



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 01:56 AM UTC

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BMRB ID : 30026  
Title : NMR structure of the 5'-terminal hairpin of the 7SK snRNA  
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Deposited on : 2016-02-25

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

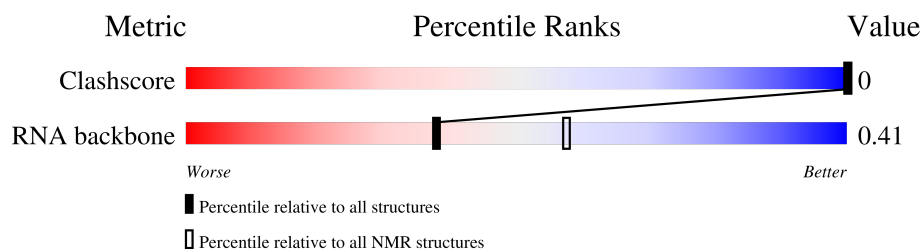
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 30%.

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                     |
| RNA backbone | 8273                        | 777                       |

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     | 57     | <br>77% 23%      |

## 2 Ensemble composition and analysis ⓘ

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1820 atoms, of which 614 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 7SK snRNA.

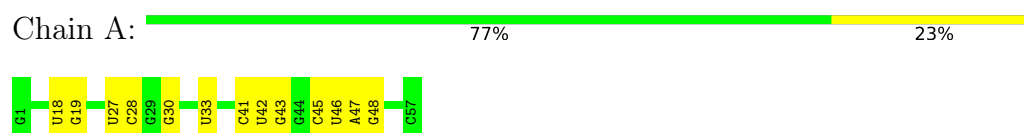
| Mol | Chain | Residues | Atoms |     |     |     |     |    | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|-------|
| 1   | A     | 57       | Total | C   | H   | N   | O   | P  | 0     |
|     |       |          | 1820  | 538 | 614 | 207 | 405 | 56 |       |

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

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

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: 7SK snRNA

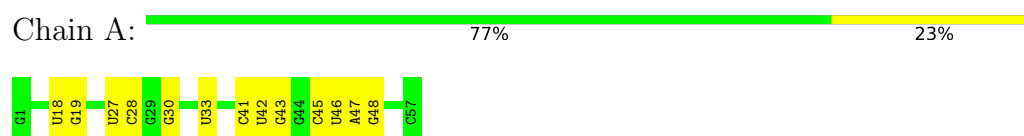


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

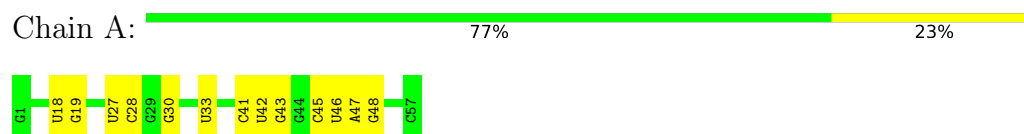
#### 4.2.1 Score per residue for model 1

- Molecule 1: 7SK snRNA



#### 4.2.2 Score per residue for model 2

- Molecule 1: 7SK snRNA



### 4.2.3 Score per residue for model 3

- Molecule 1: 7SK snRNA

Chain A:  77% 23%



### 4.2.4 Score per residue for model 4

- Molecule 1: 7SK snRNA

Chain A:  77% 23%



### 4.2.5 Score per residue for model 5

- Molecule 1: 7SK snRNA

Chain A:  77% 23%



### 4.2.6 Score per residue for model 6

- Molecule 1: 7SK snRNA

Chain A:  77% 23%



### 4.2.7 Score per residue for model 7

- Molecule 1: 7SK snRNA

Chain A:  77% 23%



#### 4.2.8 Score per residue for model 8

- Molecule 1: 7SK snRNA

Chain A:  77% 23%



#### 4.2.9 Score per residue for model 9

- Molecule 1: 7SK snRNA

Chain A:  77% 23%



#### 4.2.10 Score per residue for model 10

- Molecule 1: 7SK snRNA

Chain A:  77% 23%



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations, lowest energy*.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| CNS           | refinement     |         |

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                       | 347            |
| Number of shifts mapped to atoms             | 347            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 30%            |

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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   | 12060 | 6140     | 6150     | -       |

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](#)

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers | Suiteness |
|-----|-------|---------------|-------------------|-----------------|-----------|
| 1   | A     | 56/57 (98%)   | 12±0 (21±0%)      | 7±0 (12±0%)     | 0.51±0.00 |
| All | All   | 560/570 (98%) | 120 (21%)         | 70 (12%)        | 0.51      |

The overall RNA backbone suiteness is 0.41.

All unique RNA backbone outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 18  | U    | 10             |
| 1   | A     | 19  | G    | 10             |
| 1   | A     | 28  | C    | 10             |
| 1   | A     | 30  | G    | 10             |
| 1   | A     | 33  | U    | 10             |
| 1   | A     | 41  | C    | 10             |
| 1   | A     | 42  | U    | 10             |
| 1   | A     | 43  | G    | 10             |
| 1   | A     | 45  | C    | 10             |
| 1   | A     | 46  | U    | 10             |
| 1   | A     | 47  | A    | 10             |
| 1   | A     | 48  | G    | 10             |

All unique RNA pucker outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 18  | U    | 10             |
| 1   | A     | 27  | U    | 10             |
| 1   | A     | 41  | C    | 10             |
| 1   | A     | 42  | U    | 10             |
| 1   | A     | 45  | C    | 10             |
| 1   | A     | 46  | U    | 10             |
| 1   | A     | 47  | A    | 10             |

## 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 30% for the well-defined parts and 30% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *ChemicalShifts160225.rtf*

#### 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                  | 347 |
| Number of shifts mapped to atoms        | 347 |
| 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 30%, i.e. 324 atoms were assigned a chemical shift out of a possible 1074. 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   | 123/627 (20%)  | 104/342 (30%)  | 19/285 (7%)     | 0/0 (—%)        |
| Base    | 201/447 (45%)  | 138/276 (50%)  | 40/95 (42%)     | 23/76 (30%)     |
| Overall | 324/1074 (30%) | 242/618 (39%)  | 59/380 (16%)    | 23/76 (30%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 30%, i.e. 324 atoms were assigned a chemical shift out of a possible 1074. 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   | 123/627 (20%)  | 104/342 (30%)        | 19/285 (7%)           | 0/0 (—%)              |
| Base    | 201/447 (45%)  | 138/276 (50%)        | 40/95 (42%)           | 23/76 (30%)           |
| Overall | 324/1074 (30%) | 242/618 (39%)        | 59/380 (16%)          | 23/76 (30%)           |

#### 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     | 28  | C    | H5'  | 2.72              | 2.74 – 5.79                | -5.1    |

#### 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                                | 880   |
| Intra-residue ( $ i-j =0$ )                              | 357   |
| Sequential ( $ i-j =1$ )                                 | 295   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 28    |
| Long range ( $ i-j \geq 5$ )                             | 82    |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 118   |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 484   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 23.9  |
| Number of long range restraints per residue <sup>1</sup> | 3.4   |

<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)  | 30.7                                   | 0.2     |
| 0.2-0.5 (Medium) | 68.1                                   | 0.5     |
| >0.5 (Large)     | 45.5                                   | 1.72    |

### 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)   | 15.4                                   | 2.88    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

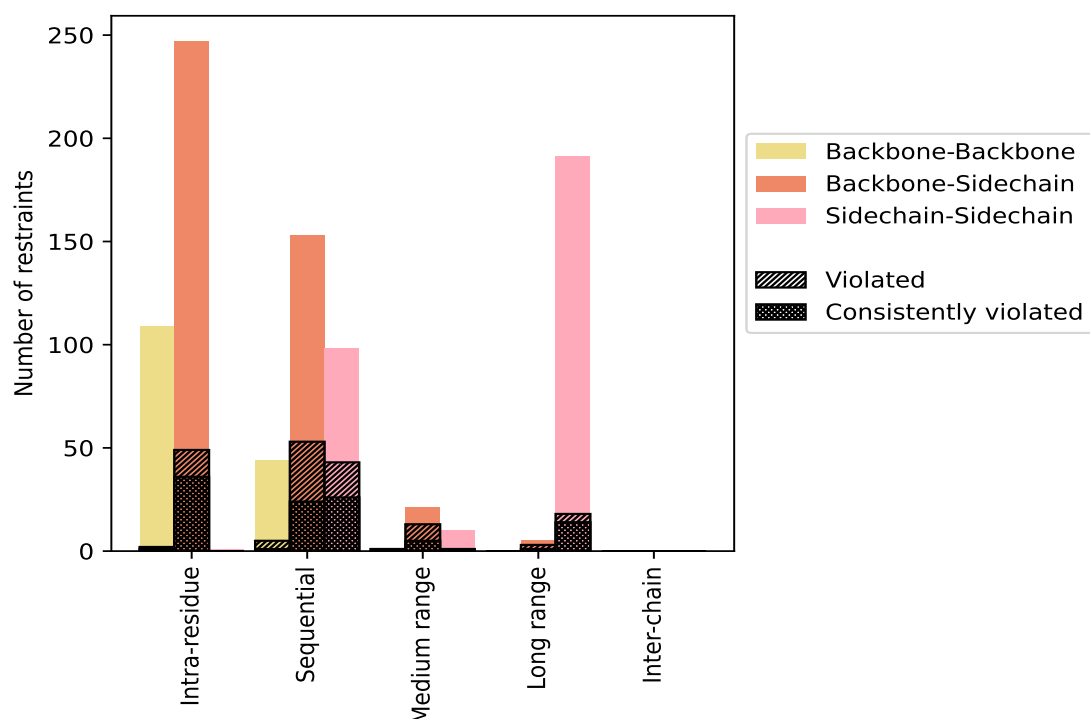
### 9.1 Summary of distance violations ⓘ

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="#">357</a> | <a href="#">40.6</a>  | <a href="#">51</a>    | <a href="#">14.3</a> | <a href="#">5.8</a>  | <a href="#">37</a>                 | <a href="#">10.4</a> | <a href="#">4.2</a>  |
| Backbone-Backbone                                          | 109                 | 12.4                  | 2                     | 1.8                  | 0.2                  | 1                                  | 0.9                  | 0.1                  |
| Backbone-Sidechain                                         | 247                 | 28.1                  | 49                    | 19.8                 | 5.6                  | 36                                 | 14.6                 | 4.1                  |
| Sidechain-Sidechain                                        | 1                   | 0.1                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">295</a> | <a href="#">33.5</a>  | <a href="#">101</a>   | <a href="#">34.2</a> | <a href="#">11.5</a> | <a href="#">51</a>                 | <a href="#">17.3</a> | <a href="#">5.8</a>  |
| Backbone-Backbone                                          | 44                  | 5.0                   | 5                     | 11.4                 | 0.6                  | 1                                  | 2.3                  | 0.1                  |
| Backbone-Sidechain                                         | 153                 | 17.4                  | 53                    | 34.6                 | 6.0                  | 24                                 | 15.7                 | 2.7                  |
| Sidechain-Sidechain                                        | 98                  | 11.1                  | 43                    | 43.9                 | 4.9                  | 26                                 | 26.5                 | 3.0                  |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">28</a>  | <a href="#">3.2</a>   | <a href="#">15</a>    | <a href="#">53.6</a> | <a href="#">1.7</a>  | <a href="#">7</a>                  | <a href="#">25.0</a> | <a href="#">0.8</a>  |
| Backbone-Backbone                                          | 1                   | 0.1                   | 1                     | 100.0                | 0.1                  | 1                                  | 100.0                | 0.1                  |
| Backbone-Sidechain                                         | 20                  | 2.3                   | 13                    | 65.0                 | 1.5                  | 5                                  | 25.0                 | 0.6                  |
| Sidechain-Sidechain                                        | 7                   | 0.8                   | 1                     | 14.3                 | 0.1                  | 1                                  | 14.3                 | 0.1                  |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">82</a>  | <a href="#">9.3</a>   | <a href="#">21</a>    | <a href="#">25.6</a> | <a href="#">2.4</a>  | <a href="#">15</a>                 | <a href="#">18.3</a> | <a href="#">1.7</a>  |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Backbone-Sidechain                                         | 5                   | 0.6                   | 3                     | 60.0                 | 0.3                  | 1                                  | 20.0                 | 0.1                  |
| Sidechain-Sidechain                                        | 77                  | 8.8                   | 18                    | 23.4                 | 2.0                  | 14                                 | 18.2                 | 1.6                  |
| <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="#">118</a> | <a href="#">13.4</a>  | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| <a href="#">Total</a>                                      | <a href="#">880</a> | <a href="#">100.0</a> | <a href="#">188</a>   | <a href="#">21.4</a> | <a href="#">21.4</a> | <a href="#">110</a>                | <a href="#">12.5</a> | <a href="#">12.5</a> |
| Backbone-Backbone                                          | 154                 | 17.5                  | 8                     | 5.2                  | 0.9                  | 3                                  | 1.9                  | 0.3                  |
| Backbone-Sidechain                                         | 426                 | 48.4                  | 118                   | 27.7                 | 13.4                 | 66                                 | 15.5                 | 7.5                  |
| Sidechain-Sidechain                                        | 300                 | 34.1                  | 62                    | 20.7                 | 7.0                  | 41                                 | 13.7                 | 4.7                  |

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

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



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

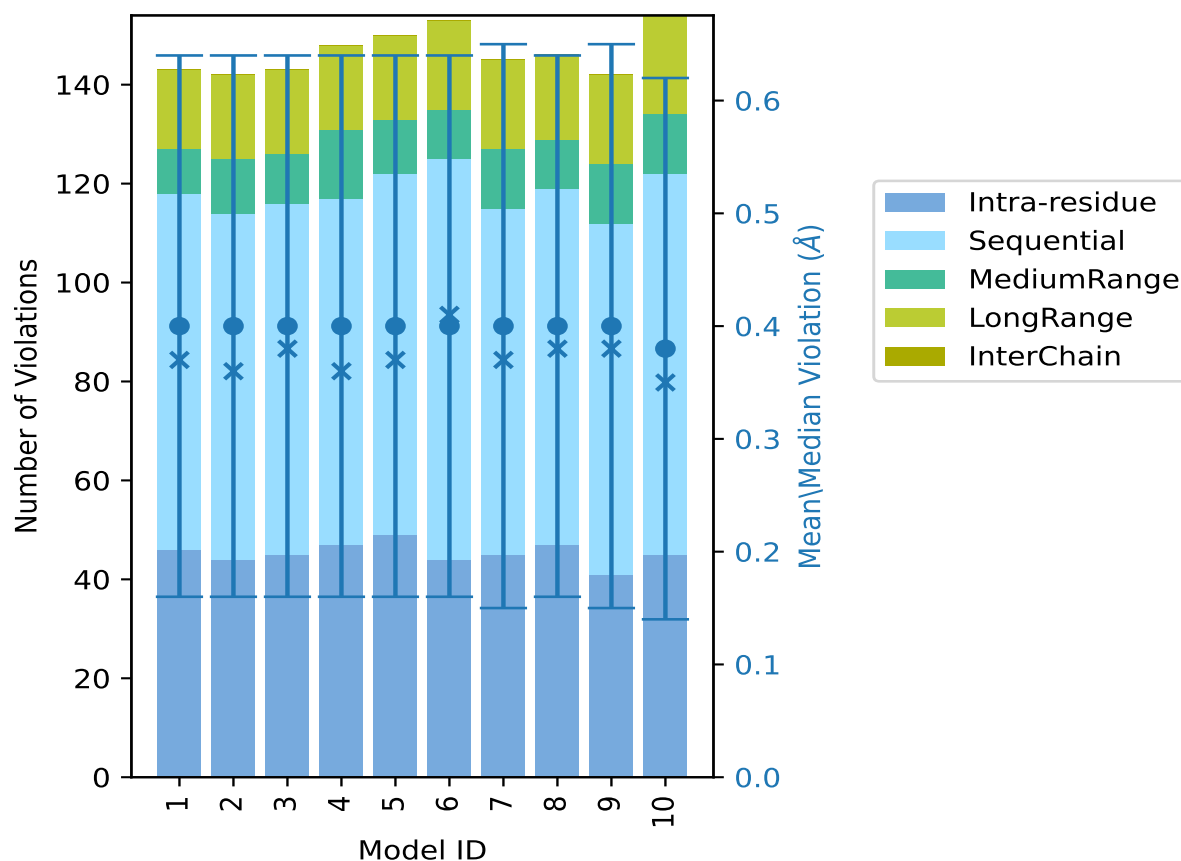
## 9.2 Distance violation statistics for each model [i](#)

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 46                   | 72              | 9               | 16              | 0               | 143   | 0.4      | 1.7     | 0.24                | 0.37       |
| 2        | 44                   | 70              | 11              | 17              | 0               | 142   | 0.4      | 1.7     | 0.24                | 0.36       |
| 3        | 45                   | 71              | 10              | 17              | 0               | 143   | 0.4      | 1.67    | 0.24                | 0.38       |
| 4        | 47                   | 70              | 14              | 17              | 0               | 148   | 0.4      | 1.7     | 0.24                | 0.36       |
| 5        | 49                   | 73              | 11              | 17              | 0               | 150   | 0.4      | 1.68    | 0.24                | 0.37       |
| 6        | 44                   | 81              | 10              | 18              | 0               | 153   | 0.4      | 1.67    | 0.24                | 0.41       |
| 7        | 45                   | 70              | 12              | 18              | 0               | 145   | 0.4      | 1.69    | 0.25                | 0.37       |
| 8        | 47                   | 72              | 10              | 17              | 0               | 146   | 0.4      | 1.72    | 0.24                | 0.38       |
| 9        | 41                   | 71              | 12              | 18              | 0               | 142   | 0.4      | 1.68    | 0.25                | 0.38       |
| 10       | 45                   | 77              | 12              | 20              | 0               | 154   | 0.38     | 1.68    | 0.24                | 0.35       |

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 574(IR:306, SQ:194, MR:13, LR:61, 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>       | %    |
| 2                             | 13              | 1               | 2               | 0               | 18    | 1                        | 10.0 |
| 0                             | 7               | 0               | 1               | 0               | 8     | 2                        | 20.0 |
| 2                             | 5               | 1               | 0               | 0               | 8     | 3                        | 30.0 |

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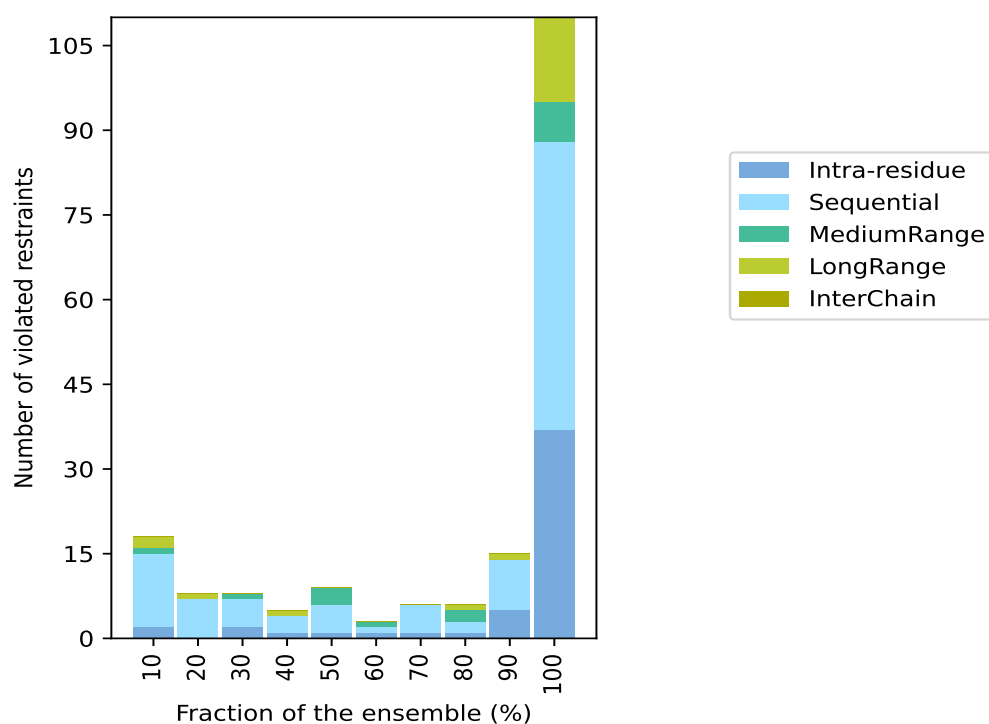
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 1                             | 3               | 0               | 1               | 0               | 5     | 4                        | 40.0  |
| 1                             | 5               | 3               | 0               | 0               | 9     | 5                        | 50.0  |
| 1                             | 1               | 1               | 0               | 0               | 3     | 6                        | 60.0  |
| 1                             | 5               | 0               | 0               | 0               | 6     | 7                        | 70.0  |
| 1                             | 2               | 2               | 1               | 0               | 6     | 8                        | 80.0  |
| 5                             | 9               | 0               | 1               | 0               | 15    | 9                        | 90.0  |
| 37                            | 51              | 7               | 15              | 0               | 110   | 10                       | 100.0 |

