |
| (1,79)  | 1:8:A:DG:H2'  | 1:9:A:DT:H6   | 2        | 0.11          |
| (1,79)  | 1:8:A:DG:H2'  | 1:9:A:DT:H6   | 15       | 0.11          |
| (1,68)  | 1:7:A:DA:H1'  | 1:8:A:DG:H8   | 2        | 0.11          |
| (1,68)  | 1:7:A:DA:H1'  | 1:8:A:DG:H8   | 11       | 0.11          |
| (1,42)  | 1:5:A:DG:H1'  | 1:6:A:DC:H5   | 7        | 0.11          |
| (1,42)  | 1:5:A:DG:H1'  | 1:6:A:DC:H5   | 10       | 0.11          |
| (1,41)  | 1:5:A:DG:H3'  | 1:5:A:DG:H8   | 5        | 0.11          |
| (1,41)  | 1:5:A:DG:H3'  | 1:5:A:DG:H8   | 12       | 0.11          |
| (1,11)  | 1:2:A:DG:H3'  | 1:2:A:DG:H8   | 9        | 0.11          |
| (1,11)  | 1:2:A:DG:H3'  | 1:2:A:DG:H8   | 10       | 0.11          |
| (1,11)  | 1:2:A:DG:H3'  | 1:2:A:DG:H8   | 12       | 0.11          |
| (1,11)  | 1:2:A:DG:H3'  | 1:2:A:DG:H8   | 17       | 0.11          |
| (4,2)   | 1:4:A:DC:H2'  | 1:4:A:DC:H6   | 9        | 0.1           |
| (4,2)   | 1:4:A:DC:H2'  | 1:4:A:DC:H6   | 9        | 0.1           |
| (4,2)   | 1:4:A:DC:H2'' | 1:4:A:DC:H6   | 9        | 0.1           |
| (3,29)  | 1:3:A:DC:C1'  | 1:10:A:DG:C1' | 15       | 0.1           |
| (3,28)  | 1:2:A:DG:C1'  | 1:11:A:DC:C1' | 4        | 0.1           |
| (2,59)  | 1:3:A:DC:O2   | 1:10:A:DG:N2  | 7        | 0.1           |
| (2,58)  | 1:3:A:DC:N4   | 1:10:A:DG:O6  | 17       | 0.1           |
| (2,52)  | 1:1:A:DG:N2   | 1:12:A:DC:O2  | 3        | 0.1           |
| (2,49)  | 1:5:A:DG:N2   | 1:7:A:DA:N7   | 14       | 0.1           |
| (2,25)  | 1:5:A:DG:N2   | 1:7:A:DA:N7   | 14       | 0.1           |
| (1,139) | 1:7:A:DA:H2'  | 1:7:A:DA:H8   | 8        | 0.1           |
| (1,42)  | 1:5:A:DG:H1'  | 1:6:A:DC:H5   | 14       | 0.1           |
| (1,41)  | 1:5:A:DG:H3'  | 1:5:A:DG:H8   | 2        | 0.1           |
| (1,41)  | 1:5:A:DG:H3'  | 1:5:A:DG:H8   | 10       | 0.1           |
| (1,41)  | 1:5:A:DG:H3'  | 1:5:A:DG:H8   | 11       | 0.1           |
| (1,41)  | 1:5:A:DG:H3'  | 1:5:A:DG:H8   | 18       | 0.1           |