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

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

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

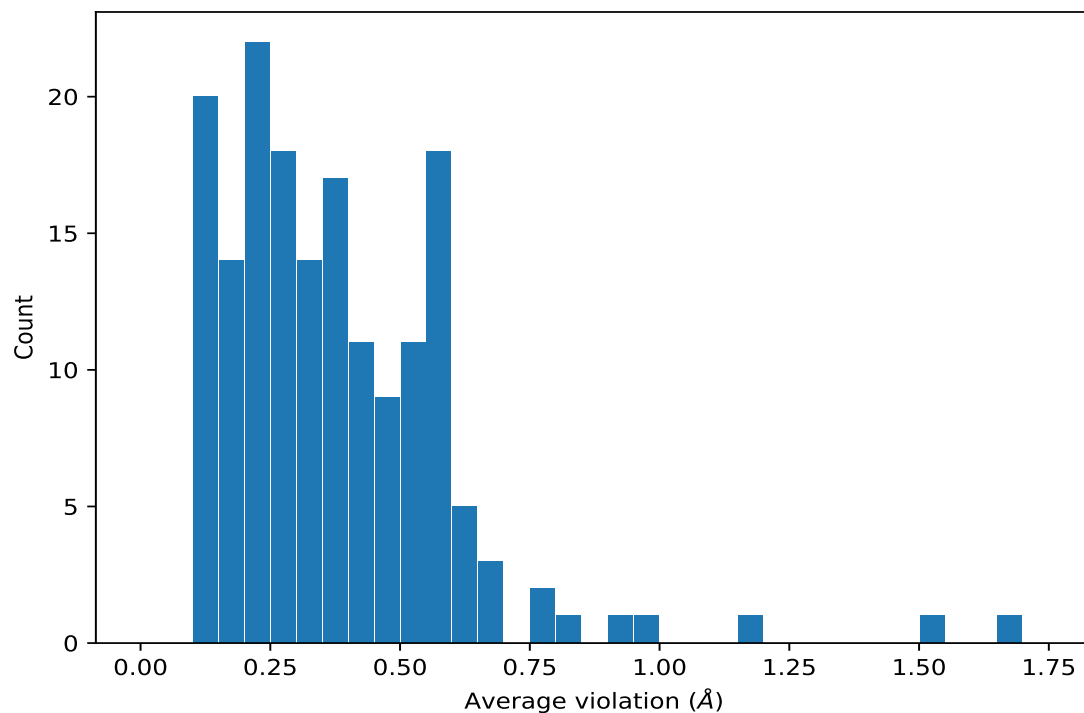


## 9.4 Most violated distance restraints in the ensemble ⓘ

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

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

in the ensemble



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

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

| Key     | Atom-1       | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|--------------|---------------|---------------------|----------|---------------------|------------|
| (1,28)  | 1:1:A:G:H1   | 1:56:A:C:H42  | 10                  | 1.69     | 0.02                | 1.68       |
| (1,626) | 1:49:A:G:H1  | 1:50:A:C:H5   | 10                  | 1.54     | 0.03                | 1.54       |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41  | 10                  | 1.16     | 0.02                | 1.16       |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5    | 10                  | 0.98     | 0.03                | 0.98       |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2'  | 10                  | 0.9      | 0.02                | 0.9        |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1'  | 10                  | 0.81     | 0.03                | 0.81       |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1'  | 10                  | 0.77     | 0.02                | 0.77       |
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41  | 10                  | 0.75     | 0.04                | 0.73       |
| (1,557) | 1:43:A:G:H8  | 1:41:A:C:H2'  | 10                  | 0.68     | 0.02                | 0.68       |
| (1,604) | 1:48:A:G:H8  | 1:48:A:G:H5'' | 10                  | 0.67     | 0.01                | 0.67       |
| (1,680) | 1:53:A:G:H8  | 1:53:A:G:H5'' | 10                  | 0.66     | 0.01                | 0.66       |
| (1,504) | 1:38:A:U:H6  | 1:37:A:C:H42  | 10                  | 0.64     | 0.06                | 0.64       |
| (1,605) | 1:48:A:G:H8  | 1:47:A:A:H8   | 10                  | 0.62     | 0.02                | 0.62       |
| (1,616) | 1:49:A:G:H8  | 1:49:A:G:H5'' | 10                  | 0.62     | 0.01                | 0.62       |
| (1,627) | 1:49:A:G:H1  | 1:50:A:C:H1'  | 10                  | 0.61     | 0.03                | 0.62       |

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| Key     | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,550) | 1:43:A:G:H8   | 1:43:A:G:H3'  | 10                  | 0.6      | 0.02                | 0.59       |
| (1,628) | 1:49:A:G:H1   | 1:50:A:C:H42  | 10                  | 0.59     | 0.03                | 0.59       |
| (1,295) | 1:21:A:U:H3   | 1:22:A:C:H6   | 10                  | 0.58     | 0.01                | 0.58       |
| (1,232) | 1:16:A:A:H8   | 1:16:A:A:H5'' | 10                  | 0.58     | 0.01                | 0.58       |
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 10                  | 0.58     | 0.01                | 0.57       |
| (1,553) | 1:43:A:G:H8   | 1:42:A:U:H5'' | 10                  | 0.58     | 0.02                | 0.57       |
| (1,411) | 1:29:A:G:H1   | 1:28:A:C:H5   | 10                  | 0.58     | 0.01                | 0.57       |
| (1,439) | 1:31:A:G:H1   | 1:32:A:C:H5   | 10                  | 0.57     | 0.01                | 0.57       |
| (1,484) | 1:35:A:A:H2   | 1:36:A:U:H1'  | 10                  | 0.57     | 0.01                | 0.57       |
| (1,646) | 1:51:A:G:H8   | 1:51:A:G:H5'' | 10                  | 0.57     | 0.01                | 0.56       |
| (1,566) | 1:44:A:G:H8   | 1:44:A:G:H2'  | 10                  | 0.56     | 0.01                | 0.56       |
| (1,394) | 1:28:A:C:H5   | 1:26:A:U:HO2' | 10                  | 0.56     | 0.01                | 0.56       |
| (1,196) | 1:12:A:C:H6   | 1:11:A:A:H2'  | 10                  | 0.56     | 0.01                | 0.56       |
| (1,570) | 1:44:A:G:H8   | 1:43:A:G:H1'  | 10                  | 0.55     | 0.01                | 0.56       |
| (1,406) | 1:29:A:G:H1   | 1:30:A:G:H8   | 10                  | 0.55     | 0.01                | 0.55       |
| (1,528) | 1:40:A:G:H8   | 1:40:A:G:H5'' | 10                  | 0.55     | 0.01                | 0.54       |
| (1,524) | 1:39:A:G:H1   | 1:38:A:U:H3   | 10                  | 0.54     | 0.01                | 0.55       |
| (1,240) | 1:16:A:A:H2   | 1:17:A:U:H1'  | 10                  | 0.54     | 0.01                | 0.54       |
| (1,306) | 1:23:A:G:H8   | 1:22:A:C:H1'  | 10                  | 0.53     | 0.1                 | 0.58       |
| (1,460) | 1:33:A:U:H6   | 1:32:A:C:H6   | 10                  | 0.53     | 0.01                | 0.53       |
| (1,265) | 1:19:A:G:H8   | 1:17:A:U:H6   | 10                  | 0.53     | 0.02                | 0.52       |
| (1,325) | 1:24:A:C:H6   | 1:23:A:G:H8   | 10                  | 0.52     | 0.04                | 0.54       |
| (1,425) | 1:30:A:G:H1   | 1:26:A:U:H1'  | 10                  | 0.52     | 0.04                | 0.52       |
| (1,149) | 1:9:A:U:H3    | 1:50:A:C:H42  | 10                  | 0.52     | 0.04                | 0.52       |
| (1,598) | 1:47:A:A:H8   | 1:47:A:A:H5'  | 10                  | 0.51     | 0.01                | 0.51       |
| (1,538) | 1:40:A:G:H1   | 1:15:A:C:H41  | 10                  | 0.5      | 0.02                | 0.5        |
| (1,18)  | 1:2:A:G:H8    | 1:2:A:G:H5''  | 10                  | 0.49     | 0.01                | 0.48       |
| (1,294) | 1:21:A:U:H3   | 1:22:A:C:H41  | 10                  | 0.48     | 0.05                | 0.5        |
| (1,544) | 1:41:A:C:H6   | 1:40:A:G:H2'  | 10                  | 0.48     | 0.13                | 0.56       |
| (1,518) | 1:39:A:G:H8   | 1:38:A:U:H5   | 10                  | 0.48     | 0.03                | 0.47       |
| (1,527) | 1:40:A:G:H8   | 1:40:A:G:H3'  | 10                  | 0.46     | 0.07                | 0.48       |
| (1,571) | 1:44:A:G:H8   | 1:43:A:G:H2'  | 10                  | 0.46     | 0.03                | 0.46       |
| (1,271) | 1:19:A:G:H1   | 1:36:A:U:H3   | 10                  | 0.44     | 0.07                | 0.46       |
| (1,202) | 1:13:A:C:H6   | 1:13:A:C:H5'' | 10                  | 0.44     | 0.03                | 0.44       |
| (1,49)  | 1:4:A:A:H8    | 1:4:A:A:H5''  | 10                  | 0.44     | 0.02                | 0.43       |
| (1,322) | 1:24:A:C:H6   | 1:23:A:G:H1'  | 10                  | 0.44     | 0.05                | 0.44       |
| (1,585) | 1:45:A:C:H6   | 1:44:A:G:H1'  | 10                  | 0.44     | 0.01                | 0.44       |
| (1,431) | 1:31:A:G:H8   | 1:31:A:G:H5'' | 10                  | 0.44     | 0.03                | 0.45       |
| (1,661) | 1:52:A:G:H8   | 1:52:A:G:H5'' | 10                  | 0.42     | 0.02                | 0.42       |
| (1,33)  | 1:3:A:G:H8    | 1:3:A:G:H5''  | 10                  | 0.41     | 0.02                | 0.4        |
| (1,751) | 1:57:A:C:H6   | 1:57:A:C:H5'' | 10                  | 0.4      | 0.0                 | 0.4        |
| (1,195) | 1:12:A:C:H6   | 1:11:A:A:H1'  | 10                  | 0.39     | 0.02                | 0.39       |

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| Key     | Atom-1       | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|--------------|---------------|---------------------|----------|---------------------|------------|
| (1,273) | 1:19:A:G:H1  | 1:20:A:A:H2   | 10                  | 0.38     | 0.13                | 0.42       |
| (1,250) | 1:17:A:U:H6  | 1:16:A:A:H8   | 10                  | 0.38     | 0.02                | 0.38       |
| (1,578) | 1:45:A:C:H6  | 1:45:A:C:H3'  | 10                  | 0.38     | 0.02                | 0.38       |
| (1,264) | 1:19:A:G:H8  | 1:19:A:G:H3'  | 10                  | 0.38     | 0.07                | 0.39       |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 10                  | 0.38     | 0.05                | 0.36       |
| (1,78)  | 1:5:A:U:H3   | 1:6:A:C:H5    | 10                  | 0.37     | 0.02                | 0.38       |
| (1,98)  | 1:6:A:C:H5   | 1:5:A:U:H3    | 10                  | 0.37     | 0.02                | 0.38       |
| (1,158) | 1:10:A:C:H6  | 1:10:A:C:H5'' | 10                  | 0.37     | 0.01                | 0.37       |
| (1,461) | 1:33:A:U:H6  | 1:32:A:C:H1'  | 10                  | 0.37     | 0.08                | 0.37       |
| (1,736) | 1:56:A:C:H6  | 1:56:A:C:H5'' | 10                  | 0.37     | 0.03                | 0.36       |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 10                  | 0.37     | 0.07                | 0.33       |
| (1,292) | 1:21:A:U:H3  | 1:22:A:C:H5   | 10                  | 0.36     | 0.04                | 0.38       |
| (1,483) | 1:35:A:A:H8  | 1:34:A:G:H8   | 10                  | 0.36     | 0.1                 | 0.38       |
| (1,453) | 1:32:A:C:H6  | 1:31:A:G:H8   | 10                  | 0.34     | 0.1                 | 0.38       |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 10                  | 0.34     | 0.01                | 0.34       |
| (1,248) | 1:17:A:U:H6  | 1:16:A:A:H1'  | 10                  | 0.34     | 0.07                | 0.36       |
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1'  | 10                  | 0.34     | 0.11                | 0.34       |
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 10                  | 0.34     | 0.01                | 0.33       |
| (1,286) | 1:21:A:U:H6  | 1:20:A:A:H1'  | 10                  | 0.33     | 0.06                | 0.32       |
| (1,572) | 1:44:A:G:H8  | 1:43:A:G:H8   | 10                  | 0.33     | 0.05                | 0.3        |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 10                  | 0.32     | 0.01                | 0.32       |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5   | 10                  | 0.32     | 0.13                | 0.23       |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 10                  | 0.31     | 0.02                | 0.32       |
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 10                  | 0.31     | 0.06                | 0.3        |
| (1,463) | 1:33:A:U:H6  | 1:32:A:C:H3'  | 10                  | 0.31     | 0.12                | 0.24       |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 10                  | 0.3      | 0.06                | 0.32       |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1'  | 10                  | 0.29     | 0.08                | 0.28       |
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 10                  | 0.28     | 0.02                | 0.28       |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 10                  | 0.28     | 0.06                | 0.28       |
| (1,490) | 1:36:A:U:H6  | 1:36:A:U:H5'' | 10                  | 0.27     | 0.04                | 0.26       |
| (1,415) | 1:30:A:G:H8  | 1:30:A:G:H3'  | 10                  | 0.27     | 0.05                | 0.28       |
| (1,492) | 1:36:A:U:H6  | 1:35:A:A:H1'  | 10                  | 0.26     | 0.05                | 0.26       |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 10                  | 0.25     | 0.0                 | 0.25       |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 10                  | 0.25     | 0.06                | 0.26       |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 10                  | 0.24     | 0.03                | 0.26       |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 10                  | 0.24     | 0.04                | 0.24       |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 10                  | 0.24     | 0.05                | 0.23       |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 10                  | 0.22     | 0.02                | 0.23       |
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 10                  | 0.22     | 0.02                | 0.22       |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 10                  | 0.21     | 0.01                | 0.21       |
| (1,224) | 1:15:A:C:H6  | 1:14:A:C:H1'  | 10                  | 0.21     | 0.03                | 0.21       |
| (1,116) | 1:7:A:U:H3   | 1:6:A:C:H42   | 10                  | 0.2      | 0.04                | 0.2        |

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| Key     | Atom-1       | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|--------------|---------------|---------------------|----------|---------------------|------------|
| (1,529) | 1:40:A:G:H8  | 1:39:A:G:H8   | 10                  | 0.2      | 0.06                | 0.2        |
| (1,190) | 1:12:A:C:H6  | 1:12:A:C:H5'' | 10                  | 0.2      | 0.03                | 0.2        |
| (1,424) | 1:30:A:G:H1  | 1:25:A:C:H5   | 10                  | 0.2      | 0.05                | 0.2        |
| (1,293) | 1:21:A:U:H3  | 1:22:A:C:H42  | 10                  | 0.19     | 0.04                | 0.2        |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 10                  | 0.19     | 0.01                | 0.2        |
| (1,596) | 1:47:A:A:H8  | 1:47:A:A:H3'  | 10                  | 0.18     | 0.04                | 0.17       |
| (1,537) | 1:40:A:G:H1  | 1:15:A:C:H42  | 10                  | 0.17     | 0.02                | 0.17       |
| (1,242) | 1:17:A:U:H6  | 1:17:A:U:H2'  | 10                  | 0.16     | 0.02                | 0.16       |
| (1,229) | 1:16:A:A:H8  | 1:16:A:A:H3'  | 10                  | 0.16     | 0.02                | 0.16       |
| (1,712) | 1:54:A:U:H3  | 1:3:A:G:H1    | 10                  | 0.14     | 0.01                | 0.14       |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 10                  | 0.11     | 0.01                | 0.11       |
| (1,607) | 1:48:A:G:H8  | 1:47:A:A:H2'  | 9                   | 0.6      | 0.02                | 0.59       |
| (1,403) | 1:29:A:G:H1' | 1:28:A:C:H5'  | 9                   | 0.39     | 0.16                | 0.45       |
| (1,351) | 1:26:A:U:H6  | 1:25:A:C:H1'  | 9                   | 0.38     | 0.18                | 0.53       |
| (1,455) | 1:32:A:C:H5  | 1:31:A:G:H1'  | 9                   | 0.35     | 0.08                | 0.37       |
| (1,287) | 1:21:A:U:H6  | 1:20:A:A:H8   | 9                   | 0.3      | 0.08                | 0.33       |
| (1,238) | 1:16:A:A:H8  | 1:15:A:C:H6   | 9                   | 0.29     | 0.07                | 0.32       |
| (1,601) | 1:47:A:A:H2  | 1:48:A:G:H8   | 9                   | 0.25     | 0.1                 | 0.24       |
| (1,486) | 1:34:A:G:H1  | 1:35:A:A:H2   | 9                   | 0.22     | 0.05                | 0.22       |
| (1,418) | 1:30:A:G:H8  | 1:30:A:G:H5'' | 9                   | 0.22     | 0.04                | 0.23       |
| (1,428) | 1:31:A:G:H8  | 1:31:A:G:H3'  | 9                   | 0.2      | 0.03                | 0.21       |
| (1,321) | 1:24:A:C:H5  | 1:24:A:C:H2'  | 9                   | 0.15     | 0.02                | 0.15       |
| (1,633) | 1:50:A:C:H6  | 1:50:A:C:H5'' | 9                   | 0.14     | 0.02                | 0.15       |
| (1,305) | 1:23:A:G:H1' | 1:23:A:G:H4'  | 9                   | 0.14     | 0.04                | 0.12       |
| (1,282) | 1:20:A:A:H2  | 1:37:A:C:H1'  | 9                   | 0.13     | 0.01                | 0.13       |
| (1,655) | 1:51:A:G:H3' | 1:50:A:C:H2'  | 9                   | 0.11     | 0.01                | 0.11       |
| (1,391) | 1:28:A:C:H42 | 1:26:A:U:H3'  | 8                   | 0.4      | 0.13                | 0.46       |
| (1,409) | 1:29:A:G:H1  | 1:26:A:U:H2'  | 8                   | 0.3      | 0.08                | 0.32       |
| (1,451) | 1:32:A:C:H6  | 1:31:A:G:H1'  | 8                   | 0.16     | 0.03                | 0.16       |
| (1,563) | 1:43:A:G:H1  | 1:12:A:C:H41  | 8                   | 0.16     | 0.06                | 0.15       |
| (1,301) | 1:23:A:G:H8  | 1:23:A:G:H2'  | 8                   | 0.13     | 0.01                | 0.12       |
| (1,69)  | 1:5:A:U:H6   | 1:4:A:A:H1'   | 8                   | 0.11     | 0.01                | 0.11       |
| (1,547) | 1:42:A:U:H6  | 1:42:A:U:H5'  | 7                   | 0.5      | 0.02                | 0.5        |
| (1,586) | 1:45:A:C:H42 | 1:44:A:G:H1   | 7                   | 0.47     | 0.05                | 0.5        |
| (1,469) | 1:34:A:G:H8  | 1:33:A:U:H1'  | 7                   | 0.23     | 0.08                | 0.16       |
| (1,237) | 1:16:A:A:H8  | 1:15:A:C:H3'  | 7                   | 0.16     | 0.03                | 0.17       |
| (1,249) | 1:17:A:U:H6  | 1:16:A:A:H2'  | 7                   | 0.16     | 0.03                | 0.16       |
| (1,500) | 1:37:A:C:H6  | 1:36:A:U:H1'  | 7                   | 0.15     | 0.03                | 0.16       |
| (1,372) | 1:28:A:C:H6  | 1:28:A:C:H3'  | 6                   | 0.2      | 0.06                | 0.23       |
| (1,323) | 1:24:A:C:H6  | 1:23:A:G:H2'  | 6                   | 0.15     | 0.04                | 0.15       |
| (1,267) | 1:19:A:G:H8  | 1:17:A:U:H4'  | 6                   | 0.12     | 0.01                | 0.12       |
| (1,508) | 1:38:A:U:H6  | 1:38:A:U:H5'' | 5                   | 0.63     | 0.01                | 0.64       |

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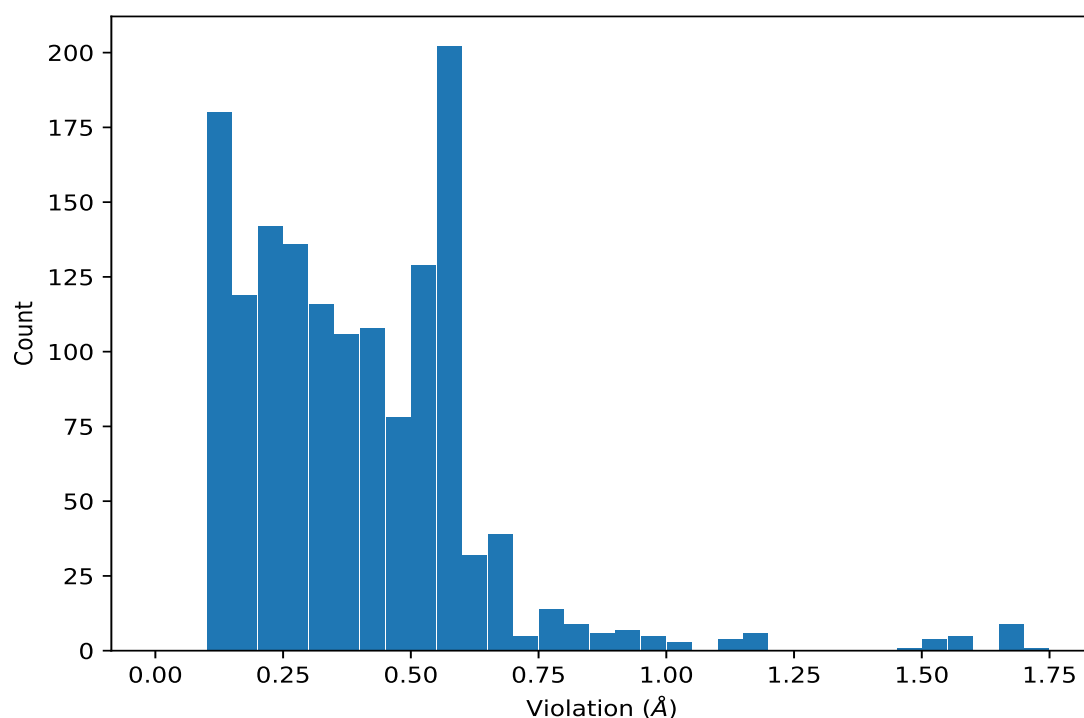
| Key     | Atom-1       | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|--------------|---------------|---------------------|----------|---------------------|------------|
| (1,354) | 1:26:A:U:H6  | 1:25:A:C:H2'  | 5                   | 0.47     | 0.03                | 0.46       |
| (1,353) | 1:26:A:U:H6  | 1:25:A:C:H3'  | 5                   | 0.4      | 0.03                | 0.41       |
| (1,435) | 1:31:A:G:H8  | 1:30:A:G:H1'  | 5                   | 0.37     | 0.12                | 0.38       |
| (1,390) | 1:28:A:C:H41 | 1:26:A:U:H3'  | 5                   | 0.25     | 0.02                | 0.24       |
| (1,384) | 1:28:A:C:H5  | 1:26:A:U:H1'  | 5                   | 0.22     | 0.06                | 0.25       |
| (1,385) | 1:28:A:C:H6  | 1:26:A:U:H2'  | 5                   | 0.22     | 0.07                | 0.19       |
| (1,380) | 1:28:A:C:H5  | 1:27:A:U:H2'  | 5                   | 0.2      | 0.04                | 0.21       |
| (1,279) | 1:20:A:A:H8  | 1:19:A:G:H3'  | 5                   | 0.11     | 0.0                 | 0.11       |
| (1,373) | 1:28:A:C:H6  | 1:28:A:C:H5'  | 4                   | 0.56     | 0.01                | 0.56       |
| (1,404) | 1:29:A:G:H8  | 1:28:A:C:H5'  | 4                   | 0.34     | 0.03                | 0.33       |
| (1,438) | 1:31:A:G:H1  | 1:30:A:G:H1   | 4                   | 0.27     | 0.07                | 0.27       |
| (1,536) | 1:40:A:G:H1  | 1:14:A:C:H5   | 4                   | 0.16     | 0.03                | 0.17       |
| (1,410) | 1:29:A:G:H1  | 1:28:A:C:H1'  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,556) | 1:43:A:G:H8  | 1:41:A:C:H1'  | 3                   | 0.47     | 0.01                | 0.47       |
| (1,277) | 1:20:A:A:H8  | 1:19:A:G:H1'  | 3                   | 0.25     | 0.04                | 0.25       |
| (1,278) | 1:20:A:A:H8  | 1:19:A:G:H2'  | 3                   | 0.22     | 0.07                | 0.2        |
| (1,434) | 1:31:A:G:H8  | 1:30:A:G:H8   | 3                   | 0.19     | 0.09                | 0.15       |
| (1,545) | 1:41:A:C:H1' | 1:40:A:G:H2'  | 3                   | 0.16     | 0.04                | 0.18       |
| (1,208) | 1:13:A:C:H6  | 1:12:A:C:H6   | 3                   | 0.16     | 0.03                | 0.16       |
| (1,417) | 1:30:A:G:H8  | 1:30:A:G:H5'  | 3                   | 0.14     | 0.01                | 0.15       |
| (1,477) | 1:35:A:A:H8  | 1:35:A:A:H5'' | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,339) | 1:25:A:C:H5  | 1:24:A:C:H5   | 2                   | 0.3      | 0.06                | 0.3        |
| (1,444) | 1:31:A:G:H1  | 1:25:A:C:H41  | 2                   | 0.28     | 0.06                | 0.28       |
| (1,462) | 1:33:A:U:H6  | 1:32:A:C:H2'  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,474) | 1:34:A:G:H1  | 1:33:A:U:H3   | 2                   | 0.2      | 0.02                | 0.2        |
| (1,352) | 1:26:A:U:H5  | 1:25:A:C:H5   | 2                   | 0.14     | 0.03                | 0.14       |
| (1,209) | 1:13:A:C:H5  | 1:12:A:C:H5   | 2                   | 0.13     | 0.02                | 0.13       |
| (1,412) | 1:29:A:G:H1  | 1:28:A:C:H6   | 2                   | 0.13     | 0.01                | 0.13       |
| (1,742) | 1:56:A:C:H5  | 1:55:A:C:H3'  | 2                   | 0.1      | 0.0                 | 0.1        |

<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) |
|---------|-------------|--------------|----------|---------------|
| (1,28)  | 1:1:A:G:H1  | 1:56:A:C:H42 | 8        | 1.72          |
| (1,28)  | 1:1:A:G:H1  | 1:56:A:C:H42 | 1        | 1.7           |
| (1,28)  | 1:1:A:G:H1  | 1:56:A:C:H42 | 2        | 1.7           |
| (1,28)  | 1:1:A:G:H1  | 1:56:A:C:H42 | 4        | 1.7           |
| (1,28)  | 1:1:A:G:H1  | 1:56:A:C:H42 | 7        | 1.69          |
| (1,28)  | 1:1:A:G:H1  | 1:56:A:C:H42 | 5        | 1.68          |
| (1,28)  | 1:1:A:G:H1  | 1:56:A:C:H42 | 9        | 1.68          |
| (1,28)  | 1:1:A:G:H1  | 1:56:A:C:H42 | 10       | 1.68          |
| (1,28)  | 1:1:A:G:H1  | 1:56:A:C:H42 | 3        | 1.67          |
| (1,28)  | 1:1:A:G:H1  | 1:56:A:C:H42 | 6        | 1.67          |
| (1,626) | 1:49:A:G:H1 | 1:50:A:C:H5  | 8        | 1.59          |
| (1,626) | 1:49:A:G:H1 | 1:50:A:C:H5  | 9        | 1.59          |
| (1,626) | 1:49:A:G:H1 | 1:50:A:C:H5  | 7        | 1.58          |
| (1,626) | 1:49:A:G:H1 | 1:50:A:C:H5  | 10       | 1.57          |
| (1,626) | 1:49:A:G:H1 | 1:50:A:C:H5  | 5        | 1.55          |
| (1,626) | 1:49:A:G:H1 | 1:50:A:C:H5  | 6        | 1.53          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (1,626) | 1:49:A:G:H1  | 1:50:A:C:H5  | 2        | 1.52          |
| (1,626) | 1:49:A:G:H1  | 1:50:A:C:H5  | 3        | 1.52          |
| (1,626) | 1:49:A:G:H1  | 1:50:A:C:H5  | 1        | 1.51          |
| (1,626) | 1:49:A:G:H1  | 1:50:A:C:H5  | 4        | 1.49          |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41 | 1        | 1.18          |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41 | 4        | 1.18          |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41 | 8        | 1.18          |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41 | 2        | 1.17          |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41 | 7        | 1.16          |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41 | 9        | 1.16          |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41 | 10       | 1.15          |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41 | 3        | 1.14          |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41 | 5        | 1.14          |
| (1,29)  | 1:1:A:G:H1   | 1:56:A:C:H41 | 6        | 1.14          |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5   | 5        | 1.02          |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5   | 7        | 1.02          |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5   | 3        | 1.01          |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5   | 9        | 0.99          |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5   | 8        | 0.98          |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5   | 10       | 0.98          |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5   | 2        | 0.97          |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5   | 6        | 0.96          |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5   | 4        | 0.94          |
| (1,693) | 1:53:A:G:H1  | 1:6:A:C:H5   | 1        | 0.93          |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2' | 4        | 0.93          |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2' | 5        | 0.93          |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2' | 3        | 0.91          |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2' | 7        | 0.9           |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2' | 9        | 0.9           |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2' | 2        | 0.89          |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2' | 10       | 0.89          |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2' | 1        | 0.88          |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2' | 6        | 0.88          |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1' | 6        | 0.87          |
| (1,281) | 1:20:A:A:H2  | 1:18:A:U:H2' | 8        | 0.87          |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1' | 2        | 0.82          |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1' | 4        | 0.82          |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1' | 1        | 0.81          |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1' | 5        | 0.81          |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1' | 8        | 0.81          |
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41 | 8        | 0.81          |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1' | 6        | 0.8           |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41  | 7        | 0.8           |
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41  | 9        | 0.8           |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1'  | 3        | 0.79          |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1'  | 7        | 0.79          |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1'  | 2        | 0.79          |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1'  | 3        | 0.79          |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1'  | 10       | 0.78          |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1'  | 4        | 0.78          |
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41  | 10       | 0.78          |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1'  | 1        | 0.77          |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1'  | 5        | 0.77          |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1'  | 10       | 0.77          |
| (1,558) | 1:43:A:G:H2' | 1:41:A:C:H1'  | 9        | 0.76          |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1'  | 7        | 0.76          |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1'  | 8        | 0.75          |
| (1,280) | 1:20:A:A:H2  | 1:18:A:U:H1'  | 9        | 0.75          |
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41  | 1        | 0.73          |
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41  | 6        | 0.73          |
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41  | 5        | 0.72          |
| (1,504) | 1:38:A:U:H6  | 1:37:A:C:H42  | 5        | 0.71          |
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41  | 4        | 0.71          |
| (1,557) | 1:43:A:G:H8  | 1:41:A:C:H2'  | 4        | 0.7           |
| (1,557) | 1:43:A:G:H8  | 1:41:A:C:H2'  | 10       | 0.7           |
| (1,504) | 1:38:A:U:H6  | 1:37:A:C:H42  | 4        | 0.7           |
| (1,504) | 1:38:A:U:H6  | 1:37:A:C:H42  | 7        | 0.7           |
| (1,504) | 1:38:A:U:H6  | 1:37:A:C:H42  | 9        | 0.7           |
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41  | 2        | 0.7           |
| (1,604) | 1:48:A:G:H8  | 1:48:A:G:H5'' | 5        | 0.69          |
| (1,504) | 1:38:A:U:H6  | 1:37:A:C:H42  | 10       | 0.69          |
| (1,604) | 1:48:A:G:H8  | 1:48:A:G:H5'' | 2        | 0.68          |
| (1,604) | 1:48:A:G:H8  | 1:48:A:G:H5'' | 3        | 0.68          |
| (1,604) | 1:48:A:G:H8  | 1:48:A:G:H5'' | 4        | 0.68          |
| (1,557) | 1:43:A:G:H8  | 1:41:A:C:H2'  | 6        | 0.68          |
| (1,557) | 1:43:A:G:H8  | 1:41:A:C:H2'  | 7        | 0.68          |
| (1,557) | 1:43:A:G:H8  | 1:41:A:C:H2'  | 9        | 0.68          |
| (1,148) | 1:9:A:U:H3   | 1:50:A:C:H41  | 3        | 0.68          |
| (1,680) | 1:53:A:G:H8  | 1:53:A:G:H5'' | 2        | 0.67          |
| (1,680) | 1:53:A:G:H8  | 1:53:A:G:H5'' | 3        | 0.67          |
| (1,680) | 1:53:A:G:H8  | 1:53:A:G:H5'' | 4        | 0.67          |
| (1,680) | 1:53:A:G:H8  | 1:53:A:G:H5'' | 5        | 0.67          |
| (1,680) | 1:53:A:G:H8  | 1:53:A:G:H5'' | 6        | 0.67          |
| (1,604) | 1:48:A:G:H8  | 1:48:A:G:H5'' | 1        | 0.67          |

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| Key     | Atom-1      | Atom-2        | Model ID | Violation (Å) |
|---------|-------------|---------------|----------|---------------|
| (1,604) | 1:48:A:G:H8 | 1:48:A:G:H5'' | 6        | 0.67          |
| (1,604) | 1:48:A:G:H8 | 1:48:A:G:H5'' | 7        | 0.67          |
| (1,604) | 1:48:A:G:H8 | 1:48:A:G:H5'' | 9        | 0.67          |
| (1,557) | 1:43:A:G:H8 | 1:41:A:C:H2'  | 3        | 0.67          |
| (1,557) | 1:43:A:G:H8 | 1:41:A:C:H2'  | 8        | 0.67          |
| (1,680) | 1:53:A:G:H8 | 1:53:A:G:H5'' | 1        | 0.66          |
| (1,680) | 1:53:A:G:H8 | 1:53:A:G:H5'' | 7        | 0.66          |
| (1,680) | 1:53:A:G:H8 | 1:53:A:G:H5'' | 8        | 0.66          |
| (1,605) | 1:48:A:G:H8 | 1:47:A:A:H8   | 8        | 0.66          |
| (1,604) | 1:48:A:G:H8 | 1:48:A:G:H5'' | 10       | 0.66          |
| (1,557) | 1:43:A:G:H8 | 1:41:A:C:H2'  | 1        | 0.66          |
| (1,557) | 1:43:A:G:H8 | 1:41:A:C:H2'  | 5        | 0.66          |
| (1,680) | 1:53:A:G:H8 | 1:53:A:G:H5'' | 9        | 0.65          |
| (1,680) | 1:53:A:G:H8 | 1:53:A:G:H5'' | 10       | 0.65          |
| (1,627) | 1:49:A:G:H1 | 1:50:A:C:H1'  | 5        | 0.65          |
| (1,604) | 1:48:A:G:H8 | 1:48:A:G:H5'' | 8        | 0.65          |
| (1,557) | 1:43:A:G:H8 | 1:41:A:C:H2'  | 2        | 0.65          |
| (1,508) | 1:38:A:U:H6 | 1:38:A:U:H5'' | 9        | 0.65          |
| (1,628) | 1:49:A:G:H1 | 1:50:A:C:H42  | 9        | 0.64          |
| (1,628) | 1:49:A:G:H1 | 1:50:A:C:H42  | 10       | 0.64          |
| (1,627) | 1:49:A:G:H1 | 1:50:A:C:H1'  | 3        | 0.64          |
| (1,607) | 1:48:A:G:H8 | 1:47:A:A:H2'  | 6        | 0.64          |
| (1,508) | 1:38:A:U:H6 | 1:38:A:U:H5'' | 7        | 0.64          |
| (1,508) | 1:38:A:U:H6 | 1:38:A:U:H5'' | 10       | 0.64          |
| (1,627) | 1:49:A:G:H1 | 1:50:A:C:H1'  | 7        | 0.63          |
| (1,616) | 1:49:A:G:H8 | 1:49:A:G:H5'' | 5        | 0.63          |
| (1,616) | 1:49:A:G:H8 | 1:49:A:G:H5'' | 6        | 0.63          |
| (1,605) | 1:48:A:G:H8 | 1:47:A:A:H8   | 1        | 0.63          |
| (1,605) | 1:48:A:G:H8 | 1:47:A:A:H8   | 5        | 0.63          |
| (1,550) | 1:43:A:G:H8 | 1:43:A:G:H3'  | 6        | 0.63          |
| (1,627) | 1:49:A:G:H1 | 1:50:A:C:H1'  | 2        | 0.62          |
| (1,627) | 1:49:A:G:H1 | 1:50:A:C:H1'  | 8        | 0.62          |
| (1,616) | 1:49:A:G:H8 | 1:49:A:G:H5'' | 1        | 0.62          |
| (1,616) | 1:49:A:G:H8 | 1:49:A:G:H5'' | 2        | 0.62          |
| (1,616) | 1:49:A:G:H8 | 1:49:A:G:H5'' | 3        | 0.62          |
| (1,616) | 1:49:A:G:H8 | 1:49:A:G:H5'' | 4        | 0.62          |
| (1,605) | 1:48:A:G:H8 | 1:47:A:A:H8   | 2        | 0.62          |
| (1,605) | 1:48:A:G:H8 | 1:47:A:A:H8   | 3        | 0.62          |
| (1,605) | 1:48:A:G:H8 | 1:47:A:A:H8   | 4        | 0.62          |
| (1,550) | 1:43:A:G:H8 | 1:43:A:G:H3'  | 4        | 0.62          |
| (1,508) | 1:38:A:U:H6 | 1:38:A:U:H5'' | 4        | 0.62          |
| (1,628) | 1:49:A:G:H1 | 1:50:A:C:H42  | 6        | 0.61          |