## 10 Dihedral-angle violation analysis [i](#)

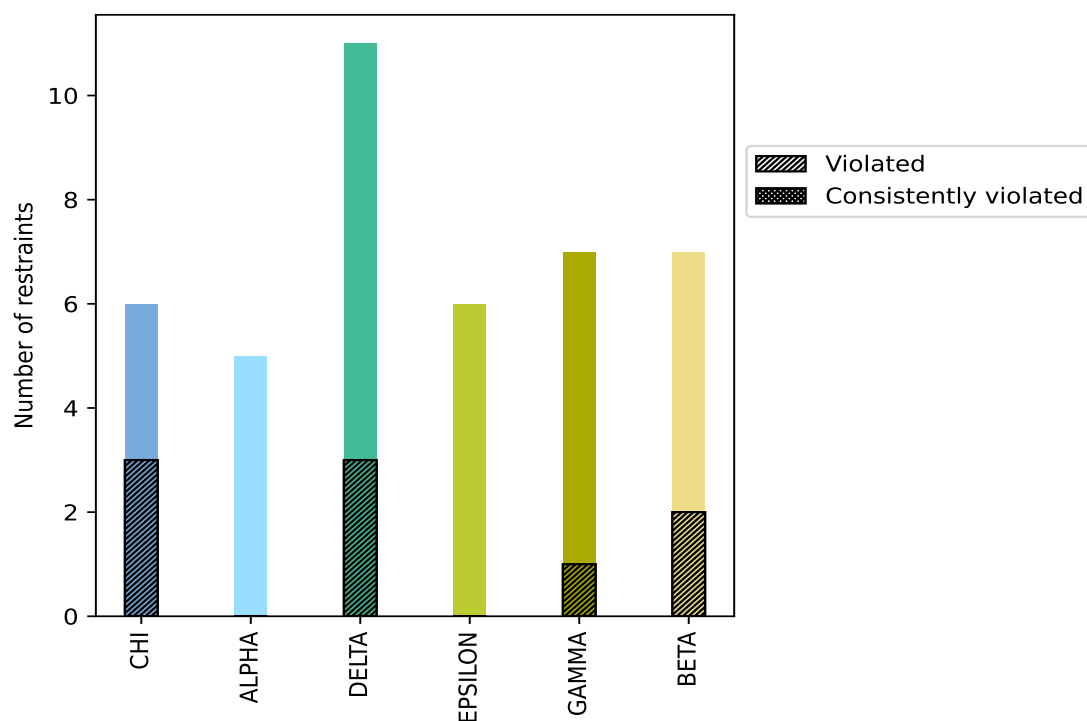
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

| Angle 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> |
| CHI        | 6     | 14.3           | 3                     | 50.0           | 7.1            | 0                                  | 0.0            | 0.0            |
| ALPHA      | 5     | 11.9           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| DELTA      | 11    | 26.2           | 3                     | 27.3           | 7.1            | 0                                  | 0.0            | 0.0            |
| EPSILON    | 6     | 14.3           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| GAMMA      | 7     | 16.7           | 1                     | 14.3           | 2.4            | 0                                  | 0.0            | 0.0            |
| BETA       | 7     | 16.7           | 2                     | 28.6           | 4.8            | 0                                  | 0.0            | 0.0            |
| Total      | 42    | 100.0          | 9                     | 21.4           | 21.4           | 0                                  | 0.0            | 0.0            |

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

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their

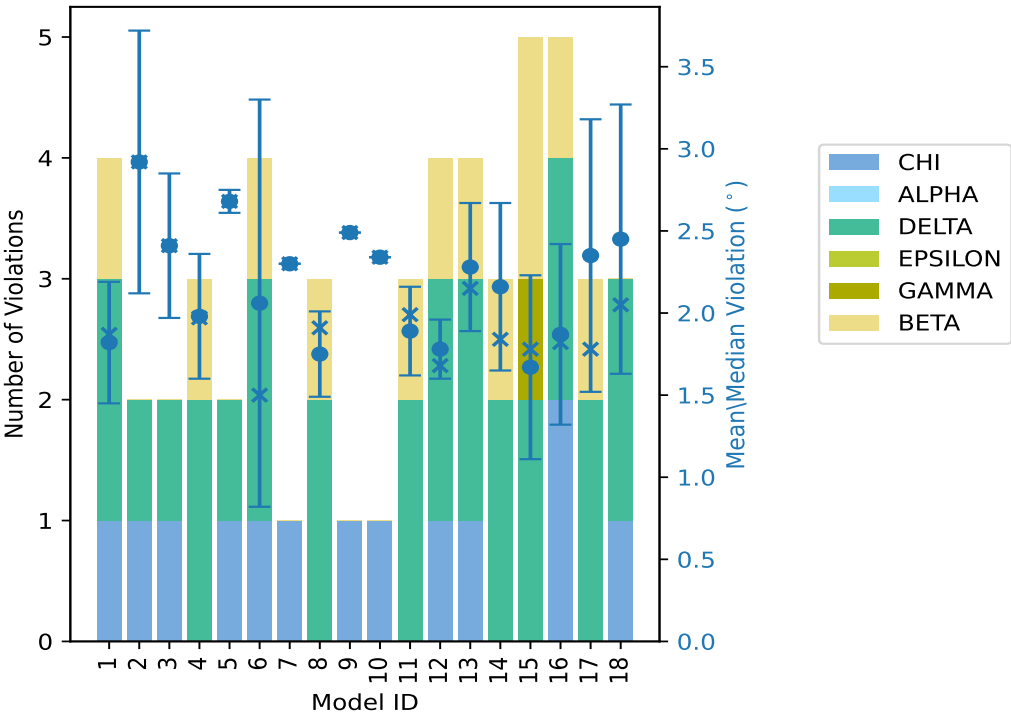
respective categories

## 10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

| Model ID | Number of violations |       |       |         |       |      |       | Mean (°) | Max (°) | S |
|----------|----------------------|-------|-------|---------|-------|------|-------|----------|---------|---|
|          | CHI                  | ALPHA | DELTA | EPSILON | GAMMA | BETA | Total |          |         |   |
| 1        | 1                    | 0     | 2     | 0       | 0     | 1    | 4     | 1.82     | 2.3     |   |
| 2        | 1                    | 0     | 1     | 0       | 0     | 0    | 2     | 2.92     | 3.71    |   |
| 3        | 1                    | 0     | 1     | 0       | 0     | 0    | 2     | 2.41     | 2.85    |   |
| 4        | 0                    | 0     | 2     | 0       | 0     | 1    | 3     | 1.98     | 2.45    |   |
| 5        | 1                    | 0     | 1     | 0       | 0     | 0    | 2     | 2.68     | 2.75    |   |
| 6        | 1                    | 0     | 2     | 0       | 0     | 1    | 4     | 2.06     | 4.19    |   |
| 7        | 1                    | 0     | 0     | 0       | 0     | 0    | 1     | 2.3      | 2.3     |   |
| 8        | 0                    | 0     | 2     | 0       | 0     | 1    | 3     | 1.75     | 1.95    |   |
| 9        | 1                    | 0     | 0     | 0       | 0     | 0    | 1     | 2.49     | 2.49    |   |
| 10       | 1                    | 0     | 0     | 0       | 0     | 0    | 1     | 2.34     | 2.34    |   |
| 11       | 0                    | 0     | 2     | 0       | 0     | 1    | 3     | 1.89     | 2.16    |   |
| 12       | 1                    | 0     | 2     | 0       | 0     | 1    | 4     | 1.78     | 2.09    |   |
| 13       | 1                    | 0     | 2     | 0       | 0     | 1    | 4     | 2.28     | 2.92    |   |
| 14       | 0                    | 0     | 2     | 0       | 0     | 1    | 3     | 2.16     | 2.88    |   |
| 15       | 0                    | 0     | 2     | 0       | 1     | 2    | 5     | 1.67     | 2.56    |   |
| 16       | 2                    | 0     | 2     | 0       | 0     | 1    | 5     | 1.87     | 2.78    |   |
| 17       | 0                    | 0     | 2     | 0       | 0     | 1    | 3     | 2.35     | 3.53    |   |
| 18       | 1                    | 0     | 2     | 0       | 0     | 0    | 3     | 2.45     | 3.6     |   |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in very 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 ensemble.