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| Key     | Atom-1      | Atom-2        | Model ID | Violation (Å) |
|---------|-------------|---------------|----------|---------------|
| (1,627) | 1:49:A:G:H1 | 1:50:A:C:H1'  | 6        | 0.61          |
| (1,627) | 1:49:A:G:H1 | 1:50:A:C:H1'  | 9        | 0.61          |
| (1,616) | 1:49:A:G:H8 | 1:49:A:G:H5'' | 10       | 0.61          |
| (1,607) | 1:48:A:G:H8 | 1:47:A:A:H2'  | 4        | 0.61          |
| (1,605) | 1:48:A:G:H8 | 1:47:A:A:H8   | 9        | 0.61          |
| (1,553) | 1:43:A:G:H8 | 1:42:A:U:H5'' | 6        | 0.61          |
| (1,550) | 1:43:A:G:H8 | 1:43:A:G:H3'  | 10       | 0.61          |
| (1,508) | 1:38:A:U:H6 | 1:38:A:U:H5'' | 5        | 0.61          |
| (1,628) | 1:49:A:G:H1 | 1:50:A:C:H42  | 7        | 0.6           |
| (1,628) | 1:49:A:G:H1 | 1:50:A:C:H42  | 8        | 0.6           |
| (1,616) | 1:49:A:G:H8 | 1:49:A:G:H5'' | 7        | 0.6           |
| (1,616) | 1:49:A:G:H8 | 1:49:A:G:H5'' | 8        | 0.6           |
| (1,616) | 1:49:A:G:H8 | 1:49:A:G:H5'' | 9        | 0.6           |
| (1,607) | 1:48:A:G:H8 | 1:47:A:A:H2'  | 7        | 0.6           |
| (1,605) | 1:48:A:G:H8 | 1:47:A:A:H8   | 6        | 0.6           |
| (1,605) | 1:48:A:G:H8 | 1:47:A:A:H8   | 7        | 0.6           |
| (1,605) | 1:48:A:G:H8 | 1:47:A:A:H8   | 10       | 0.6           |
| (1,550) | 1:43:A:G:H8 | 1:43:A:G:H3'  | 3        | 0.6           |
| (1,504) | 1:38:A:U:H6 | 1:37:A:C:H42  | 3        | 0.6           |
| (1,411) | 1:29:A:G:H1 | 1:28:A:C:H5   | 2        | 0.6           |
| (1,306) | 1:23:A:G:H8 | 1:22:A:C:H1'  | 8        | 0.6           |
| (1,295) | 1:21:A:U:H3 | 1:22:A:C:H6   | 8        | 0.6           |
| (1,232) | 1:16:A:A:H8 | 1:16:A:A:H5'' | 3        | 0.6           |
| (1,627) | 1:49:A:G:H1 | 1:50:A:C:H1'  | 10       | 0.59          |
| (1,607) | 1:48:A:G:H8 | 1:47:A:A:H2'  | 1        | 0.59          |
| (1,607) | 1:48:A:G:H8 | 1:47:A:A:H2'  | 3        | 0.59          |
| (1,607) | 1:48:A:G:H8 | 1:47:A:A:H2'  | 5        | 0.59          |
| (1,607) | 1:48:A:G:H8 | 1:47:A:A:H2'  | 10       | 0.59          |
| (1,566) | 1:44:A:G:H8 | 1:44:A:G:H2'  | 9        | 0.59          |
| (1,553) | 1:43:A:G:H8 | 1:42:A:U:H5'' | 3        | 0.59          |
| (1,553) | 1:43:A:G:H8 | 1:42:A:U:H5'' | 5        | 0.59          |
| (1,550) | 1:43:A:G:H8 | 1:43:A:G:H3'  | 1        | 0.59          |
| (1,550) | 1:43:A:G:H8 | 1:43:A:G:H3'  | 2        | 0.59          |
| (1,550) | 1:43:A:G:H8 | 1:43:A:G:H3'  | 5        | 0.59          |
| (1,550) | 1:43:A:G:H8 | 1:43:A:G:H3'  | 9        | 0.59          |
| (1,504) | 1:38:A:U:H6 | 1:37:A:C:H42  | 2        | 0.59          |
| (1,484) | 1:35:A:A:H2 | 1:36:A:U:H1'  | 9        | 0.59          |
| (1,439) | 1:31:A:G:H1 | 1:32:A:C:H5   | 5        | 0.59          |
| (1,439) | 1:31:A:G:H1 | 1:32:A:C:H5   | 7        | 0.59          |
| (1,439) | 1:31:A:G:H1 | 1:32:A:C:H5   | 10       | 0.59          |
| (1,411) | 1:29:A:G:H1 | 1:28:A:C:H5   | 4        | 0.59          |
| (1,411) | 1:29:A:G:H1 | 1:28:A:C:H5   | 9        | 0.59          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 2        | 0.59          |
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 4        | 0.59          |
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 9        | 0.59          |
| (1,306) | 1:23:A:G:H8   | 1:22:A:C:H1'  | 6        | 0.59          |
| (1,306) | 1:23:A:G:H8   | 1:22:A:C:H1'  | 7        | 0.59          |
| (1,295) | 1:21:A:U:H3   | 1:22:A:C:H6   | 2        | 0.59          |
| (1,295) | 1:21:A:U:H3   | 1:22:A:C:H6   | 5        | 0.59          |
| (1,232) | 1:16:A:A:H8   | 1:16:A:A:H5'' | 2        | 0.59          |
| (1,232) | 1:16:A:A:H8   | 1:16:A:A:H5'' | 10       | 0.59          |
| (1,646) | 1:51:A:G:H8   | 1:51:A:G:H5'' | 3        | 0.58          |
| (1,646) | 1:51:A:G:H8   | 1:51:A:G:H5'' | 4        | 0.58          |
| (1,646) | 1:51:A:G:H8   | 1:51:A:G:H5'' | 6        | 0.58          |
| (1,628) | 1:49:A:G:H1   | 1:50:A:C:H42  | 3        | 0.58          |
| (1,607) | 1:48:A:G:H8   | 1:47:A:A:H2'  | 2        | 0.58          |
| (1,607) | 1:48:A:G:H8   | 1:47:A:A:H2'  | 9        | 0.58          |
| (1,566) | 1:44:A:G:H8   | 1:44:A:G:H2'  | 10       | 0.58          |
| (1,553) | 1:43:A:G:H8   | 1:42:A:U:H5'' | 1        | 0.58          |
| (1,550) | 1:43:A:G:H8   | 1:43:A:G:H3'  | 8        | 0.58          |
| (1,544) | 1:41:A:C:H6   | 1:40:A:G:H2'  | 6        | 0.58          |
| (1,504) | 1:38:A:U:H6   | 1:37:A:C:H42  | 1        | 0.58          |
| (1,439) | 1:31:A:G:H1   | 1:32:A:C:H5   | 3        | 0.58          |
| (1,439) | 1:31:A:G:H1   | 1:32:A:C:H5   | 9        | 0.58          |
| (1,411) | 1:29:A:G:H1   | 1:28:A:C:H5   | 5        | 0.58          |
| (1,411) | 1:29:A:G:H1   | 1:28:A:C:H5   | 7        | 0.58          |
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 7        | 0.58          |
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 10       | 0.58          |
| (1,306) | 1:23:A:G:H8   | 1:22:A:C:H1'  | 1        | 0.58          |
| (1,306) | 1:23:A:G:H8   | 1:22:A:C:H1'  | 4        | 0.58          |
| (1,306) | 1:23:A:G:H8   | 1:22:A:C:H1'  | 5        | 0.58          |
| (1,295) | 1:21:A:U:H3   | 1:22:A:C:H6   | 1        | 0.58          |
| (1,295) | 1:21:A:U:H3   | 1:22:A:C:H6   | 3        | 0.58          |
| (1,295) | 1:21:A:U:H3   | 1:22:A:C:H6   | 4        | 0.58          |
| (1,295) | 1:21:A:U:H3   | 1:22:A:C:H6   | 7        | 0.58          |
| (1,295) | 1:21:A:U:H3   | 1:22:A:C:H6   | 10       | 0.58          |
| (1,232) | 1:16:A:A:H8   | 1:16:A:A:H5'' | 4        | 0.58          |
| (1,232) | 1:16:A:A:H8   | 1:16:A:A:H5'' | 7        | 0.58          |
| (1,232) | 1:16:A:A:H8   | 1:16:A:A:H5'' | 8        | 0.58          |
| (1,149) | 1:9:A:U:H3    | 1:50:A:C:H42  | 9        | 0.58          |
| (1,646) | 1:51:A:G:H8   | 1:51:A:G:H5'' | 1        | 0.57          |
| (1,646) | 1:51:A:G:H8   | 1:51:A:G:H5'' | 5        | 0.57          |
| (1,628) | 1:49:A:G:H1   | 1:50:A:C:H42  | 1        | 0.57          |
| (1,627) | 1:49:A:G:H1   | 1:50:A:C:H1'  | 1        | 0.57          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,570) | 1:44:A:G:H8   | 1:43:A:G:H1'  | 4        | 0.57          |
| (1,566) | 1:44:A:G:H8   | 1:44:A:G:H2'  | 6        | 0.57          |
| (1,566) | 1:44:A:G:H8   | 1:44:A:G:H2'  | 7        | 0.57          |
| (1,553) | 1:43:A:G:H8   | 1:42:A:U:H5'' | 7        | 0.57          |
| (1,553) | 1:43:A:G:H8   | 1:42:A:U:H5'' | 8        | 0.57          |
| (1,553) | 1:43:A:G:H8   | 1:42:A:U:H5'' | 9        | 0.57          |
| (1,553) | 1:43:A:G:H8   | 1:42:A:U:H5'' | 10       | 0.57          |
| (1,550) | 1:43:A:G:H8   | 1:43:A:G:H3'  | 7        | 0.57          |
| (1,544) | 1:41:A:C:H6   | 1:40:A:G:H2'  | 4        | 0.57          |
| (1,524) | 1:39:A:G:H1   | 1:38:A:U:H3   | 6        | 0.57          |
| (1,504) | 1:38:A:U:H6   | 1:37:A:C:H42  | 6        | 0.57          |
| (1,504) | 1:38:A:U:H6   | 1:37:A:C:H42  | 8        | 0.57          |
| (1,484) | 1:35:A:A:H2   | 1:36:A:U:H1'  | 2        | 0.57          |
| (1,484) | 1:35:A:A:H2   | 1:36:A:U:H1'  | 3        | 0.57          |
| (1,484) | 1:35:A:A:H2   | 1:36:A:U:H1'  | 5        | 0.57          |
| (1,484) | 1:35:A:A:H2   | 1:36:A:U:H1'  | 6        | 0.57          |
| (1,484) | 1:35:A:A:H2   | 1:36:A:U:H1'  | 8        | 0.57          |
| (1,439) | 1:31:A:G:H1   | 1:32:A:C:H5   | 6        | 0.57          |
| (1,439) | 1:31:A:G:H1   | 1:32:A:C:H5   | 8        | 0.57          |
| (1,425) | 1:30:A:G:H1   | 1:26:A:U:H1'  | 9        | 0.57          |
| (1,411) | 1:29:A:G:H1   | 1:28:A:C:H5   | 1        | 0.57          |
| (1,411) | 1:29:A:G:H1   | 1:28:A:C:H5   | 10       | 0.57          |
| (1,406) | 1:29:A:G:H1   | 1:30:A:G:H8   | 4        | 0.57          |
| (1,403) | 1:29:A:G:H1'  | 1:28:A:C:H5'  | 5        | 0.57          |
| (1,394) | 1:28:A:C:H5   | 1:26:A:U:HO2' | 3        | 0.57          |
| (1,394) | 1:28:A:C:H5   | 1:26:A:U:HO2' | 6        | 0.57          |
| (1,373) | 1:28:A:C:H6   | 1:28:A:C:H5'  | 1        | 0.57          |
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 1        | 0.57          |
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 3        | 0.57          |
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 6        | 0.57          |
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 8        | 0.57          |
| (1,325) | 1:24:A:C:H6   | 1:23:A:G:H8   | 8        | 0.57          |
| (1,306) | 1:23:A:G:H8   | 1:22:A:C:H1'  | 2        | 0.57          |
| (1,306) | 1:23:A:G:H8   | 1:22:A:C:H1'  | 3        | 0.57          |
| (1,295) | 1:21:A:U:H3   | 1:22:A:C:H6   | 9        | 0.57          |
| (1,232) | 1:16:A:A:H8   | 1:16:A:A:H5'' | 1        | 0.57          |
| (1,232) | 1:16:A:A:H8   | 1:16:A:A:H5'' | 5        | 0.57          |
| (1,232) | 1:16:A:A:H8   | 1:16:A:A:H5'' | 9        | 0.57          |
| (1,196) | 1:12:A:C:H6   | 1:11:A:A:H2'  | 2        | 0.57          |
| (1,196) | 1:12:A:C:H6   | 1:11:A:A:H2'  | 4        | 0.57          |
| (1,149) | 1:9:A:U:H3    | 1:50:A:C:H42  | 8        | 0.57          |
| (1,646) | 1:51:A:G:H8   | 1:51:A:G:H5'' | 2        | 0.56          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,646) | 1:51:A:G:H8   | 1:51:A:G:H5'' | 7        | 0.56          |
| (1,646) | 1:51:A:G:H8   | 1:51:A:G:H5'' | 8        | 0.56          |
| (1,646) | 1:51:A:G:H8   | 1:51:A:G:H5'' | 10       | 0.56          |
| (1,628) | 1:49:A:G:H1   | 1:50:A:C:H42  | 4        | 0.56          |
| (1,628) | 1:49:A:G:H1   | 1:50:A:C:H42  | 5        | 0.56          |
| (1,570) | 1:44:A:G:H8   | 1:43:A:G:H1'  | 6        | 0.56          |
| (1,570) | 1:44:A:G:H8   | 1:43:A:G:H1'  | 7        | 0.56          |
| (1,570) | 1:44:A:G:H8   | 1:43:A:G:H1'  | 8        | 0.56          |
| (1,570) | 1:44:A:G:H8   | 1:43:A:G:H1'  | 9        | 0.56          |
| (1,566) | 1:44:A:G:H8   | 1:44:A:G:H2'  | 2        | 0.56          |
| (1,566) | 1:44:A:G:H8   | 1:44:A:G:H2'  | 5        | 0.56          |
| (1,553) | 1:43:A:G:H8   | 1:42:A:U:H5'' | 2        | 0.56          |
| (1,544) | 1:41:A:C:H6   | 1:40:A:G:H2'  | 1        | 0.56          |
| (1,544) | 1:41:A:C:H6   | 1:40:A:G:H2'  | 3        | 0.56          |
| (1,544) | 1:41:A:C:H6   | 1:40:A:G:H2'  | 5        | 0.56          |
| (1,544) | 1:41:A:C:H6   | 1:40:A:G:H2'  | 8        | 0.56          |
| (1,528) | 1:40:A:G:H8   | 1:40:A:G:H5'' | 4        | 0.56          |
| (1,528) | 1:40:A:G:H8   | 1:40:A:G:H5'' | 8        | 0.56          |
| (1,524) | 1:39:A:G:H1   | 1:38:A:U:H3   | 1        | 0.56          |
| (1,484) | 1:35:A:A:H2   | 1:36:A:U:H1'  | 1        | 0.56          |
| (1,484) | 1:35:A:A:H2   | 1:36:A:U:H1'  | 7        | 0.56          |
| (1,484) | 1:35:A:A:H2   | 1:36:A:U:H1'  | 10       | 0.56          |
| (1,439) | 1:31:A:G:H1   | 1:32:A:C:H5   | 1        | 0.56          |
| (1,439) | 1:31:A:G:H1   | 1:32:A:C:H5   | 2        | 0.56          |
| (1,439) | 1:31:A:G:H1   | 1:32:A:C:H5   | 4        | 0.56          |
| (1,411) | 1:29:A:G:H1   | 1:28:A:C:H5   | 3        | 0.56          |
| (1,411) | 1:29:A:G:H1   | 1:28:A:C:H5   | 6        | 0.56          |
| (1,411) | 1:29:A:G:H1   | 1:28:A:C:H5   | 8        | 0.56          |
| (1,406) | 1:29:A:G:H1   | 1:30:A:G:H8   | 2        | 0.56          |
| (1,394) | 1:28:A:C:H5   | 1:26:A:U:HO2' | 1        | 0.56          |
| (1,394) | 1:28:A:C:H5   | 1:26:A:U:HO2' | 5        | 0.56          |
| (1,394) | 1:28:A:C:H5   | 1:26:A:U:HO2' | 7        | 0.56          |
| (1,394) | 1:28:A:C:H5   | 1:26:A:U:HO2' | 10       | 0.56          |
| (1,373) | 1:28:A:C:H6   | 1:28:A:C:H5'  | 8        | 0.56          |
| (1,357) | 1:26:A:U:HO2' | 1:27:A:U:H1'  | 5        | 0.56          |
| (1,351) | 1:26:A:U:H6   | 1:25:A:C:H1'  | 1        | 0.56          |
| (1,351) | 1:26:A:U:H6   | 1:25:A:C:H1'  | 8        | 0.56          |
| (1,295) | 1:21:A:U:H3   | 1:22:A:C:H6   | 6        | 0.56          |
| (1,265) | 1:19:A:G:H8   | 1:17:A:U:H6   | 7        | 0.56          |
| (1,240) | 1:16:A:A:H2   | 1:17:A:U:H1'  | 5        | 0.56          |
| (1,232) | 1:16:A:A:H8   | 1:16:A:A:H5'' | 6        | 0.56          |
| (1,196) | 1:12:A:C:H6   | 1:11:A:A:H2'  | 1        | 0.56          |