| Number of violated restraints |       |       |         |       |      |       | Fraction of the ensemble |      |
|-------------------------------|-------|-------|---------|-------|------|-------|--------------------------|------|
| CHI                           | ALPHA | DELTA | EPSILON | GAMMA | BETA | Total | Count <sup>1</sup>       | %    |
| 1                             | 0     | 1     | 0       | 1     | 1    | 4     | 1                        | 5.6  |
| 0                             | 0     | 0     | 0       | 0     | 0    | 0     | 2                        | 11.1 |
| 0                             | 0     | 0     | 0       | 0     | 0    | 0     | 3                        | 16.7 |
| 0                             | 0     | 0     | 0       | 0     | 0    | 0     | 4                        | 22.2 |
| 1                             | 0     | 0     | 0       | 0     | 0    | 1     | 5                        | 27.8 |
| 0                             | 0     | 0     | 0       | 0     | 0    | 0     | 6                        | 33.3 |
| 1                             | 0     | 0     | 0       | 0     | 0    | 1     | 7                        | 38.9 |
| 0                             | 0     | 0     | 0       | 0     | 0    | 0     | 8                        | 44.4 |
| 0                             | 0     | 0     | 0       | 0     | 0    | 0     | 9                        | 50.0 |
| 0                             | 0     | 0     | 0       | 0     | 0    | 0     | 10                       | 55.6 |
| 0                             | 0     | 1     | 0       | 0     | 1    | 2     | 11                       | 61.1 |

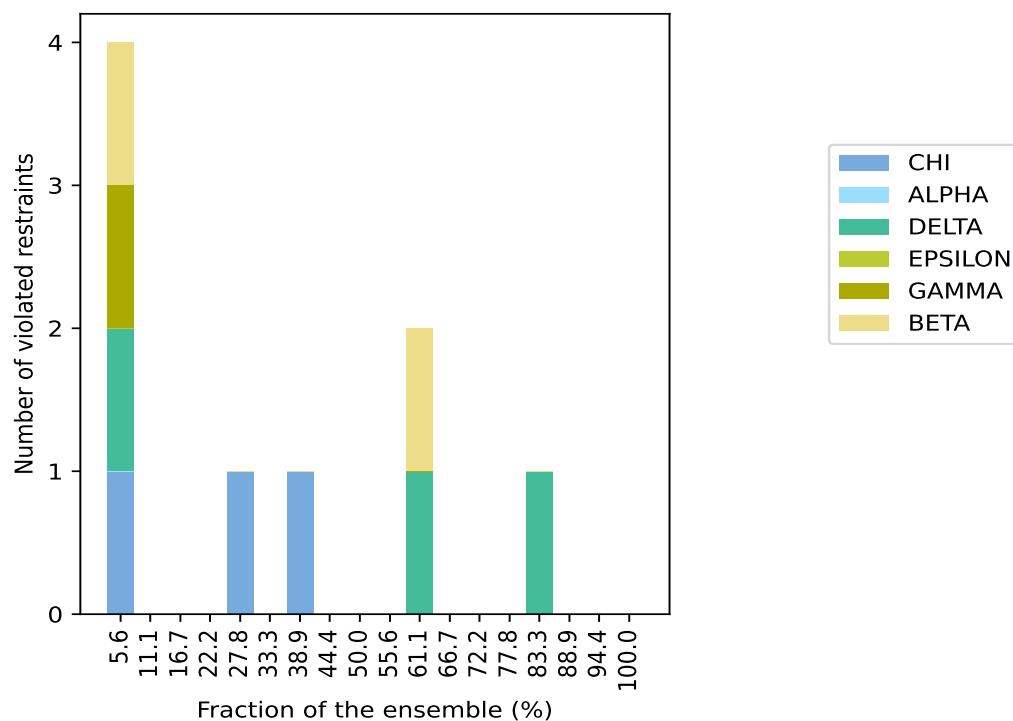
Continued on next page...