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| Key     | Atom-1      | Atom-2        | Model ID | Violation (Å) |
|---------|-------------|---------------|----------|---------------|
| (1,196) | 1:12:A:C:H6 | 1:11:A:A:H2'  | 7        | 0.56          |
| (1,196) | 1:12:A:C:H6 | 1:11:A:A:H2'  | 10       | 0.56          |
| (1,149) | 1:9:A:U:H3  | 1:50:A:C:H42  | 7        | 0.56          |
| (1,646) | 1:51:A:G:H8 | 1:51:A:G:H5'' | 9        | 0.55          |
| (1,628) | 1:49:A:G:H1 | 1:50:A:C:H42  | 2        | 0.55          |
| (1,627) | 1:49:A:G:H1 | 1:50:A:C:H1'  | 4        | 0.55          |
| (1,570) | 1:44:A:G:H8 | 1:43:A:G:H1'  | 2        | 0.55          |
| (1,570) | 1:44:A:G:H8 | 1:43:A:G:H1'  | 3        | 0.55          |
| (1,570) | 1:44:A:G:H8 | 1:43:A:G:H1'  | 5        | 0.55          |
| (1,570) | 1:44:A:G:H8 | 1:43:A:G:H1'  | 10       | 0.55          |
| (1,566) | 1:44:A:G:H8 | 1:44:A:G:H2'  | 1        | 0.55          |
| (1,566) | 1:44:A:G:H8 | 1:44:A:G:H2'  | 3        | 0.55          |
| (1,566) | 1:44:A:G:H8 | 1:44:A:G:H2'  | 8        | 0.55          |
| (1,553) | 1:43:A:G:H8 | 1:42:A:U:H5'' | 4        | 0.55          |
| (1,544) | 1:41:A:C:H6 | 1:40:A:G:H2'  | 2        | 0.55          |
| (1,528) | 1:40:A:G:H8 | 1:40:A:G:H5'' | 5        | 0.55          |
| (1,528) | 1:40:A:G:H8 | 1:40:A:G:H5'' | 7        | 0.55          |
| (1,524) | 1:39:A:G:H1 | 1:38:A:U:H3   | 2        | 0.55          |
| (1,524) | 1:39:A:G:H1 | 1:38:A:U:H3   | 4        | 0.55          |
| (1,524) | 1:39:A:G:H1 | 1:38:A:U:H3   | 8        | 0.55          |
| (1,484) | 1:35:A:A:H2 | 1:36:A:U:H1'  | 4        | 0.55          |
| (1,463) | 1:33:A:U:H6 | 1:32:A:C:H3'  | 6        | 0.55          |
| (1,460) | 1:33:A:U:H6 | 1:32:A:C:H6   | 3        | 0.55          |
| (1,460) | 1:33:A:U:H6 | 1:32:A:C:H6   | 7        | 0.55          |
| (1,406) | 1:29:A:G:H1 | 1:30:A:G:H8   | 1        | 0.55          |
| (1,406) | 1:29:A:G:H1 | 1:30:A:G:H8   | 5        | 0.55          |
| (1,406) | 1:29:A:G:H1 | 1:30:A:G:H8   | 6        | 0.55          |
| (1,406) | 1:29:A:G:H1 | 1:30:A:G:H8   | 8        | 0.55          |
| (1,394) | 1:28:A:C:H5 | 1:26:A:U:HO2' | 2        | 0.55          |
| (1,394) | 1:28:A:C:H5 | 1:26:A:U:HO2' | 8        | 0.55          |
| (1,394) | 1:28:A:C:H5 | 1:26:A:U:HO2' | 9        | 0.55          |
| (1,373) | 1:28:A:C:H6 | 1:28:A:C:H5'  | 4        | 0.55          |
| (1,373) | 1:28:A:C:H6 | 1:28:A:C:H5'  | 5        | 0.55          |
| (1,351) | 1:26:A:U:H6 | 1:25:A:C:H1'  | 3        | 0.55          |
| (1,325) | 1:24:A:C:H6 | 1:23:A:G:H8   | 4        | 0.55          |
| (1,325) | 1:24:A:C:H6 | 1:23:A:G:H8   | 7        | 0.55          |
| (1,240) | 1:16:A:A:H2 | 1:17:A:U:H1'  | 3        | 0.55          |
| (1,196) | 1:12:A:C:H6 | 1:11:A:A:H2'  | 3        | 0.55          |
| (1,196) | 1:12:A:C:H6 | 1:11:A:A:H2'  | 5        | 0.55          |
| (1,196) | 1:12:A:C:H6 | 1:11:A:A:H2'  | 6        | 0.55          |
| (1,196) | 1:12:A:C:H6 | 1:11:A:A:H2'  | 9        | 0.55          |
| (1,149) | 1:9:A:U:H3  | 1:50:A:C:H42  | 10       | 0.55          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,570) | 1:44:A:G:H8  | 1:43:A:G:H1'  | 1        | 0.54          |
| (1,566) | 1:44:A:G:H8  | 1:44:A:G:H2'  | 4        | 0.54          |
| (1,528) | 1:40:A:G:H8  | 1:40:A:G:H5'' | 1        | 0.54          |
| (1,528) | 1:40:A:G:H8  | 1:40:A:G:H5'' | 2        | 0.54          |
| (1,528) | 1:40:A:G:H8  | 1:40:A:G:H5'' | 3        | 0.54          |
| (1,528) | 1:40:A:G:H8  | 1:40:A:G:H5'' | 6        | 0.54          |
| (1,528) | 1:40:A:G:H8  | 1:40:A:G:H5'' | 9        | 0.54          |
| (1,528) | 1:40:A:G:H8  | 1:40:A:G:H5'' | 10       | 0.54          |
| (1,524) | 1:39:A:G:H1  | 1:38:A:U:H3   | 3        | 0.54          |
| (1,463) | 1:33:A:U:H6  | 1:32:A:C:H3'  | 10       | 0.54          |
| (1,460) | 1:33:A:U:H6  | 1:32:A:C:H6   | 5        | 0.54          |
| (1,425) | 1:30:A:G:H1  | 1:26:A:U:H1'  | 4        | 0.54          |
| (1,425) | 1:30:A:G:H1  | 1:26:A:U:H1'  | 7        | 0.54          |
| (1,425) | 1:30:A:G:H1  | 1:26:A:U:H1'  | 10       | 0.54          |
| (1,406) | 1:29:A:G:H1  | 1:30:A:G:H8   | 7        | 0.54          |
| (1,406) | 1:29:A:G:H1  | 1:30:A:G:H8   | 9        | 0.54          |
| (1,406) | 1:29:A:G:H1  | 1:30:A:G:H8   | 10       | 0.54          |
| (1,403) | 1:29:A:G:H1' | 1:28:A:C:H5'  | 8        | 0.54          |
| (1,394) | 1:28:A:C:H5  | 1:26:A:U:HO2' | 4        | 0.54          |
| (1,351) | 1:26:A:U:H6  | 1:25:A:C:H1'  | 6        | 0.54          |
| (1,325) | 1:24:A:C:H6  | 1:23:A:G:H8   | 1        | 0.54          |
| (1,325) | 1:24:A:C:H6  | 1:23:A:G:H8   | 5        | 0.54          |
| (1,265) | 1:19:A:G:H8  | 1:17:A:U:H6   | 1        | 0.54          |
| (1,265) | 1:19:A:G:H8  | 1:17:A:U:H6   | 2        | 0.54          |
| (1,265) | 1:19:A:G:H8  | 1:17:A:U:H6   | 3        | 0.54          |
| (1,240) | 1:16:A:A:H2  | 1:17:A:U:H1'  | 2        | 0.54          |
| (1,240) | 1:16:A:A:H2  | 1:17:A:U:H1'  | 7        | 0.54          |
| (1,240) | 1:16:A:A:H2  | 1:17:A:U:H1'  | 9        | 0.54          |
| (1,240) | 1:16:A:A:H2  | 1:17:A:U:H1'  | 10       | 0.54          |
| (1,196) | 1:12:A:C:H6  | 1:11:A:A:H2'  | 8        | 0.54          |
| (1,598) | 1:47:A:A:H8  | 1:47:A:A:H5'  | 8        | 0.53          |
| (1,547) | 1:42:A:U:H6  | 1:42:A:U:H5'  | 4        | 0.53          |
| (1,547) | 1:42:A:U:H6  | 1:42:A:U:H5'  | 6        | 0.53          |
| (1,527) | 1:40:A:G:H8  | 1:40:A:G:H3'  | 4        | 0.53          |
| (1,524) | 1:39:A:G:H1  | 1:38:A:U:H3   | 7        | 0.53          |
| (1,524) | 1:39:A:G:H1  | 1:38:A:U:H3   | 9        | 0.53          |
| (1,524) | 1:39:A:G:H1  | 1:38:A:U:H3   | 10       | 0.53          |
| (1,460) | 1:33:A:U:H6  | 1:32:A:C:H6   | 1        | 0.53          |
| (1,460) | 1:33:A:U:H6  | 1:32:A:C:H6   | 2        | 0.53          |
| (1,460) | 1:33:A:U:H6  | 1:32:A:C:H6   | 9        | 0.53          |
| (1,460) | 1:33:A:U:H6  | 1:32:A:C:H6   | 10       | 0.53          |
| (1,425) | 1:30:A:G:H1  | 1:26:A:U:H1'  | 2        | 0.53          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (1,403) | 1:29:A:G:H1' | 1:28:A:C:H5' | 1        | 0.53          |
| (1,403) | 1:29:A:G:H1' | 1:28:A:C:H5' | 4        | 0.53          |
| (1,351) | 1:26:A:U:H6  | 1:25:A:C:H1' | 5        | 0.53          |
| (1,325) | 1:24:A:C:H6  | 1:23:A:G:H8  | 2        | 0.53          |
| (1,325) | 1:24:A:C:H6  | 1:23:A:G:H8  | 3        | 0.53          |
| (1,265) | 1:19:A:G:H8  | 1:17:A:U:H6  | 6        | 0.53          |
| (1,240) | 1:16:A:A:H2  | 1:17:A:U:H1' | 1        | 0.53          |
| (1,240) | 1:16:A:A:H2  | 1:17:A:U:H1' | 4        | 0.53          |
| (1,240) | 1:16:A:A:H2  | 1:17:A:U:H1' | 6        | 0.53          |
| (1,240) | 1:16:A:A:H2  | 1:17:A:U:H1' | 8        | 0.53          |
| (1,571) | 1:44:A:G:H8  | 1:43:A:G:H2' | 6        | 0.52          |
| (1,538) | 1:40:A:G:H1  | 1:15:A:C:H41 | 2        | 0.52          |
| (1,538) | 1:40:A:G:H1  | 1:15:A:C:H41 | 9        | 0.52          |
| (1,527) | 1:40:A:G:H8  | 1:40:A:G:H3' | 6        | 0.52          |
| (1,524) | 1:39:A:G:H1  | 1:38:A:U:H3  | 5        | 0.52          |
| (1,518) | 1:39:A:G:H8  | 1:38:A:U:H5  | 8        | 0.52          |
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1' | 9        | 0.52          |
| (1,460) | 1:33:A:U:H6  | 1:32:A:C:H6  | 4        | 0.52          |
| (1,460) | 1:33:A:U:H6  | 1:32:A:C:H6  | 8        | 0.52          |
| (1,425) | 1:30:A:G:H1  | 1:26:A:U:H1' | 3        | 0.52          |
| (1,425) | 1:30:A:G:H1  | 1:26:A:U:H1' | 5        | 0.52          |
| (1,406) | 1:29:A:G:H1  | 1:30:A:G:H8  | 3        | 0.52          |
| (1,391) | 1:28:A:C:H42 | 1:26:A:U:H3' | 9        | 0.52          |
| (1,354) | 1:26:A:U:H6  | 1:25:A:C:H2' | 6        | 0.52          |
| (1,325) | 1:24:A:C:H6  | 1:23:A:G:H8  | 6        | 0.52          |
| (1,294) | 1:21:A:U:H3  | 1:22:A:C:H41 | 3        | 0.52          |
| (1,294) | 1:21:A:U:H3  | 1:22:A:C:H41 | 5        | 0.52          |
| (1,273) | 1:19:A:G:H1  | 1:20:A:A:H2  | 3        | 0.52          |
| (1,265) | 1:19:A:G:H8  | 1:17:A:U:H6  | 10       | 0.52          |
| (1,149) | 1:9:A:U:H3   | 1:50:A:C:H42 | 6        | 0.52          |
| (1,598) | 1:47:A:A:H8  | 1:47:A:A:H5' | 1        | 0.51          |
| (1,598) | 1:47:A:A:H8  | 1:47:A:A:H5' | 2        | 0.51          |
| (1,598) | 1:47:A:A:H8  | 1:47:A:A:H5' | 3        | 0.51          |
| (1,598) | 1:47:A:A:H8  | 1:47:A:A:H5' | 5        | 0.51          |
| (1,598) | 1:47:A:A:H8  | 1:47:A:A:H5' | 6        | 0.51          |
| (1,586) | 1:45:A:C:H42 | 1:44:A:G:H1  | 4        | 0.51          |
| (1,547) | 1:42:A:U:H6  | 1:42:A:U:H5' | 2        | 0.51          |
| (1,538) | 1:40:A:G:H1  | 1:15:A:C:H41 | 5        | 0.51          |
| (1,527) | 1:40:A:G:H8  | 1:40:A:G:H3' | 3        | 0.51          |
| (1,518) | 1:39:A:G:H8  | 1:38:A:U:H5  | 4        | 0.51          |
| (1,518) | 1:39:A:G:H8  | 1:38:A:U:H5  | 9        | 0.51          |
| (1,483) | 1:35:A:A:H8  | 1:34:A:G:H8  | 4        | 0.51          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (1,461) | 1:33:A:U:H6  | 1:32:A:C:H1' | 6        | 0.51          |
| (1,460) | 1:33:A:U:H6  | 1:32:A:C:H6  | 6        | 0.51          |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5  | 10       | 0.51          |
| (1,435) | 1:31:A:G:H8  | 1:30:A:G:H1' | 10       | 0.51          |
| (1,425) | 1:30:A:G:H1  | 1:26:A:U:H1' | 1        | 0.51          |
| (1,391) | 1:28:A:C:H42 | 1:26:A:U:H3' | 7        | 0.51          |
| (1,391) | 1:28:A:C:H42 | 1:26:A:U:H3' | 10       | 0.51          |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1' | 6        | 0.51          |
| (1,322) | 1:24:A:C:H6  | 1:23:A:G:H1' | 9        | 0.51          |
| (1,322) | 1:24:A:C:H6  | 1:23:A:G:H1' | 10       | 0.51          |
| (1,294) | 1:21:A:U:H3  | 1:22:A:C:H41 | 1        | 0.51          |
| (1,294) | 1:21:A:U:H3  | 1:22:A:C:H41 | 2        | 0.51          |
| (1,294) | 1:21:A:U:H3  | 1:22:A:C:H41 | 4        | 0.51          |
| (1,273) | 1:19:A:G:H1  | 1:20:A:A:H2  | 6        | 0.51          |
| (1,265) | 1:19:A:G:H8  | 1:17:A:U:H6  | 4        | 0.51          |
| (1,265) | 1:19:A:G:H8  | 1:17:A:U:H6  | 5        | 0.51          |
| (1,265) | 1:19:A:G:H8  | 1:17:A:U:H6  | 9        | 0.51          |
| (1,149) | 1:9:A:U:H3   | 1:50:A:C:H42 | 1        | 0.51          |
| (1,18)  | 1:2:A:G:H8   | 1:2:A:G:H5'' | 6        | 0.51          |
| (1,598) | 1:47:A:A:H8  | 1:47:A:A:H5' | 4        | 0.5           |
| (1,598) | 1:47:A:A:H8  | 1:47:A:A:H5' | 7        | 0.5           |
| (1,598) | 1:47:A:A:H8  | 1:47:A:A:H5' | 10       | 0.5           |
| (1,586) | 1:45:A:C:H42 | 1:44:A:G:H1  | 1        | 0.5           |
| (1,586) | 1:45:A:C:H42 | 1:44:A:G:H1  | 6        | 0.5           |
| (1,586) | 1:45:A:C:H42 | 1:44:A:G:H1  | 8        | 0.5           |
| (1,547) | 1:42:A:U:H6  | 1:42:A:U:H5' | 3        | 0.5           |
| (1,538) | 1:40:A:G:H1  | 1:15:A:C:H41 | 1        | 0.5           |
| (1,538) | 1:40:A:G:H1  | 1:15:A:C:H41 | 3        | 0.5           |
| (1,538) | 1:40:A:G:H1  | 1:15:A:C:H41 | 7        | 0.5           |
| (1,538) | 1:40:A:G:H1  | 1:15:A:C:H41 | 8        | 0.5           |
| (1,538) | 1:40:A:G:H1  | 1:15:A:C:H41 | 10       | 0.5           |
| (1,527) | 1:40:A:G:H8  | 1:40:A:G:H3' | 8        | 0.5           |
| (1,518) | 1:39:A:G:H8  | 1:38:A:U:H5  | 7        | 0.5           |
| (1,461) | 1:33:A:U:H6  | 1:32:A:C:H1' | 10       | 0.5           |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5  | 6        | 0.5           |
| (1,425) | 1:30:A:G:H1  | 1:26:A:U:H1' | 8        | 0.5           |
| (1,391) | 1:28:A:C:H42 | 1:26:A:U:H3' | 2        | 0.5           |
| (1,322) | 1:24:A:C:H6  | 1:23:A:G:H1' | 6        | 0.5           |
| (1,294) | 1:21:A:U:H3  | 1:22:A:C:H41 | 6        | 0.5           |
| (1,273) | 1:19:A:G:H1  | 1:20:A:A:H2  | 1        | 0.5           |
| (1,273) | 1:19:A:G:H1  | 1:20:A:A:H2  | 2        | 0.5           |
| (1,265) | 1:19:A:G:H8  | 1:17:A:U:H6  | 8        | 0.5           |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,18)  | 1:2:A:G:H8   | 1:2:A:G:H5''  | 7        | 0.5           |
| (1,18)  | 1:2:A:G:H8   | 1:2:A:G:H5''  | 9        | 0.5           |
| (1,18)  | 1:2:A:G:H8   | 1:2:A:G:H5''  | 10       | 0.5           |
| (1,601) | 1:47:A:A:H2  | 1:48:A:G:H8   | 8        | 0.49          |
| (1,598) | 1:47:A:A:H8  | 1:47:A:A:H5'  | 9        | 0.49          |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 6        | 0.49          |
| (1,571) | 1:44:A:G:H8  | 1:43:A:G:H2'  | 8        | 0.49          |
| (1,556) | 1:43:A:G:H8  | 1:41:A:C:H1'  | 10       | 0.49          |
| (1,547) | 1:42:A:U:H6  | 1:42:A:U:H5'  | 5        | 0.49          |
| (1,527) | 1:40:A:G:H8  | 1:40:A:G:H3'  | 1        | 0.49          |
| (1,453) | 1:32:A:C:H6  | 1:31:A:G:H8   | 6        | 0.49          |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5   | 9        | 0.49          |
| (1,294) | 1:21:A:U:H3  | 1:22:A:C:H41  | 8        | 0.49          |
| (1,271) | 1:19:A:G:H1  | 1:36:A:U:H3   | 2        | 0.49          |
| (1,271) | 1:19:A:G:H1  | 1:36:A:U:H3   | 6        | 0.49          |
| (1,271) | 1:19:A:G:H1  | 1:36:A:U:H3   | 7        | 0.49          |
| (1,202) | 1:13:A:C:H6  | 1:13:A:C:H5'' | 6        | 0.49          |
| (1,18)  | 1:2:A:G:H8   | 1:2:A:G:H5''  | 8        | 0.49          |
| (1,586) | 1:45:A:C:H42 | 1:44:A:G:H1   | 2        | 0.48          |
| (1,571) | 1:44:A:G:H8  | 1:43:A:G:H2'  | 5        | 0.48          |
| (1,547) | 1:42:A:U:H6  | 1:42:A:U:H5'  | 8        | 0.48          |
| (1,538) | 1:40:A:G:H1  | 1:15:A:C:H41  | 4        | 0.48          |
| (1,527) | 1:40:A:G:H8  | 1:40:A:G:H3'  | 2        | 0.48          |
| (1,527) | 1:40:A:G:H8  | 1:40:A:G:H3'  | 5        | 0.48          |
| (1,431) | 1:31:A:G:H8  | 1:31:A:G:H5'' | 1        | 0.48          |
| (1,431) | 1:31:A:G:H8  | 1:31:A:G:H5'' | 8        | 0.48          |
| (1,294) | 1:21:A:U:H3  | 1:22:A:C:H41  | 7        | 0.48          |
| (1,271) | 1:19:A:G:H1  | 1:36:A:U:H3   | 10       | 0.48          |
| (1,202) | 1:13:A:C:H6  | 1:13:A:C:H5'' | 3        | 0.48          |
| (1,149) | 1:9:A:U:H3   | 1:50:A:C:H42  | 4        | 0.48          |
| (1,149) | 1:9:A:U:H3   | 1:50:A:C:H42  | 5        | 0.48          |
| (1,49)  | 1:4:A:A:H8   | 1:4:A:A:H5''  | 6        | 0.48          |
| (1,18)  | 1:2:A:G:H8   | 1:2:A:G:H5''  | 1        | 0.48          |
| (1,18)  | 1:2:A:G:H8   | 1:2:A:G:H5''  | 3        | 0.48          |
| (1,18)  | 1:2:A:G:H8   | 1:2:A:G:H5''  | 4        | 0.48          |
| (1,599) | 1:47:A:A:H8  | 1:46:A:U:H1'  | 8        | 0.47          |
| (1,571) | 1:44:A:G:H8  | 1:43:A:G:H2'  | 3        | 0.47          |
| (1,556) | 1:43:A:G:H8  | 1:41:A:C:H1'  | 9        | 0.47          |
| (1,518) | 1:39:A:G:H8  | 1:38:A:U:H5   | 1        | 0.47          |
| (1,518) | 1:39:A:G:H8  | 1:38:A:U:H5   | 6        | 0.47          |
| (1,518) | 1:39:A:G:H8  | 1:38:A:U:H5   | 10       | 0.47          |
| (1,419) | 1:30:A:G:H8  | 1:29:A:G:H2'  | 9        | 0.47          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,354) | 1:26:A:U:H6  | 1:25:A:C:H2'  | 1        | 0.47          |
| (1,322) | 1:24:A:C:H6  | 1:23:A:G:H1'  | 7        | 0.47          |
| (1,271) | 1:19:A:G:H1  | 1:36:A:U:H3   | 3        | 0.47          |
| (1,202) | 1:13:A:C:H6  | 1:13:A:C:H5'' | 4        | 0.47          |
| (1,149) | 1:9:A:U:H3   | 1:50:A:C:H42  | 3        | 0.47          |
| (1,18)  | 1:2:A:G:H8   | 1:2:A:G:H5''  | 2        | 0.47          |
| (1,18)  | 1:2:A:G:H8   | 1:2:A:G:H5''  | 5        | 0.47          |
| (1,571) | 1:44:A:G:H8  | 1:43:A:G:H2'  | 1        | 0.46          |
| (1,556) | 1:43:A:G:H8  | 1:41:A:C:H1'  | 7        | 0.46          |
| (1,547) | 1:42:A:U:H6  | 1:42:A:U:H5'  | 1        | 0.46          |
| (1,538) | 1:40:A:G:H1  | 1:15:A:C:H41  | 6        | 0.46          |
| (1,518) | 1:39:A:G:H8  | 1:38:A:U:H5   | 5        | 0.46          |
| (1,435) | 1:31:A:G:H8  | 1:30:A:G:H1'  | 9        | 0.46          |
| (1,431) | 1:31:A:G:H8  | 1:31:A:G:H5'' | 3        | 0.46          |
| (1,431) | 1:31:A:G:H8  | 1:31:A:G:H5'' | 4        | 0.46          |
| (1,431) | 1:31:A:G:H8  | 1:31:A:G:H5'' | 5        | 0.46          |
| (1,354) | 1:26:A:U:H6  | 1:25:A:C:H2'  | 8        | 0.46          |
| (1,325) | 1:24:A:C:H6  | 1:23:A:G:H8   | 10       | 0.46          |
| (1,264) | 1:19:A:G:H8  | 1:19:A:G:H3'  | 6        | 0.46          |
| (1,202) | 1:13:A:C:H6  | 1:13:A:C:H5'' | 5        | 0.46          |
| (1,149) | 1:9:A:U:H3   | 1:50:A:C:H42  | 2        | 0.46          |
| (1,33)  | 1:3:A:G:H8   | 1:3:A:G:H5''  | 6        | 0.46          |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 7        | 0.45          |
| (1,585) | 1:45:A:C:H6  | 1:44:A:G:H1'  | 4        | 0.45          |
| (1,585) | 1:45:A:C:H6  | 1:44:A:G:H1'  | 6        | 0.45          |
| (1,585) | 1:45:A:C:H6  | 1:44:A:G:H1'  | 8        | 0.45          |
| (1,571) | 1:44:A:G:H8  | 1:43:A:G:H2'  | 2        | 0.45          |
| (1,518) | 1:39:A:G:H8  | 1:38:A:U:H5   | 2        | 0.45          |
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1'  | 10       | 0.45          |
| (1,483) | 1:35:A:A:H8  | 1:34:A:G:H8   | 5        | 0.45          |
| (1,403) | 1:29:A:G:H1' | 1:28:A:C:H5'  | 2        | 0.45          |
| (1,354) | 1:26:A:U:H6  | 1:25:A:C:H2'  | 3        | 0.45          |
| (1,353) | 1:26:A:U:H6  | 1:25:A:C:H3'  | 6        | 0.45          |
| (1,325) | 1:24:A:C:H6  | 1:23:A:G:H8   | 9        | 0.45          |
| (1,271) | 1:19:A:G:H1  | 1:36:A:U:H3   | 1        | 0.45          |
| (1,271) | 1:19:A:G:H1  | 1:36:A:U:H3   | 5        | 0.45          |
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 6        | 0.45          |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 6        | 0.45          |
| (1,49)  | 1:4:A:A:H8   | 1:4:A:A:H5''  | 3        | 0.45          |
| (1,661) | 1:52:A:G:H8  | 1:52:A:G:H5'' | 2        | 0.44          |
| (1,661) | 1:52:A:G:H8  | 1:52:A:G:H5'' | 6        | 0.44          |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 10       | 0.44          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,585) | 1:45:A:C:H6  | 1:44:A:G:H1'  | 1        | 0.44          |
| (1,585) | 1:45:A:C:H6  | 1:44:A:G:H1'  | 2        | 0.44          |
| (1,585) | 1:45:A:C:H6  | 1:44:A:G:H1'  | 3        | 0.44          |
| (1,455) | 1:32:A:C:H5  | 1:31:A:G:H1'  | 5        | 0.44          |
| (1,455) | 1:32:A:C:H5  | 1:31:A:G:H1'  | 6        | 0.44          |
| (1,431) | 1:31:A:G:H8  | 1:31:A:G:H5'' | 2        | 0.44          |
| (1,354) | 1:26:A:U:H6  | 1:25:A:C:H2'  | 5        | 0.44          |
| (1,322) | 1:24:A:C:H6  | 1:23:A:G:H1'  | 2        | 0.44          |
| (1,264) | 1:19:A:G:H8  | 1:19:A:G:H3'  | 1        | 0.44          |
| (1,248) | 1:17:A:U:H6  | 1:16:A:A:H1'  | 6        | 0.44          |
| (1,202) | 1:13:A:C:H6  | 1:13:A:C:H5'' | 2        | 0.44          |
| (1,202) | 1:13:A:C:H6  | 1:13:A:C:H5'' | 8        | 0.44          |
| (1,49)  | 1:4:A:A:H8   | 1:4:A:A:H5''  | 5        | 0.44          |
| (1,49)  | 1:4:A:A:H8   | 1:4:A:A:H5''  | 7        | 0.44          |
| (1,736) | 1:56:A:C:H6  | 1:56:A:C:H5'' | 6        | 0.43          |
| (1,661) | 1:52:A:G:H8  | 1:52:A:G:H5'' | 4        | 0.43          |
| (1,661) | 1:52:A:G:H8  | 1:52:A:G:H5'' | 5        | 0.43          |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 9        | 0.43          |
| (1,585) | 1:45:A:C:H6  | 1:44:A:G:H1'  | 5        | 0.43          |
| (1,585) | 1:45:A:C:H6  | 1:44:A:G:H1'  | 7        | 0.43          |
| (1,585) | 1:45:A:C:H6  | 1:44:A:G:H1'  | 10       | 0.43          |
| (1,571) | 1:44:A:G:H8  | 1:43:A:G:H2'  | 4        | 0.43          |
| (1,571) | 1:44:A:G:H8  | 1:43:A:G:H2'  | 7        | 0.43          |
| (1,425) | 1:30:A:G:H1  | 1:26:A:U:H1'  | 6        | 0.43          |
| (1,322) | 1:24:A:C:H6  | 1:23:A:G:H1'  | 3        | 0.43          |
| (1,273) | 1:19:A:G:H1  | 1:20:A:A:H2   | 8        | 0.43          |
| (1,271) | 1:19:A:G:H1  | 1:36:A:U:H3   | 8        | 0.43          |
| (1,264) | 1:19:A:G:H8  | 1:19:A:G:H3'  | 8        | 0.43          |
| (1,202) | 1:13:A:C:H6  | 1:13:A:C:H5'' | 1        | 0.43          |
| (1,49)  | 1:4:A:A:H8   | 1:4:A:A:H5''  | 2        | 0.43          |
| (1,49)  | 1:4:A:A:H8   | 1:4:A:A:H5''  | 4        | 0.43          |
| (1,49)  | 1:4:A:A:H8   | 1:4:A:A:H5''  | 8        | 0.43          |
| (1,49)  | 1:4:A:A:H8   | 1:4:A:A:H5''  | 9        | 0.43          |
| (1,49)  | 1:4:A:A:H8   | 1:4:A:A:H5''  | 10       | 0.43          |
| (1,33)  | 1:3:A:G:H8   | 1:3:A:G:H5''  | 7        | 0.43          |
| (1,33)  | 1:3:A:G:H8   | 1:3:A:G:H5''  | 10       | 0.43          |
| (1,661) | 1:52:A:G:H8  | 1:52:A:G:H5'' | 1        | 0.42          |
| (1,661) | 1:52:A:G:H8  | 1:52:A:G:H5'' | 3        | 0.42          |
| (1,661) | 1:52:A:G:H8  | 1:52:A:G:H5'' | 8        | 0.42          |
| (1,586) | 1:45:A:C:H42 | 1:44:A:G:H1   | 5        | 0.42          |
| (1,585) | 1:45:A:C:H6  | 1:44:A:G:H1'  | 9        | 0.42          |
| (1,571) | 1:44:A:G:H8  | 1:43:A:G:H2'  | 9        | 0.42          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,483) | 1:35:A:A:H8  | 1:34:A:G:H8   | 7        | 0.42          |
| (1,391) | 1:28:A:C:H42 | 1:26:A:U:H3'  | 4        | 0.42          |
| (1,353) | 1:26:A:U:H6  | 1:25:A:C:H3'  | 1        | 0.42          |
| (1,287) | 1:21:A:U:H6  | 1:20:A:A:H8   | 6        | 0.42          |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 7        | 0.42          |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 9        | 0.42          |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 10       | 0.42          |
| (1,49)  | 1:4:A:A:H8   | 1:4:A:A:H5''  | 1        | 0.42          |
| (1,33)  | 1:3:A:G:H8   | 1:3:A:G:H5''  | 9        | 0.42          |
| (1,751) | 1:57:A:C:H6  | 1:57:A:C:H5'' | 6        | 0.41          |
| (1,661) | 1:52:A:G:H8  | 1:52:A:G:H5'' | 7        | 0.41          |
| (1,578) | 1:45:A:C:H6  | 1:45:A:C:H3'  | 6        | 0.41          |
| (1,572) | 1:44:A:G:H8  | 1:43:A:G:H8   | 9        | 0.41          |
| (1,572) | 1:44:A:G:H8  | 1:43:A:G:H8   | 10       | 0.41          |
| (1,518) | 1:39:A:G:H8  | 1:38:A:U:H5   | 3        | 0.41          |
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1'  | 5        | 0.41          |
| (1,453) | 1:32:A:C:H6  | 1:31:A:G:H8   | 3        | 0.41          |
| (1,453) | 1:32:A:C:H6  | 1:31:A:G:H8   | 5        | 0.41          |
| (1,431) | 1:31:A:G:H8  | 1:31:A:G:H5'' | 6        | 0.41          |
| (1,409) | 1:29:A:G:H1  | 1:26:A:U:H2'  | 9        | 0.41          |
| (1,353) | 1:26:A:U:H6  | 1:25:A:C:H3'  | 8        | 0.41          |
| (1,294) | 1:21:A:U:H3  | 1:22:A:C:H41  | 9        | 0.41          |
| (1,286) | 1:21:A:U:H6  | 1:20:A:A:H1'  | 4        | 0.41          |
| (1,286) | 1:21:A:U:H6  | 1:20:A:A:H1'  | 7        | 0.41          |
| (1,271) | 1:19:A:G:H1  | 1:36:A:U:H3   | 4        | 0.41          |
| (1,264) | 1:19:A:G:H8  | 1:19:A:G:H3'  | 3        | 0.41          |
| (1,250) | 1:17:A:U:H6  | 1:16:A:A:H8   | 7        | 0.41          |
| (1,250) | 1:17:A:U:H6  | 1:16:A:A:H8   | 8        | 0.41          |
| (1,248) | 1:17:A:U:H6  | 1:16:A:A:H1'  | 8        | 0.41          |
| (1,33)  | 1:3:A:G:H8   | 1:3:A:G:H5''  | 8        | 0.41          |
| (1,751) | 1:57:A:C:H6  | 1:57:A:C:H5'' | 1        | 0.4           |
| (1,751) | 1:57:A:C:H6  | 1:57:A:C:H5'' | 2        | 0.4           |
| (1,751) | 1:57:A:C:H6  | 1:57:A:C:H5'' | 3        | 0.4           |
| (1,751) | 1:57:A:C:H6  | 1:57:A:C:H5'' | 4        | 0.4           |
| (1,751) | 1:57:A:C:H6  | 1:57:A:C:H5'' | 5        | 0.4           |
| (1,751) | 1:57:A:C:H6  | 1:57:A:C:H5'' | 7        | 0.4           |
| (1,751) | 1:57:A:C:H6  | 1:57:A:C:H5'' | 8        | 0.4           |
| (1,751) | 1:57:A:C:H6  | 1:57:A:C:H5'' | 9        | 0.4           |
| (1,751) | 1:57:A:C:H6  | 1:57:A:C:H5'' | 10       | 0.4           |
| (1,578) | 1:45:A:C:H6  | 1:45:A:C:H3'  | 7        | 0.4           |
| (1,571) | 1:44:A:G:H8  | 1:43:A:G:H2'  | 10       | 0.4           |
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1'  | 2        | 0.4           |

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| Key     | Atom-1      | Atom-2        | Model ID | Violation (Å) |
|---------|-------------|---------------|----------|---------------|
| (1,483) | 1:35:A:A:H8 | 1:34:A:G:H8   | 1        | 0.4           |
| (1,483) | 1:35:A:A:H8 | 1:34:A:G:H8   | 8        | 0.4           |
| (1,431) | 1:31:A:G:H8 | 1:31:A:G:H5'' | 7        | 0.4           |
| (1,306) | 1:23:A:G:H8 | 1:22:A:C:H1'  | 9        | 0.4           |
| (1,292) | 1:21:A:U:H3 | 1:22:A:C:H5   | 3        | 0.4           |
| (1,286) | 1:21:A:U:H6 | 1:20:A:A:H1'  | 5        | 0.4           |
| (1,273) | 1:19:A:G:H1 | 1:20:A:A:H2   | 7        | 0.4           |
| (1,273) | 1:19:A:G:H1 | 1:20:A:A:H2   | 10       | 0.4           |
| (1,250) | 1:17:A:U:H6 | 1:16:A:A:H8   | 3        | 0.4           |
| (1,250) | 1:17:A:U:H6 | 1:16:A:A:H8   | 9        | 0.4           |
| (1,248) | 1:17:A:U:H6 | 1:16:A:A:H1'  | 2        | 0.4           |
| (1,202) | 1:13:A:C:H6 | 1:13:A:C:H5'' | 7        | 0.4           |
| (1,195) | 1:12:A:C:H6 | 1:11:A:A:H1'  | 3        | 0.4           |
| (1,195) | 1:12:A:C:H6 | 1:11:A:A:H1'  | 4        | 0.4           |
| (1,195) | 1:12:A:C:H6 | 1:11:A:A:H1'  | 7        | 0.4           |
| (1,195) | 1:12:A:C:H6 | 1:11:A:A:H1'  | 10       | 0.4           |
| (1,98)  | 1:6:A:C:H5  | 1:5:A:U:H3    | 8        | 0.4           |
| (1,78)  | 1:5:A:U:H3  | 1:6:A:C:H5    | 8        | 0.4           |
| (1,33)  | 1:3:A:G:H8  | 1:3:A:G:H5''  | 1        | 0.4           |
| (1,33)  | 1:3:A:G:H8  | 1:3:A:G:H5''  | 2        | 0.4           |
| (1,33)  | 1:3:A:G:H8  | 1:3:A:G:H5''  | 3        | 0.4           |
| (1,736) | 1:56:A:C:H6 | 1:56:A:C:H5'' | 9        | 0.39          |
| (1,736) | 1:56:A:C:H6 | 1:56:A:C:H5'' | 10       | 0.39          |
| (1,661) | 1:52:A:G:H8 | 1:52:A:G:H5'' | 9        | 0.39          |
| (1,661) | 1:52:A:G:H8 | 1:52:A:G:H5'' | 10       | 0.39          |
| (1,578) | 1:45:A:C:H6 | 1:45:A:C:H3'  | 3        | 0.39          |
| (1,578) | 1:45:A:C:H6 | 1:45:A:C:H3'  | 5        | 0.39          |
| (1,455) | 1:32:A:C:H5 | 1:31:A:G:H1'  | 3        | 0.39          |
| (1,453) | 1:32:A:C:H6 | 1:31:A:G:H8   | 1        | 0.39          |
| (1,453) | 1:32:A:C:H6 | 1:31:A:G:H8   | 8        | 0.39          |
| (1,431) | 1:31:A:G:H8 | 1:31:A:G:H5'' | 9        | 0.39          |
| (1,431) | 1:31:A:G:H8 | 1:31:A:G:H5'' | 10       | 0.39          |
| (1,409) | 1:29:A:G:H1 | 1:26:A:U:H2'  | 2        | 0.39          |
| (1,322) | 1:24:A:C:H6 | 1:23:A:G:H1'  | 1        | 0.39          |
| (1,322) | 1:24:A:C:H6 | 1:23:A:G:H1'  | 8        | 0.39          |
| (1,292) | 1:21:A:U:H3 | 1:22:A:C:H5   | 5        | 0.39          |
| (1,264) | 1:19:A:G:H8 | 1:19:A:G:H3'  | 2        | 0.39          |
| (1,264) | 1:19:A:G:H8 | 1:19:A:G:H3'  | 7        | 0.39          |
| (1,250) | 1:17:A:U:H6 | 1:16:A:A:H8   | 2        | 0.39          |
| (1,202) | 1:13:A:C:H6 | 1:13:A:C:H5'' | 9        | 0.39          |
| (1,202) | 1:13:A:C:H6 | 1:13:A:C:H5'' | 10       | 0.39          |
| (1,195) | 1:12:A:C:H6 | 1:11:A:A:H1'  | 2        | 0.39          |