Continued from previous page...

| CHI | Number of violated restraints |       |         |       |      |       | Fraction of the ensemble |       |
|-----|-------------------------------|-------|---------|-------|------|-------|--------------------------|-------|
|     | ALPHA                         | DELTA | EPSILON | GAMMA | BETA | Total | Count <sup>1</sup>       | %     |
| 0   | 0                             | 0     | 0       | 0     | 0    | 0     | 12                       | 66.7  |
| 0   | 0                             | 0     | 0       | 0     | 0    | 0     | 13                       | 72.2  |
| 0   | 0                             | 0     | 0       | 0     | 0    | 0     | 14                       | 77.8  |
| 0   | 0                             | 1     | 0       | 0     | 0    | 1     | 15                       | 83.3  |
| 0   | 0                             | 0     | 0       | 0     | 0    | 0     | 16                       | 88.9  |
| 0   | 0                             | 0     | 0       | 0     | 0    | 0     | 17                       | 94.4  |
| 0   | 0                             | 0     | 0       | 0     | 0    | 0     | 18                       | 100.0 |

<sup>1</sup> Number of models with violations

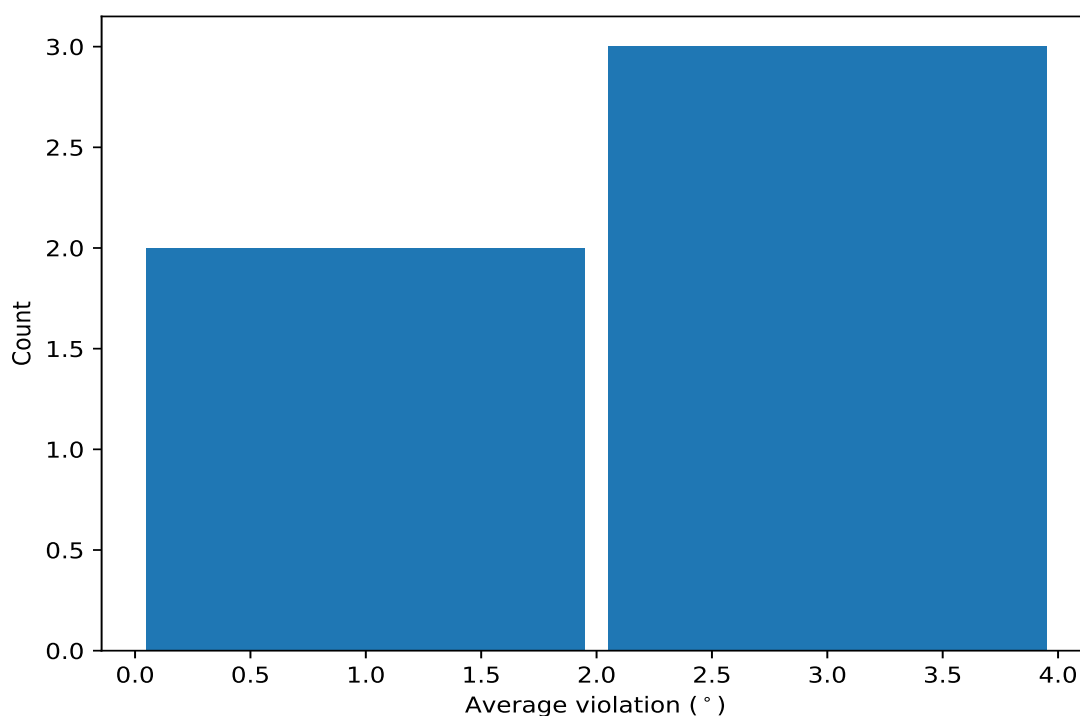
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