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| Key     | Atom-1      | Atom-2        | Model ID | Violation (Å) |
|---------|-------------|---------------|----------|---------------|
| (1,195) | 1:12:A:C:H6 | 1:11:A:A:H1'  | 5        | 0.39          |
| (1,195) | 1:12:A:C:H6 | 1:11:A:A:H1'  | 9        | 0.39          |
| (1,158) | 1:10:A:C:H6 | 1:10:A:C:H5'' | 3        | 0.39          |
| (1,158) | 1:10:A:C:H6 | 1:10:A:C:H5'' | 4        | 0.39          |
| (1,98)  | 1:6:A:C:H5  | 1:5:A:U:H3    | 5        | 0.39          |
| (1,98)  | 1:6:A:C:H5  | 1:5:A:U:H3    | 9        | 0.39          |
| (1,78)  | 1:5:A:U:H3  | 1:6:A:C:H5    | 5        | 0.39          |
| (1,78)  | 1:5:A:U:H3  | 1:6:A:C:H5    | 9        | 0.39          |
| (1,33)  | 1:3:A:G:H8  | 1:3:A:G:H5''  | 4        | 0.39          |
| (1,33)  | 1:3:A:G:H8  | 1:3:A:G:H5''  | 5        | 0.39          |
| (1,736) | 1:56:A:C:H6 | 1:56:A:C:H5'' | 7        | 0.38          |
| (1,578) | 1:45:A:C:H6 | 1:45:A:C:H3'  | 1        | 0.38          |
| (1,578) | 1:45:A:C:H6 | 1:45:A:C:H3'  | 4        | 0.38          |
| (1,578) | 1:45:A:C:H6 | 1:45:A:C:H3'  | 8        | 0.38          |
| (1,572) | 1:44:A:G:H8 | 1:43:A:G:H8   | 7        | 0.38          |
| (1,490) | 1:36:A:U:H6 | 1:36:A:U:H5'' | 9        | 0.38          |
| (1,461) | 1:33:A:U:H6 | 1:32:A:C:H1'  | 3        | 0.38          |
| (1,455) | 1:32:A:C:H5 | 1:31:A:G:H1'  | 4        | 0.38          |
| (1,435) | 1:31:A:G:H8 | 1:30:A:G:H1'  | 7        | 0.38          |
| (1,404) | 1:29:A:G:H8 | 1:28:A:C:H5'  | 4        | 0.38          |
| (1,322) | 1:24:A:C:H6 | 1:23:A:G:H1'  | 4        | 0.38          |
| (1,294) | 1:21:A:U:H3 | 1:22:A:C:H41  | 10       | 0.38          |
| (1,292) | 1:21:A:U:H3 | 1:22:A:C:H5   | 1        | 0.38          |
| (1,292) | 1:21:A:U:H3 | 1:22:A:C:H5   | 2        | 0.38          |
| (1,292) | 1:21:A:U:H3 | 1:22:A:C:H5   | 4        | 0.38          |
| (1,292) | 1:21:A:U:H3 | 1:22:A:C:H5   | 8        | 0.38          |
| (1,286) | 1:21:A:U:H6 | 1:20:A:A:H1'  | 9        | 0.38          |
| (1,264) | 1:19:A:G:H8 | 1:19:A:G:H3'  | 10       | 0.38          |
| (1,250) | 1:17:A:U:H6 | 1:16:A:A:H8   | 5        | 0.38          |
| (1,238) | 1:16:A:A:H8 | 1:15:A:C:H6   | 6        | 0.38          |
| (1,195) | 1:12:A:C:H6 | 1:11:A:A:H1'  | 6        | 0.38          |
| (1,158) | 1:10:A:C:H6 | 1:10:A:C:H5'' | 2        | 0.38          |
| (1,98)  | 1:6:A:C:H5  | 1:5:A:U:H3    | 3        | 0.38          |
| (1,98)  | 1:6:A:C:H5  | 1:5:A:U:H3    | 7        | 0.38          |
| (1,98)  | 1:6:A:C:H5  | 1:5:A:U:H3    | 10       | 0.38          |
| (1,78)  | 1:5:A:U:H3  | 1:6:A:C:H5    | 3        | 0.38          |
| (1,78)  | 1:5:A:U:H3  | 1:6:A:C:H5    | 7        | 0.38          |
| (1,78)  | 1:5:A:U:H3  | 1:6:A:C:H5    | 10       | 0.38          |
| (1,578) | 1:45:A:C:H6 | 1:45:A:C:H3'  | 9        | 0.37          |
| (1,461) | 1:33:A:U:H6 | 1:32:A:C:H1'  | 1        | 0.37          |
| (1,461) | 1:33:A:U:H6 | 1:32:A:C:H1'  | 4        | 0.37          |
| (1,461) | 1:33:A:U:H6 | 1:32:A:C:H1'  | 8        | 0.37          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,455) | 1:32:A:C:H5  | 1:31:A:G:H1'  | 8        | 0.37          |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5   | 7        | 0.37          |
| (1,409) | 1:29:A:G:H1  | 1:26:A:U:H2'  | 7        | 0.37          |
| (1,353) | 1:26:A:U:H6  | 1:25:A:C:H3'  | 3        | 0.37          |
| (1,353) | 1:26:A:U:H6  | 1:25:A:C:H3'  | 5        | 0.37          |
| (1,292) | 1:21:A:U:H3  | 1:22:A:C:H5   | 7        | 0.37          |
| (1,264) | 1:19:A:G:H8  | 1:19:A:G:H3'  | 4        | 0.37          |
| (1,250) | 1:17:A:U:H6  | 1:16:A:A:H8   | 4        | 0.37          |
| (1,250) | 1:17:A:U:H6  | 1:16:A:A:H8   | 10       | 0.37          |
| (1,248) | 1:17:A:U:H6  | 1:16:A:A:H1'  | 1        | 0.37          |
| (1,248) | 1:17:A:U:H6  | 1:16:A:A:H1'  | 3        | 0.37          |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 6        | 0.37          |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 9        | 0.37          |
| (1,195) | 1:12:A:C:H6  | 1:11:A:A:H1'  | 1        | 0.37          |
| (1,158) | 1:10:A:C:H6  | 1:10:A:C:H5'' | 1        | 0.37          |
| (1,158) | 1:10:A:C:H6  | 1:10:A:C:H5'' | 5        | 0.37          |
| (1,158) | 1:10:A:C:H6  | 1:10:A:C:H5'' | 6        | 0.37          |
| (1,158) | 1:10:A:C:H6  | 1:10:A:C:H5'' | 7        | 0.37          |
| (1,158) | 1:10:A:C:H6  | 1:10:A:C:H5'' | 9        | 0.37          |
| (1,158) | 1:10:A:C:H6  | 1:10:A:C:H5'' | 10       | 0.37          |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 6        | 0.37          |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 5        | 0.37          |
| (1,736) | 1:56:A:C:H6  | 1:56:A:C:H5'' | 3        | 0.36          |
| (1,736) | 1:56:A:C:H6  | 1:56:A:C:H5'' | 4        | 0.36          |
| (1,586) | 1:45:A:C:H42 | 1:44:A:G:H1   | 3        | 0.36          |
| (1,578) | 1:45:A:C:H6  | 1:45:A:C:H3'  | 2        | 0.36          |
| (1,527) | 1:40:A:G:H8  | 1:40:A:G:H3'  | 7        | 0.36          |
| (1,527) | 1:40:A:G:H8  | 1:40:A:G:H3'  | 9        | 0.36          |
| (1,461) | 1:33:A:U:H6  | 1:32:A:C:H1'  | 5        | 0.36          |
| (1,453) | 1:32:A:C:H6  | 1:31:A:G:H8   | 4        | 0.36          |
| (1,339) | 1:25:A:C:H5  | 1:24:A:C:H5   | 6        | 0.36          |
| (1,322) | 1:24:A:C:H6  | 1:23:A:G:H1'  | 5        | 0.36          |
| (1,250) | 1:17:A:U:H6  | 1:16:A:A:H8   | 6        | 0.36          |
| (1,248) | 1:17:A:U:H6  | 1:16:A:A:H1'  | 7        | 0.36          |
| (1,238) | 1:16:A:A:H8  | 1:15:A:C:H6   | 1        | 0.36          |
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 5        | 0.36          |
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 7        | 0.36          |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 7        | 0.36          |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 3        | 0.36          |
| (1,98)  | 1:6:A:C:H5   | 1:5:A:U:H3    | 2        | 0.36          |
| (1,98)  | 1:6:A:C:H5   | 1:5:A:U:H3    | 6        | 0.36          |
| (1,78)  | 1:5:A:U:H3   | 1:6:A:C:H5    | 2        | 0.36          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,78)  | 1:5:A:U:H3   | 1:6:A:C:H5    | 6        | 0.36          |
| (1,736) | 1:56:A:C:H6  | 1:56:A:C:H5'' | 1        | 0.35          |
| (1,736) | 1:56:A:C:H6  | 1:56:A:C:H5'' | 2        | 0.35          |
| (1,736) | 1:56:A:C:H6  | 1:56:A:C:H5'' | 8        | 0.35          |
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 6        | 0.35          |
| (1,578) | 1:45:A:C:H6  | 1:45:A:C:H3'  | 10       | 0.35          |
| (1,527) | 1:40:A:G:H8  | 1:40:A:G:H3'  | 10       | 0.35          |
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1'  | 3        | 0.35          |
| (1,483) | 1:35:A:A:H8  | 1:34:A:G:H8   | 3        | 0.35          |
| (1,469) | 1:34:A:G:H8  | 1:33:A:U:H1'  | 2        | 0.35          |
| (1,455) | 1:32:A:C:H5  | 1:31:A:G:H1'  | 1        | 0.35          |
| (1,444) | 1:31:A:G:H1  | 1:25:A:C:H41  | 10       | 0.35          |
| (1,438) | 1:31:A:G:H1  | 1:30:A:G:H1   | 10       | 0.35          |
| (1,409) | 1:29:A:G:H1  | 1:26:A:U:H2'  | 10       | 0.35          |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 6        | 0.35          |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 4        | 0.35          |
| (1,287) | 1:21:A:U:H6  | 1:20:A:A:H8   | 1        | 0.35          |
| (1,287) | 1:21:A:U:H6  | 1:20:A:A:H8   | 7        | 0.35          |
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 9        | 0.35          |
| (1,195) | 1:12:A:C:H6  | 1:11:A:A:H1'  | 8        | 0.35          |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 3        | 0.35          |
| (1,158) | 1:10:A:C:H6  | 1:10:A:C:H5'' | 8        | 0.35          |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 3        | 0.35          |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 5        | 0.35          |
| (1,98)  | 1:6:A:C:H5   | 1:5:A:U:H3    | 1        | 0.35          |
| (1,98)  | 1:6:A:C:H5   | 1:5:A:U:H3    | 4        | 0.35          |
| (1,78)  | 1:5:A:U:H3   | 1:6:A:C:H5    | 1        | 0.35          |
| (1,78)  | 1:5:A:U:H3   | 1:6:A:C:H5    | 4        | 0.35          |
| (1,736) | 1:56:A:C:H6  | 1:56:A:C:H5'' | 5        | 0.34          |
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 2        | 0.34          |
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 5        | 0.34          |
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 7        | 0.34          |
| (1,435) | 1:31:A:G:H8  | 1:30:A:G:H1'  | 6        | 0.34          |
| (1,404) | 1:29:A:G:H8  | 1:28:A:C:H5'  | 8        | 0.34          |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 5        | 0.34          |
| (1,292) | 1:21:A:U:H3  | 1:22:A:C:H5   | 6        | 0.34          |
| (1,264) | 1:19:A:G:H8  | 1:19:A:G:H3'  | 5        | 0.34          |
| (1,248) | 1:17:A:U:H6  | 1:16:A:A:H1'  | 10       | 0.34          |
| (1,238) | 1:16:A:A:H8  | 1:15:A:C:H6   | 8        | 0.34          |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 2        | 0.34          |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 9        | 0.34          |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 10       | 0.34          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 1        | 0.33          |
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 3        | 0.33          |
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 4        | 0.33          |
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 8        | 0.33          |
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 9        | 0.33          |
| (1,717) | 1:55:A:C:H6  | 1:55:A:C:H5'' | 10       | 0.33          |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 4        | 0.33          |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 6        | 0.33          |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 1        | 0.33          |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 4        | 0.33          |
| (1,572) | 1:44:A:G:H8  | 1:43:A:G:H8   | 4        | 0.33          |
| (1,483) | 1:35:A:A:H8  | 1:34:A:G:H8   | 6        | 0.33          |
| (1,438) | 1:31:A:G:H1  | 1:30:A:G:H1   | 9        | 0.33          |
| (1,415) | 1:30:A:G:H8  | 1:30:A:G:H3'  | 1        | 0.33          |
| (1,415) | 1:30:A:G:H8  | 1:30:A:G:H3'  | 8        | 0.33          |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 4        | 0.33          |
| (1,385) | 1:28:A:C:H6  | 1:26:A:U:H2'  | 4        | 0.33          |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 1        | 0.33          |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 6        | 0.33          |
| (1,287) | 1:21:A:U:H6  | 1:20:A:A:H8   | 2        | 0.33          |
| (1,287) | 1:21:A:U:H6  | 1:20:A:A:H8   | 3        | 0.33          |
| (1,286) | 1:21:A:U:H6  | 1:20:A:A:H1'  | 6        | 0.33          |
| (1,250) | 1:17:A:U:H6  | 1:16:A:A:H8   | 1        | 0.33          |
| (1,238) | 1:16:A:A:H8  | 1:15:A:C:H6   | 3        | 0.33          |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 1        | 0.33          |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 4        | 0.33          |
| (1,123) | 1:8:A:G:H8   | 1:8:A:G:H5''  | 8        | 0.33          |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 1        | 0.33          |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 2        | 0.33          |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 4        | 0.33          |
| (1,601) | 1:47:A:A:H2  | 1:48:A:G:H8   | 3        | 0.32          |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 1        | 0.32          |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 2        | 0.32          |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 3        | 0.32          |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 5        | 0.32          |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 7        | 0.32          |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 10       | 0.32          |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 5        | 0.32          |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 8        | 0.32          |
| (1,572) | 1:44:A:G:H8  | 1:43:A:G:H8   | 6        | 0.32          |
| (1,492) | 1:36:A:U:H6  | 1:35:A:A:H1'  | 6        | 0.32          |
| (1,486) | 1:34:A:G:H1  | 1:35:A:A:H2   | 5        | 0.32          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1'  | 4        | 0.32          |
| (1,483) | 1:35:A:A:H8  | 1:34:A:G:H8   | 2        | 0.32          |
| (1,434) | 1:31:A:G:H8  | 1:30:A:G:H8   | 10       | 0.32          |
| (1,420) | 1:30:A:G:H8  | 1:29:A:G:H3'  | 9        | 0.32          |
| (1,404) | 1:29:A:G:H8  | 1:28:A:C:H5'  | 5        | 0.32          |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 2        | 0.32          |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 3        | 0.32          |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 7        | 0.32          |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 9        | 0.32          |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 10       | 0.32          |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 2        | 0.32          |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 3        | 0.32          |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 7        | 0.32          |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 8        | 0.32          |
| (1,278) | 1:20:A:A:H8  | 1:19:A:G:H2'  | 5        | 0.32          |
| (1,238) | 1:16:A:A:H8  | 1:15:A:C:H6   | 2        | 0.32          |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 5        | 0.32          |
| (1,117) | 1:7:A:U:H3   | 1:6:A:C:H41   | 8        | 0.32          |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 9        | 0.31          |
| (1,469) | 1:34:A:G:H8  | 1:33:A:U:H1'  | 7        | 0.31          |
| (1,463) | 1:33:A:U:H6  | 1:32:A:C:H3'  | 9        | 0.31          |
| (1,461) | 1:33:A:U:H6  | 1:32:A:C:H1'  | 2        | 0.31          |
| (1,455) | 1:32:A:C:H5  | 1:31:A:G:H1'  | 7        | 0.31          |
| (1,453) | 1:32:A:C:H6  | 1:31:A:G:H8   | 7        | 0.31          |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 1        | 0.31          |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 5        | 0.31          |
| (1,391) | 1:28:A:C:H42 | 1:26:A:U:H3'  | 3        | 0.31          |
| (1,391) | 1:28:A:C:H42 | 1:26:A:U:H3'  | 6        | 0.31          |
| (1,338) | 1:25:A:C:H6  | 1:24:A:C:H6   | 6        | 0.31          |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 5        | 0.31          |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 9        | 0.31          |
| (1,286) | 1:21:A:U:H6  | 1:20:A:A:H1'  | 10       | 0.31          |
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 2        | 0.31          |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 3        | 0.3           |
| (1,544) | 1:41:A:C:H6  | 1:40:A:G:H2'  | 10       | 0.3           |
| (1,490) | 1:36:A:U:H6  | 1:36:A:U:H5'' | 7        | 0.3           |
| (1,490) | 1:36:A:U:H6  | 1:36:A:U:H5'' | 10       | 0.3           |
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 3        | 0.3           |
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 4        | 0.3           |
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 5        | 0.3           |
| (1,469) | 1:34:A:G:H8  | 1:33:A:U:H1'  | 3        | 0.3           |
| (1,461) | 1:33:A:U:H6  | 1:32:A:C:H1'  | 7        | 0.3           |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,415) | 1:30:A:G:H8  | 1:30:A:G:H3'  | 4        | 0.3           |
| (1,404) | 1:29:A:G:H8  | 1:28:A:C:H5'  | 1        | 0.3           |
| (1,403) | 1:29:A:G:H1' | 1:28:A:C:H5'  | 3        | 0.3           |
| (1,317) | 1:24:A:C:H6  | 1:24:A:C:H5'' | 10       | 0.3           |
| (1,292) | 1:21:A:U:H3  | 1:22:A:C:H5   | 9        | 0.3           |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 4        | 0.3           |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 7        | 0.3           |
| (1,286) | 1:21:A:U:H6  | 1:20:A:A:H1'  | 2        | 0.3           |
| (1,248) | 1:17:A:U:H6  | 1:16:A:A:H1'  | 4        | 0.3           |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 10       | 0.3           |
| (1,596) | 1:47:A:A:H8  | 1:47:A:A:H3'  | 6        | 0.29          |
| (1,572) | 1:44:A:G:H8  | 1:43:A:G:H8   | 2        | 0.29          |
| (1,572) | 1:44:A:G:H8  | 1:43:A:G:H8   | 5        | 0.29          |
| (1,563) | 1:43:A:G:H1  | 1:12:A:C:H41  | 9        | 0.29          |
| (1,544) | 1:41:A:C:H6  | 1:40:A:G:H2'  | 7        | 0.29          |
| (1,529) | 1:40:A:G:H8  | 1:39:A:G:H8   | 9        | 0.29          |
| (1,492) | 1:36:A:U:H6  | 1:35:A:A:H1'  | 1        | 0.29          |
| (1,492) | 1:36:A:U:H6  | 1:35:A:A:H1'  | 2        | 0.29          |
| (1,492) | 1:36:A:U:H6  | 1:35:A:A:H1'  | 8        | 0.29          |
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 8        | 0.29          |
| (1,463) | 1:33:A:U:H6  | 1:32:A:C:H3'  | 7        | 0.29          |
| (1,453) | 1:32:A:C:H6  | 1:31:A:G:H8   | 2        | 0.29          |
| (1,415) | 1:30:A:G:H8  | 1:30:A:G:H3'  | 2        | 0.29          |
| (1,409) | 1:29:A:G:H1  | 1:26:A:U:H2'  | 4        | 0.29          |
| (1,390) | 1:28:A:C:H41 | 1:26:A:U:H3'  | 2        | 0.29          |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1'  | 3        | 0.29          |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 8        | 0.29          |
| (1,287) | 1:21:A:U:H6  | 1:20:A:A:H8   | 8        | 0.29          |
| (1,286) | 1:21:A:U:H6  | 1:20:A:A:H1'  | 1        | 0.29          |
| (1,277) | 1:20:A:A:H8  | 1:19:A:G:H1'  | 9        | 0.29          |
| (1,238) | 1:16:A:A:H8  | 1:15:A:C:H6   | 4        | 0.29          |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 3        | 0.29          |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 2        | 0.29          |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 7        | 0.28          |
| (1,601) | 1:47:A:A:H2  | 1:48:A:G:H8   | 1        | 0.28          |
| (1,590) | 1:46:A:U:H6  | 1:46:A:U:H5'  | 2        | 0.28          |
| (1,572) | 1:44:A:G:H8  | 1:43:A:G:H8   | 3        | 0.28          |
| (1,486) | 1:34:A:G:H1  | 1:35:A:A:H2   | 4        | 0.28          |
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1'  | 1        | 0.28          |
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1'  | 6        | 0.28          |
| (1,483) | 1:35:A:A:H8  | 1:34:A:G:H8   | 10       | 0.28          |
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 1        | 0.28          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 2        | 0.28          |
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 6        | 0.28          |
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 7        | 0.28          |
| (1,455) | 1:32:A:C:H5  | 1:31:A:G:H1'  | 2        | 0.28          |
| (1,453) | 1:32:A:C:H6  | 1:31:A:G:H8   | 10       | 0.28          |
| (1,415) | 1:30:A:G:H8  | 1:30:A:G:H3'  | 5        | 0.28          |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1'  | 1        | 0.28          |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1'  | 7        | 0.28          |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1'  | 8        | 0.28          |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 3        | 0.28          |
| (1,292) | 1:21:A:U:H3  | 1:22:A:C:H5   | 10       | 0.28          |
| (1,238) | 1:16:A:A:H8  | 1:15:A:C:H6   | 5        | 0.28          |
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 10       | 0.28          |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 7        | 0.28          |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 3        | 0.27          |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 5        | 0.27          |
| (1,572) | 1:44:A:G:H8  | 1:43:A:G:H8   | 1        | 0.27          |
| (1,572) | 1:44:A:G:H8  | 1:43:A:G:H8   | 8        | 0.27          |
| (1,490) | 1:36:A:U:H6  | 1:36:A:U:H5'' | 4        | 0.27          |
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 10       | 0.27          |
| (1,424) | 1:30:A:G:H1  | 1:25:A:C:H5   | 9        | 0.27          |
| (1,415) | 1:30:A:G:H8  | 1:30:A:G:H3'  | 3        | 0.27          |
| (1,390) | 1:28:A:C:H41 | 1:26:A:U:H3'  | 4        | 0.27          |
| (1,384) | 1:28:A:C:H5  | 1:26:A:U:H1'  | 1        | 0.27          |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1'  | 5        | 0.27          |
| (1,306) | 1:23:A:G:H8  | 1:22:A:C:H1'  | 10       | 0.27          |
| (1,287) | 1:21:A:U:H6  | 1:20:A:A:H8   | 10       | 0.27          |
| (1,224) | 1:15:A:C:H6  | 1:14:A:C:H1'  | 5        | 0.27          |
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 3        | 0.27          |
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 4        | 0.27          |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 4        | 0.27          |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 1        | 0.27          |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 4        | 0.27          |
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 8        | 0.27          |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 8        | 0.26          |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 9        | 0.26          |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 7        | 0.26          |
| (1,492) | 1:36:A:U:H6  | 1:35:A:A:H1'  | 4        | 0.26          |
| (1,492) | 1:36:A:U:H6  | 1:35:A:A:H1'  | 5        | 0.26          |
| (1,490) | 1:36:A:U:H6  | 1:36:A:U:H5'' | 8        | 0.26          |
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1'  | 8        | 0.26          |
| (1,418) | 1:30:A:G:H8  | 1:30:A:G:H5'' | 1        | 0.26          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,418) | 1:30:A:G:H8  | 1:30:A:G:H5'' | 5        | 0.26          |
| (1,418) | 1:30:A:G:H8  | 1:30:A:G:H5'' | 8        | 0.26          |
| (1,415) | 1:30:A:G:H8  | 1:30:A:G:H3'  | 7        | 0.26          |
| (1,384) | 1:28:A:C:H5  | 1:26:A:U:H1'  | 8        | 0.26          |
| (1,380) | 1:28:A:C:H5  | 1:27:A:U:H2'  | 4        | 0.26          |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1'  | 9        | 0.26          |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1'  | 10       | 0.26          |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 1        | 0.26          |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 8        | 0.26          |
| (1,293) | 1:21:A:U:H3  | 1:22:A:C:H42  | 6        | 0.26          |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 5        | 0.26          |
| (1,286) | 1:21:A:U:H6  | 1:20:A:A:H1'  | 3        | 0.26          |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 5        | 0.26          |
| (1,116) | 1:7:A:U:H3   | 1:6:A:C:H42   | 6        | 0.26          |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 10       | 0.25          |
| (1,601) | 1:47:A:A:H2  | 1:48:A:G:H8   | 5        | 0.25          |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 1        | 0.25          |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 2        | 0.25          |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 3        | 0.25          |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 4        | 0.25          |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 5        | 0.25          |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 6        | 0.25          |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 8        | 0.25          |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 9        | 0.25          |
| (1,546) | 1:42:A:U:H6  | 1:42:A:U:H1'  | 10       | 0.25          |
| (1,544) | 1:41:A:C:H6  | 1:40:A:G:H2'  | 9        | 0.25          |
| (1,529) | 1:40:A:G:H8  | 1:39:A:G:H8   | 7        | 0.25          |
| (1,529) | 1:40:A:G:H8  | 1:39:A:G:H8   | 10       | 0.25          |
| (1,492) | 1:36:A:U:H6  | 1:35:A:A:H1'  | 3        | 0.25          |
| (1,490) | 1:36:A:U:H6  | 1:36:A:U:H5'' | 1        | 0.25          |
| (1,490) | 1:36:A:U:H6  | 1:36:A:U:H5'' | 2        | 0.25          |
| (1,463) | 1:33:A:U:H6  | 1:32:A:C:H3'  | 3        | 0.25          |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5   | 3        | 0.25          |
| (1,424) | 1:30:A:G:H1  | 1:25:A:C:H5   | 2        | 0.25          |
| (1,415) | 1:30:A:G:H8  | 1:30:A:G:H3'  | 10       | 0.25          |
| (1,393) | 1:28:A:C:H41 | 1:27:A:U:H5'  | 8        | 0.25          |
| (1,385) | 1:28:A:C:H6  | 1:26:A:U:H2'  | 5        | 0.25          |
| (1,384) | 1:28:A:C:H5  | 1:26:A:U:H1'  | 5        | 0.25          |
| (1,372) | 1:28:A:C:H6  | 1:28:A:C:H3'  | 8        | 0.25          |
| (1,277) | 1:20:A:A:H8  | 1:19:A:G:H1'  | 5        | 0.25          |
| (1,248) | 1:17:A:U:H6  | 1:16:A:A:H1'  | 5        | 0.25          |
| (1,224) | 1:15:A:C:H6  | 1:14:A:C:H1'  | 4        | 0.25          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 8        | 0.25          |
| (1,601) | 1:47:A:A:H2  | 1:48:A:G:H8   | 2        | 0.24          |
| (1,529) | 1:40:A:G:H8  | 1:39:A:G:H8   | 5        | 0.24          |
| (1,490) | 1:36:A:U:H6  | 1:36:A:U:H5'' | 3        | 0.24          |
| (1,490) | 1:36:A:U:H6  | 1:36:A:U:H5'' | 6        | 0.24          |
| (1,486) | 1:34:A:G:H1  | 1:35:A:A:H2   | 9        | 0.24          |
| (1,480) | 1:35:A:A:H8  | 1:34:A:G:H1'  | 9        | 0.24          |
| (1,463) | 1:33:A:U:H6  | 1:32:A:C:H3'  | 5        | 0.24          |
| (1,463) | 1:33:A:U:H6  | 1:32:A:C:H3'  | 8        | 0.24          |
| (1,461) | 1:33:A:U:H6  | 1:32:A:C:H1'  | 9        | 0.24          |
| (1,428) | 1:31:A:G:H8  | 1:31:A:G:H3'  | 1        | 0.24          |
| (1,424) | 1:30:A:G:H1  | 1:25:A:C:H5   | 4        | 0.24          |
| (1,409) | 1:29:A:G:H1  | 1:26:A:U:H2'  | 3        | 0.24          |
| (1,390) | 1:28:A:C:H41 | 1:26:A:U:H3'  | 7        | 0.24          |
| (1,390) | 1:28:A:C:H41 | 1:26:A:U:H3'  | 10       | 0.24          |
| (1,372) | 1:28:A:C:H6  | 1:28:A:C:H3'  | 1        | 0.24          |
| (1,372) | 1:28:A:C:H6  | 1:28:A:C:H3'  | 4        | 0.24          |
| (1,339) | 1:25:A:C:H5  | 1:24:A:C:H5   | 10       | 0.24          |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 6        | 0.24          |
| (1,293) | 1:21:A:U:H3  | 1:22:A:C:H42  | 5        | 0.24          |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 1        | 0.24          |
| (1,271) | 1:19:A:G:H1  | 1:36:A:U:H3   | 9        | 0.24          |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 2        | 0.24          |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 10       | 0.24          |
| (1,116) | 1:7:A:U:H3   | 1:6:A:C:H42   | 7        | 0.24          |
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 9        | 0.24          |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 5        | 0.24          |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 8        | 0.24          |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 2        | 0.23          |
| (1,601) | 1:47:A:A:H2  | 1:48:A:G:H8   | 9        | 0.23          |
| (1,563) | 1:43:A:G:H1  | 1:12:A:C:H41  | 6        | 0.23          |
| (1,492) | 1:36:A:U:H6  | 1:35:A:A:H1'  | 10       | 0.23          |
| (1,490) | 1:36:A:U:H6  | 1:36:A:U:H5'' | 5        | 0.23          |
| (1,463) | 1:33:A:U:H6  | 1:32:A:C:H3'  | 1        | 0.23          |
| (1,463) | 1:33:A:U:H6  | 1:32:A:C:H3'  | 2        | 0.23          |
| (1,462) | 1:33:A:U:H6  | 1:32:A:C:H2'  | 6        | 0.23          |
| (1,428) | 1:31:A:G:H8  | 1:31:A:G:H3'  | 8        | 0.23          |
| (1,418) | 1:30:A:G:H8  | 1:30:A:G:H5'' | 2        | 0.23          |
| (1,418) | 1:30:A:G:H8  | 1:30:A:G:H5'' | 4        | 0.23          |
| (1,403) | 1:29:A:G:H1' | 1:28:A:C:H5'  | 10       | 0.23          |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1'  | 2        | 0.23          |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 2        | 0.23          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,273) | 1:19:A:G:H1  | 1:20:A:A:H2   | 5        | 0.23          |
| (1,217) | 1:14:A:C:H6  | 1:13:A:C:H1'  | 1        | 0.23          |
| (1,116) | 1:7:A:U:H3   | 1:6:A:C:H42   | 9        | 0.23          |
| (1,116) | 1:7:A:U:H3   | 1:6:A:C:H42   | 10       | 0.23          |
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 5        | 0.23          |
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 7        | 0.23          |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 1        | 0.23          |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 2        | 0.23          |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 3        | 0.23          |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 4        | 0.23          |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 3        | 0.23          |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 6        | 0.22          |
| (1,492) | 1:36:A:U:H6  | 1:35:A:A:H1'  | 7        | 0.22          |
| (1,486) | 1:34:A:G:H1  | 1:35:A:A:H2   | 3        | 0.22          |
| (1,486) | 1:34:A:G:H1  | 1:35:A:A:H2   | 8        | 0.22          |
| (1,474) | 1:34:A:G:H1  | 1:33:A:U:H3   | 6        | 0.22          |
| (1,462) | 1:33:A:U:H6  | 1:32:A:C:H2'  | 10       | 0.22          |
| (1,444) | 1:31:A:G:H1  | 1:25:A:C:H41  | 9        | 0.22          |
| (1,428) | 1:31:A:G:H8  | 1:31:A:G:H3'  | 4        | 0.22          |
| (1,428) | 1:31:A:G:H8  | 1:31:A:G:H3'  | 5        | 0.22          |
| (1,424) | 1:30:A:G:H1  | 1:25:A:C:H5   | 10       | 0.22          |
| (1,415) | 1:30:A:G:H8  | 1:30:A:G:H3'  | 6        | 0.22          |
| (1,409) | 1:29:A:G:H1  | 1:26:A:U:H2'  | 6        | 0.22          |
| (1,390) | 1:28:A:C:H41 | 1:26:A:U:H3'  | 9        | 0.22          |
| (1,384) | 1:28:A:C:H5  | 1:26:A:U:H1'  | 4        | 0.22          |
| (1,380) | 1:28:A:C:H5  | 1:27:A:U:H2'  | 5        | 0.22          |
| (1,372) | 1:28:A:C:H6  | 1:28:A:C:H3'  | 5        | 0.22          |
| (1,335) | 1:25:A:C:H6  | 1:24:A:C:H1'  | 4        | 0.22          |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 10       | 0.22          |
| (1,323) | 1:24:A:C:H6  | 1:23:A:G:H2'  | 6        | 0.22          |
| (1,293) | 1:21:A:U:H3  | 1:22:A:C:H42  | 4        | 0.22          |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 3        | 0.22          |
| (1,286) | 1:21:A:U:H6  | 1:20:A:A:H1'  | 8        | 0.22          |
| (1,224) | 1:15:A:C:H6  | 1:14:A:C:H1'  | 2        | 0.22          |
| (1,224) | 1:15:A:C:H6  | 1:14:A:C:H1'  | 3        | 0.22          |
| (1,190) | 1:12:A:C:H6  | 1:12:A:C:H5'' | 3        | 0.22          |
| (1,190) | 1:12:A:C:H6  | 1:12:A:C:H5'' | 4        | 0.22          |
| (1,190) | 1:12:A:C:H6  | 1:12:A:C:H5'' | 6        | 0.22          |
| (1,190) | 1:12:A:C:H6  | 1:12:A:C:H5'' | 8        | 0.22          |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 7        | 0.22          |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 9        | 0.22          |
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 3        | 0.22          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 10       | 0.22          |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 5        | 0.22          |
| (1,486) | 1:34:A:G:H1  | 1:35:A:A:H2   | 2        | 0.21          |
| (1,463) | 1:33:A:U:H6  | 1:32:A:C:H3'  | 4        | 0.21          |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5   | 1        | 0.21          |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5   | 2        | 0.21          |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5   | 4        | 0.21          |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5   | 8        | 0.21          |
| (1,438) | 1:31:A:G:H1  | 1:30:A:G:H1   | 7        | 0.21          |
| (1,428) | 1:31:A:G:H8  | 1:31:A:G:H3'  | 3        | 0.21          |
| (1,424) | 1:30:A:G:H1  | 1:25:A:C:H5   | 7        | 0.21          |
| (1,380) | 1:28:A:C:H5  | 1:27:A:U:H2'  | 1        | 0.21          |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 4        | 0.21          |
| (1,305) | 1:23:A:G:H1' | 1:23:A:G:H4'  | 9        | 0.21          |
| (1,293) | 1:21:A:U:H3  | 1:22:A:C:H42  | 2        | 0.21          |
| (1,273) | 1:19:A:G:H1  | 1:20:A:A:H2   | 4        | 0.21          |
| (1,224) | 1:15:A:C:H6  | 1:14:A:C:H1'  | 1        | 0.21          |
| (1,224) | 1:15:A:C:H6  | 1:14:A:C:H1'  | 8        | 0.21          |
| (1,224) | 1:15:A:C:H6  | 1:14:A:C:H1'  | 9        | 0.21          |
| (1,190) | 1:12:A:C:H6  | 1:12:A:C:H5'' | 1        | 0.21          |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 8        | 0.21          |
| (1,116) | 1:7:A:U:H3   | 1:6:A:C:H42   | 5        | 0.21          |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 6        | 0.21          |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 1        | 0.21          |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 2        | 0.21          |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 4        | 0.21          |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 8        | 0.21          |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 9        | 0.21          |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 4        | 0.2           |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 3        | 0.2           |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 5        | 0.2           |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 6        | 0.2           |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 7        | 0.2           |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 9        | 0.2           |
| (1,545) | 1:41:A:C:H1' | 1:40:A:G:H2'  | 7        | 0.2           |
| (1,529) | 1:40:A:G:H8  | 1:39:A:G:H8   | 4        | 0.2           |
| (1,451) | 1:32:A:C:H6  | 1:31:A:G:H1'  | 6        | 0.2           |
| (1,445) | 1:31:A:G:H1  | 1:25:A:C:H5   | 5        | 0.2           |
| (1,428) | 1:31:A:G:H8  | 1:31:A:G:H3'  | 2        | 0.2           |
| (1,418) | 1:30:A:G:H8  | 1:30:A:G:H5'' | 3        | 0.2           |
| (1,403) | 1:29:A:G:H1' | 1:28:A:C:H5'  | 7        | 0.2           |
| (1,351) | 1:26:A:U:H6  | 1:25:A:C:H1'  | 7        | 0.2           |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,305) | 1:23:A:G:H1' | 1:23:A:G:H4'  | 10       | 0.2           |
| (1,293) | 1:21:A:U:H3  | 1:22:A:C:H42  | 1        | 0.2           |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 6        | 0.2           |
| (1,278) | 1:20:A:A:H8  | 1:19:A:G:H2'  | 4        | 0.2           |
| (1,277) | 1:20:A:A:H8  | 1:19:A:G:H1'  | 4        | 0.2           |
| (1,249) | 1:17:A:U:H6  | 1:16:A:A:H2'  | 6        | 0.2           |
| (1,248) | 1:17:A:U:H6  | 1:16:A:A:H1'  | 9        | 0.2           |
| (1,237) | 1:16:A:A:H8  | 1:15:A:C:H3'  | 1        | 0.2           |
| (1,190) | 1:12:A:C:H6  | 1:12:A:C:H5'' | 2        | 0.2           |
| (1,116) | 1:7:A:U:H3   | 1:6:A:C:H42   | 3        | 0.2           |
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 2        | 0.2           |
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 6        | 0.2           |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 7        | 0.2           |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 9        | 0.2           |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 6        | 0.2           |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 7        | 0.2           |
| (1,6)   | 1:1:A:G:H8   | 1:1:A:G:H5''  | 10       | 0.2           |
| (1,690) | 1:53:A:G:H1  | 1:6:A:C:H42   | 1        | 0.19          |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 2        | 0.19          |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 8        | 0.19          |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 10       | 0.19          |
| (1,596) | 1:47:A:A:H8  | 1:47:A:A:H3'  | 7        | 0.19          |
| (1,596) | 1:47:A:A:H8  | 1:47:A:A:H3'  | 10       | 0.19          |
| (1,537) | 1:40:A:G:H1  | 1:15:A:C:H42  | 4        | 0.19          |
| (1,537) | 1:40:A:G:H1  | 1:15:A:C:H42  | 5        | 0.19          |
| (1,529) | 1:40:A:G:H8  | 1:39:A:G:H8   | 6        | 0.19          |
| (1,500) | 1:37:A:C:H6  | 1:36:A:U:H1'  | 3        | 0.19          |
| (1,451) | 1:32:A:C:H6  | 1:31:A:G:H1'  | 3        | 0.19          |
| (1,451) | 1:32:A:C:H6  | 1:31:A:G:H1'  | 5        | 0.19          |
| (1,418) | 1:30:A:G:H8  | 1:30:A:G:H5'' | 6        | 0.19          |
| (1,385) | 1:28:A:C:H6  | 1:26:A:U:H2'  | 1        | 0.19          |
| (1,385) | 1:28:A:C:H6  | 1:26:A:U:H2'  | 8        | 0.19          |
| (1,351) | 1:26:A:U:H6  | 1:25:A:C:H1'  | 4        | 0.19          |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 7        | 0.19          |
| (1,293) | 1:21:A:U:H3  | 1:22:A:C:H42  | 3        | 0.19          |
| (1,264) | 1:19:A:G:H8  | 1:19:A:G:H3'  | 9        | 0.19          |
| (1,249) | 1:17:A:U:H6  | 1:16:A:A:H2'  | 8        | 0.19          |
| (1,242) | 1:17:A:U:H6  | 1:17:A:U:H2'  | 7        | 0.19          |
| (1,229) | 1:16:A:A:H8  | 1:16:A:A:H3'  | 6        | 0.19          |
| (1,229) | 1:16:A:A:H8  | 1:16:A:A:H3'  | 7        | 0.19          |
| (1,208) | 1:13:A:C:H6  | 1:12:A:C:H6   | 9        | 0.19          |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 1        | 0.19          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,190) | 1:12:A:C:H6  | 1:12:A:C:H5'' | 5        | 0.19          |
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 1        | 0.19          |
| (1,96)  | 1:6:A:C:H41  | 1:5:A:U:H3    | 4        | 0.19          |
| (1,84)  | 1:6:A:C:H6   | 1:6:A:C:H5''  | 10       | 0.19          |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 1        | 0.18          |
| (1,673) | 1:52:A:G:H1  | 1:6:A:C:H5    | 4        | 0.18          |
| (1,601) | 1:47:A:A:H2  | 1:48:A:G:H8   | 4        | 0.18          |
| (1,596) | 1:47:A:A:H8  | 1:47:A:A:H3'  | 4        | 0.18          |
| (1,596) | 1:47:A:A:H8  | 1:47:A:A:H3'  | 9        | 0.18          |
| (1,545) | 1:41:A:C:H1' | 1:40:A:G:H2'  | 9        | 0.18          |
| (1,537) | 1:40:A:G:H1  | 1:15:A:C:H42  | 7        | 0.18          |
| (1,536) | 1:40:A:G:H1  | 1:14:A:C:H5   | 10       | 0.18          |
| (1,474) | 1:34:A:G:H1  | 1:33:A:U:H3   | 10       | 0.18          |
| (1,455) | 1:32:A:C:H5  | 1:31:A:G:H1'  | 10       | 0.18          |
| (1,438) | 1:31:A:G:H1  | 1:30:A:G:H1   | 6        | 0.18          |
| (1,424) | 1:30:A:G:H1  | 1:25:A:C:H5   | 5        | 0.18          |
| (1,387) | 1:28:A:C:H5  | 1:26:A:U:H3'  | 4        | 0.18          |
| (1,332) | 1:25:A:C:H6  | 1:25:A:C:H5'' | 9        | 0.18          |
| (1,321) | 1:24:A:C:H5  | 1:24:A:C:H2'  | 5        | 0.18          |
| (1,293) | 1:21:A:U:H3  | 1:22:A:C:H42  | 7        | 0.18          |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 2        | 0.18          |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 9        | 0.18          |
| (1,290) | 1:21:A:U:H3  | 1:35:A:A:H2   | 10       | 0.18          |
| (1,287) | 1:21:A:U:H6  | 1:20:A:A:H8   | 5        | 0.18          |
| (1,249) | 1:17:A:U:H6  | 1:16:A:A:H2'  | 2        | 0.18          |
| (1,242) | 1:17:A:U:H6  | 1:17:A:U:H2'  | 6        | 0.18          |
| (1,237) | 1:16:A:A:H8  | 1:15:A:C:H3'  | 8        | 0.18          |
| (1,229) | 1:16:A:A:H8  | 1:16:A:A:H3'  | 4        | 0.18          |
| (1,224) | 1:15:A:C:H6  | 1:14:A:C:H1'  | 10       | 0.18          |
| (1,205) | 1:13:A:C:H6  | 1:12:A:C:H1'  | 8        | 0.18          |
| (1,190) | 1:12:A:C:H6  | 1:12:A:C:H5'' | 7        | 0.18          |
| (1,537) | 1:40:A:G:H1  | 1:15:A:C:H42  | 2        | 0.17          |
| (1,537) | 1:40:A:G:H1  | 1:15:A:C:H42  | 9        | 0.17          |
| (1,537) | 1:40:A:G:H1  | 1:15:A:C:H42  | 10       | 0.17          |
| (1,536) | 1:40:A:G:H1  | 1:14:A:C:H5   | 7        | 0.17          |
| (1,536) | 1:40:A:G:H1  | 1:14:A:C:H5   | 9        | 0.17          |
| (1,486) | 1:34:A:G:H1  | 1:35:A:A:H2   | 1        | 0.17          |
| (1,486) | 1:34:A:G:H1  | 1:35:A:A:H2   | 6        | 0.17          |
| (1,451) | 1:32:A:C:H6  | 1:31:A:G:H1'  | 8        | 0.17          |
| (1,428) | 1:31:A:G:H8  | 1:31:A:G:H3'  | 6        | 0.17          |
| (1,418) | 1:30:A:G:H8  | 1:30:A:G:H5'' | 7        | 0.17          |
| (1,409) | 1:29:A:G:H1  | 1:26:A:U:H2'  | 5        | 0.17          |