#### 10.4.2 Table: Most violated dihedral-angle 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.

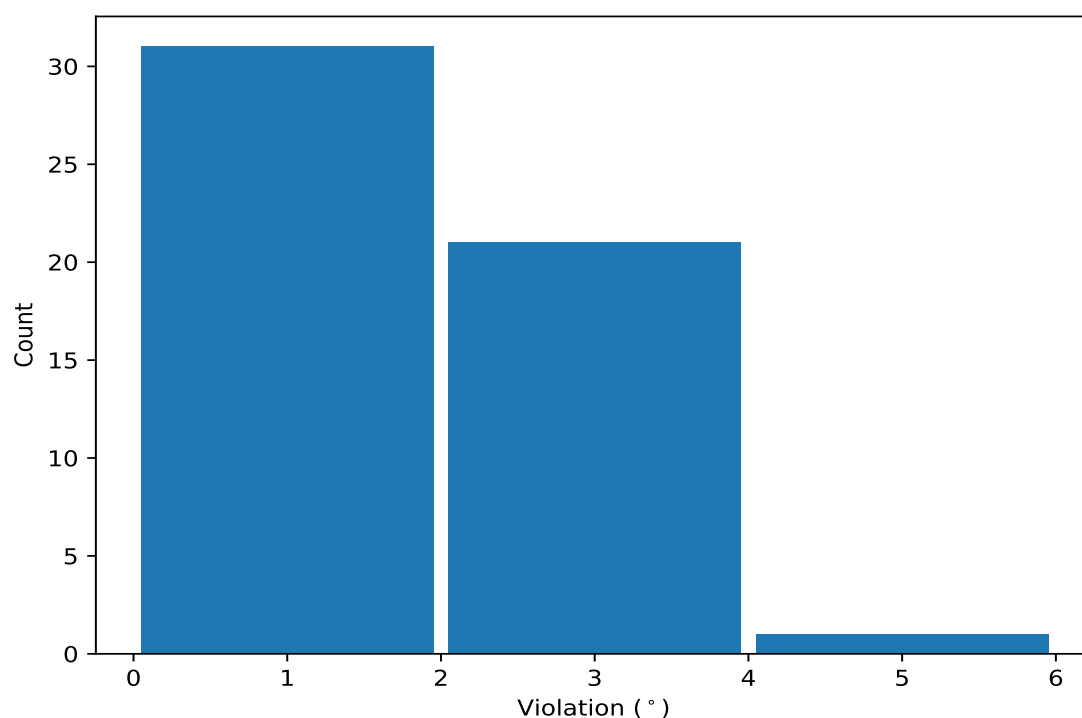
| Key    | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|---------------|---------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 15                  | 2.18 | 0.6             | 1.99   |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 11                  | 1.94 | 0.31            | 1.91   |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 11                  | 1.75 | 0.18            | 1.82   |
| (1,32) | 1:10:A:DG:O4' | 1:10:A:DG:C1' | 1:10:A:DG:N9  | 1:10:A:DG:C4  | 7                   | 2.64 | 0.5             | 2.49   |
| (1,28) | 1:8:A:DG:O4'  | 1:8:A:DG:C1'  | 1:8:A:DG:N9   | 1:8:A:DG:C4   | 5                   | 2.38 | 1.03            | 2.02   |

<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

### 10.5 All violated dihedral-angle restraints [i](#)

#### 10.5.1 Histogram : Distribution of violations [i](#)

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



### 10.5.2 Table: All violated dihedral-angle restraints [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.

| Key    | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|--------|---------------|---------------|---------------|---------------|----------|---------------|
| (1,28) | 1:8:A:DG:O4'  | 1:8:A:DG:C1'  | 1:8:A:DG:N9   | 1:8:A:DG:C4   | 6        | 4.19          |
| (1,32) | 1:10:A:DG:O4' | 1:10:A:DG:C1' | 1:10:A:DG:N9  | 1:10:A:DG:C4  | 2        | 3.71          |
| (1,31) | 1:10:A:DG:C5' | 1:10:A:DG:C4' | 1:10:A:DG:C3' | 1:10:A:DG:O3' | 18       | 3.6           |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 17       | 3.53          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 13       | 2.92          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 14       | 2.88          |
| (1,32) | 1:10:A:DG:O4' | 1:10:A:DG:C1' | 1:10:A:DG:N9  | 1:10:A:DG:C4  | 3        | 2.85          |
| (1,28) | 1:8:A:DG:O4'  | 1:8:A:DG:C1'  | 1:8:A:DG:N9   | 1:8:A:DG:C4   | 16       | 2.78          |
| (1,32) | 1:10:A:DG:O4' | 1:10:A:DG:C1' | 1:10:A:DG:N9  | 1:10:A:DG:C4  | 5        | 2.75          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 5        | 2.6           |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 15       | 2.56          |
| (1,32) | 1:10:A:DG:O4' | 1:10:A:DG:C1' | 1:10:A:DG:N9  | 1:10:A:DG:C4  | 9        | 2.49          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 4        | 2.45          |
| (1,32) | 1:10:A:DG:O4' | 1:10:A:DG:C1' | 1:10:A:DG:N9  | 1:10:A:DG:C4  | 10       | 2.34          |
| (1,32) | 1:10:A:DG:O4' | 1:10:A:DG:C1' | 1:10:A:DG:N9  | 1:10:A:DG:C4  | 7        | 2.3           |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 1        | 2.3           |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 13       | 2.28          |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 11       | 2.16          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 2        | 2.12          |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 12       | 2.09          |
| (1,32) | 1:10:A:DG:O4' | 1:10:A:DG:C1' | 1:10:A:DG:N9  | 1:10:A:DG:C4  | 18       | 2.05          |

Continued on next page...

Continued from previous page...

| Key    | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|--------|---------------|---------------|---------------|---------------|----------|---------------|
| (1,28) | 1:8:A:DG:O4'  | 1:8:A:DG:C1'  | 1:8:A:DG:N9   | 1:8:A:DG:C4   | 13       | 2.02          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 11       | 1.99          |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 4        | 1.97          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 3        | 1.97          |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 16       | 1.95          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 8        | 1.95          |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 8        | 1.91          |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 13       | 1.9           |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1        | 1.89          |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 15       | 1.88          |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 1        | 1.85          |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 14       | 1.84          |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 16       | 1.82          |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 17       | 1.78          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 15       | 1.78          |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 14       | 1.76          |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 17       | 1.74          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 16       | 1.74          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 18       | 1.71          |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 12       | 1.69          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 12       | 1.67          |
| (1,28) | 1:8:A:DG:O4'  | 1:8:A:DG:C1'  | 1:8:A:DG:N9   | 1:8:A:DG:C4   | 12       | 1.65          |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 11       | 1.53          |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 4        | 1.52          |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 6        | 1.52          |
| (1,36) | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 1:11:A:DC:C3' | 1:11:A:DC:O3' | 6        | 1.49          |
| (1,34) | 1:11:A:DC:P   | 1:11:A:DC:O5' | 1:11:A:DC:C5' | 1:11:A:DC:C4' | 8        | 1.38          |
| (1,28) | 1:8:A:DG:O4'  | 1:8:A:DG:C1'  | 1:8:A:DG:N9   | 1:8:A:DG:C4   | 1        | 1.26          |
| (1,17) | 1:4:A:DC:P    | 1:4:A:DC:O5'  | 1:4:A:DC:C5'  | 1:4:A:DC:C4'  | 15       | 1.1           |
| (1,4)  | 1:1:A:DG:O4'  | 1:1:A:DG:C1'  | 1:1:A:DG:N9   | 1:1:A:DG:C4   | 16       | 1.06          |
| (1,27) | 1:8:A:DG:C5'  | 1:8:A:DG:C4'  | 1:8:A:DG:C3'  | 1:8:A:DG:O3'  | 6        | 1.05          |
| (1,18) | 1:4:A:DC:O5'  | 1:4:A:DC:C5'  | 1:4:A:DC:C4'  | 1:4:A:DC:C3'  | 15       | 1.03          |