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| Key     | Atom-1      | Atom-2        | Model ID | Violation (Å) |
|---------|-------------|---------------|----------|---------------|
| (1,380) | 1:28:A:C:H5 | 1:27:A:U:H2'  | 6        | 0.17          |
| (1,352) | 1:26:A:U:H5 | 1:25:A:C:H5   | 10       | 0.17          |
| (1,351) | 1:26:A:U:H6 | 1:25:A:C:H1'  | 2        | 0.17          |
| (1,293) | 1:21:A:U:H3 | 1:22:A:C:H42  | 8        | 0.17          |
| (1,242) | 1:17:A:U:H6 | 1:17:A:U:H2'  | 8        | 0.17          |
| (1,242) | 1:17:A:U:H6 | 1:17:A:U:H2'  | 10       | 0.17          |
| (1,238) | 1:16:A:A:H8 | 1:15:A:C:H6   | 10       | 0.17          |
| (1,237) | 1:16:A:A:H8 | 1:15:A:C:H3'  | 2        | 0.17          |
| (1,237) | 1:16:A:A:H8 | 1:15:A:C:H3'  | 3        | 0.17          |
| (1,237) | 1:16:A:A:H8 | 1:15:A:C:H3'  | 6        | 0.17          |
| (1,116) | 1:7:A:U:H3  | 1:6:A:C:H42   | 2        | 0.17          |
| (1,116) | 1:7:A:U:H3  | 1:6:A:C:H42   | 4        | 0.17          |
| (1,633) | 1:50:A:C:H6 | 1:50:A:C:H5'' | 2        | 0.16          |
| (1,633) | 1:50:A:C:H6 | 1:50:A:C:H5'' | 4        | 0.16          |
| (1,633) | 1:50:A:C:H6 | 1:50:A:C:H5'' | 5        | 0.16          |
| (1,601) | 1:47:A:A:H2 | 1:48:A:G:H8   | 10       | 0.16          |
| (1,596) | 1:47:A:A:H8 | 1:47:A:A:H3'  | 2        | 0.16          |
| (1,596) | 1:47:A:A:H8 | 1:47:A:A:H3'  | 3        | 0.16          |
| (1,596) | 1:47:A:A:H8 | 1:47:A:A:H3'  | 5        | 0.16          |
| (1,563) | 1:43:A:G:H1 | 1:12:A:C:H41  | 5        | 0.16          |
| (1,537) | 1:40:A:G:H1 | 1:15:A:C:H42  | 8        | 0.16          |
| (1,529) | 1:40:A:G:H8 | 1:39:A:G:H8   | 1        | 0.16          |
| (1,500) | 1:37:A:C:H6 | 1:36:A:U:H1'  | 1        | 0.16          |
| (1,500) | 1:37:A:C:H6 | 1:36:A:U:H1'  | 2        | 0.16          |
| (1,500) | 1:37:A:C:H6 | 1:36:A:U:H1'  | 9        | 0.16          |
| (1,469) | 1:34:A:G:H8 | 1:33:A:U:H1'  | 8        | 0.16          |
| (1,469) | 1:34:A:G:H8 | 1:33:A:U:H1'  | 9        | 0.16          |
| (1,469) | 1:34:A:G:H8 | 1:33:A:U:H1'  | 10       | 0.16          |
| (1,451) | 1:32:A:C:H6 | 1:31:A:G:H1'  | 4        | 0.16          |
| (1,437) | 1:31:A:G:H8 | 1:30:A:G:H3'  | 10       | 0.16          |
| (1,424) | 1:30:A:G:H1 | 1:25:A:C:H5   | 1        | 0.16          |
| (1,424) | 1:30:A:G:H1 | 1:25:A:C:H5   | 3        | 0.16          |
| (1,415) | 1:30:A:G:H8 | 1:30:A:G:H3'  | 9        | 0.16          |
| (1,380) | 1:28:A:C:H5 | 1:27:A:U:H2'  | 8        | 0.16          |
| (1,351) | 1:26:A:U:H6 | 1:25:A:C:H1'  | 10       | 0.16          |
| (1,323) | 1:24:A:C:H6 | 1:23:A:G:H2'  | 10       | 0.16          |
| (1,321) | 1:24:A:C:H5 | 1:24:A:C:H2'  | 1        | 0.16          |
| (1,321) | 1:24:A:C:H5 | 1:24:A:C:H2'  | 3        | 0.16          |
| (1,293) | 1:21:A:U:H3 | 1:22:A:C:H42  | 9        | 0.16          |
| (1,287) | 1:21:A:U:H6 | 1:20:A:A:H8   | 4        | 0.16          |
| (1,249) | 1:17:A:U:H6 | 1:16:A:A:H2'  | 3        | 0.16          |
| (1,242) | 1:17:A:U:H6 | 1:17:A:U:H2'  | 2        | 0.16          |

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| Key     | Atom-1      | Atom-2        | Model ID | Violation (Å) |
|---------|-------------|---------------|----------|---------------|
| (1,242) | 1:17:A:U:H6 | 1:17:A:U:H2'  | 3        | 0.16          |
| (1,238) | 1:16:A:A:H8 | 1:15:A:C:H6   | 7        | 0.16          |
| (1,229) | 1:16:A:A:H8 | 1:16:A:A:H3'  | 3        | 0.16          |
| (1,229) | 1:16:A:A:H8 | 1:16:A:A:H3'  | 9        | 0.16          |
| (1,229) | 1:16:A:A:H8 | 1:16:A:A:H3'  | 10       | 0.16          |
| (1,224) | 1:15:A:C:H6 | 1:14:A:C:H1'  | 6        | 0.16          |
| (1,224) | 1:15:A:C:H6 | 1:14:A:C:H1'  | 7        | 0.16          |
| (1,208) | 1:13:A:C:H6 | 1:12:A:C:H6   | 10       | 0.16          |
| (1,190) | 1:12:A:C:H6 | 1:12:A:C:H5'' | 10       | 0.16          |
| (1,116) | 1:7:A:U:H3  | 1:6:A:C:H42   | 1        | 0.16          |
| (1,712) | 1:54:A:U:H3 | 1:3:A:G:H1    | 2        | 0.15          |
| (1,712) | 1:54:A:U:H3 | 1:3:A:G:H1    | 4        | 0.15          |
| (1,712) | 1:54:A:U:H3 | 1:3:A:G:H1    | 5        | 0.15          |
| (1,712) | 1:54:A:U:H3 | 1:3:A:G:H1    | 7        | 0.15          |
| (1,712) | 1:54:A:U:H3 | 1:3:A:G:H1    | 8        | 0.15          |
| (1,633) | 1:50:A:C:H6 | 1:50:A:C:H5'' | 1        | 0.15          |
| (1,633) | 1:50:A:C:H6 | 1:50:A:C:H5'' | 3        | 0.15          |
| (1,596) | 1:47:A:A:H8 | 1:47:A:A:H3'  | 1        | 0.15          |
| (1,563) | 1:43:A:G:H1 | 1:12:A:C:H41  | 8        | 0.15          |
| (1,537) | 1:40:A:G:H1 | 1:15:A:C:H42  | 1        | 0.15          |
| (1,537) | 1:40:A:G:H1 | 1:15:A:C:H42  | 3        | 0.15          |
| (1,492) | 1:36:A:U:H6 | 1:35:A:A:H1'  | 9        | 0.15          |
| (1,436) | 1:31:A:G:H8 | 1:30:A:G:H2'  | 10       | 0.15          |
| (1,435) | 1:31:A:G:H8 | 1:30:A:G:H1'  | 2        | 0.15          |
| (1,434) | 1:31:A:G:H8 | 1:30:A:G:H8   | 7        | 0.15          |
| (1,428) | 1:31:A:G:H8 | 1:31:A:G:H3'  | 7        | 0.15          |
| (1,424) | 1:30:A:G:H1 | 1:25:A:C:H5   | 8        | 0.15          |
| (1,418) | 1:30:A:G:H8 | 1:30:A:G:H5'' | 10       | 0.15          |
| (1,417) | 1:30:A:G:H8 | 1:30:A:G:H5'  | 6        | 0.15          |
| (1,417) | 1:30:A:G:H8 | 1:30:A:G:H5'  | 10       | 0.15          |
| (1,323) | 1:24:A:C:H6 | 1:23:A:G:H2'  | 7        | 0.15          |
| (1,323) | 1:24:A:C:H6 | 1:23:A:G:H2'  | 9        | 0.15          |
| (1,321) | 1:24:A:C:H5 | 1:24:A:C:H2'  | 4        | 0.15          |
| (1,321) | 1:24:A:C:H5 | 1:24:A:C:H2'  | 7        | 0.15          |
| (1,282) | 1:20:A:A:H2 | 1:37:A:C:H1'  | 3        | 0.15          |
| (1,282) | 1:20:A:A:H2 | 1:37:A:C:H1'  | 5        | 0.15          |
| (1,267) | 1:19:A:G:H8 | 1:17:A:U:H4'  | 6        | 0.15          |
| (1,242) | 1:17:A:U:H6 | 1:17:A:U:H2'  | 1        | 0.15          |
| (1,242) | 1:17:A:U:H6 | 1:17:A:U:H2'  | 4        | 0.15          |
| (1,209) | 1:13:A:C:H5 | 1:12:A:C:H5   | 9        | 0.15          |
| (1,596) | 1:47:A:A:H8 | 1:47:A:A:H3'  | 8        | 0.14          |
| (1,563) | 1:43:A:G:H1 | 1:12:A:C:H41  | 2        | 0.14          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,537) | 1:40:A:G:H1  | 1:15:A:C:H42  | 6        | 0.14          |
| (1,529) | 1:40:A:G:H8  | 1:39:A:G:H8   | 2        | 0.14          |
| (1,500) | 1:37:A:C:H6  | 1:36:A:U:H1'  | 8        | 0.14          |
| (1,469) | 1:34:A:G:H8  | 1:33:A:U:H1'  | 1        | 0.14          |
| (1,451) | 1:32:A:C:H6  | 1:31:A:G:H1'  | 1        | 0.14          |
| (1,443) | 1:31:A:G:H1  | 1:25:A:C:H42  | 10       | 0.14          |
| (1,428) | 1:31:A:G:H8  | 1:31:A:G:H3'  | 10       | 0.14          |
| (1,412) | 1:29:A:G:H1  | 1:28:A:C:H6   | 4        | 0.14          |
| (1,410) | 1:29:A:G:H1  | 1:28:A:C:H1'  | 5        | 0.14          |
| (1,391) | 1:28:A:C:H42 | 1:26:A:U:H3'  | 5        | 0.14          |
| (1,321) | 1:24:A:C:H5  | 1:24:A:C:H2'  | 2        | 0.14          |
| (1,321) | 1:24:A:C:H5  | 1:24:A:C:H2'  | 6        | 0.14          |
| (1,321) | 1:24:A:C:H5  | 1:24:A:C:H2'  | 8        | 0.14          |
| (1,301) | 1:23:A:G:H8  | 1:23:A:G:H2'  | 1        | 0.14          |
| (1,301) | 1:23:A:G:H8  | 1:23:A:G:H2'  | 4        | 0.14          |
| (1,301) | 1:23:A:G:H8  | 1:23:A:G:H2'  | 8        | 0.14          |
| (1,282) | 1:20:A:A:H2  | 1:37:A:C:H1'  | 10       | 0.14          |
| (1,278) | 1:20:A:A:H8  | 1:19:A:G:H2'  | 9        | 0.14          |
| (1,273) | 1:19:A:G:H1  | 1:20:A:A:H2   | 9        | 0.14          |
| (1,249) | 1:17:A:U:H6  | 1:16:A:A:H2'  | 1        | 0.14          |
| (1,242) | 1:17:A:U:H6  | 1:17:A:U:H2'  | 5        | 0.14          |
| (1,242) | 1:17:A:U:H6  | 1:17:A:U:H2'  | 9        | 0.14          |
| (1,229) | 1:16:A:A:H8  | 1:16:A:A:H3'  | 2        | 0.14          |
| (1,229) | 1:16:A:A:H8  | 1:16:A:A:H3'  | 8        | 0.14          |
| (1,116) | 1:7:A:U:H3   | 1:6:A:C:H42   | 8        | 0.14          |
| (1,712) | 1:54:A:U:H3  | 1:3:A:G:H1    | 1        | 0.13          |
| (1,633) | 1:50:A:C:H6  | 1:50:A:C:H5'' | 6        | 0.13          |
| (1,529) | 1:40:A:G:H8  | 1:39:A:G:H8   | 8        | 0.13          |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 6        | 0.13          |
| (1,486) | 1:34:A:G:H1  | 1:35:A:A:H2   | 10       | 0.13          |
| (1,451) | 1:32:A:C:H6  | 1:31:A:G:H1'  | 2        | 0.13          |
| (1,451) | 1:32:A:C:H6  | 1:31:A:G:H1'  | 7        | 0.13          |
| (1,417) | 1:30:A:G:H8  | 1:30:A:G:H5'  | 7        | 0.13          |
| (1,403) | 1:29:A:G:H1' | 1:28:A:C:H5'  | 9        | 0.13          |
| (1,305) | 1:23:A:G:H1' | 1:23:A:G:H4'  | 5        | 0.13          |
| (1,282) | 1:20:A:A:H2  | 1:37:A:C:H1'  | 1        | 0.13          |
| (1,282) | 1:20:A:A:H2  | 1:37:A:C:H1'  | 6        | 0.13          |
| (1,282) | 1:20:A:A:H2  | 1:37:A:C:H1'  | 7        | 0.13          |
| (1,267) | 1:19:A:G:H8  | 1:17:A:U:H4'  | 4        | 0.13          |
| (1,267) | 1:19:A:G:H8  | 1:17:A:U:H4'  | 10       | 0.13          |
| (1,229) | 1:16:A:A:H8  | 1:16:A:A:H3'  | 1        | 0.13          |
| (1,229) | 1:16:A:A:H8  | 1:16:A:A:H3'  | 5        | 0.13          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,218) | 1:14:A:C:H6  | 1:13:A:C:H2'  | 6        | 0.13          |
| (1,190) | 1:12:A:C:H6  | 1:12:A:C:H5'' | 9        | 0.13          |
| (1,712) | 1:54:A:U:H3  | 1:3:A:G:H1    | 3        | 0.12          |
| (1,712) | 1:54:A:U:H3  | 1:3:A:G:H1    | 6        | 0.12          |
| (1,712) | 1:54:A:U:H3  | 1:3:A:G:H1    | 9        | 0.12          |
| (1,712) | 1:54:A:U:H3  | 1:3:A:G:H1    | 10       | 0.12          |
| (1,655) | 1:51:A:G:H3' | 1:50:A:C:H2'  | 2        | 0.12          |
| (1,633) | 1:50:A:C:H6  | 1:50:A:C:H5'' | 8        | 0.12          |
| (1,563) | 1:43:A:G:H1  | 1:12:A:C:H41  | 10       | 0.12          |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 1        | 0.12          |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 2        | 0.12          |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 3        | 0.12          |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 8        | 0.12          |
| (1,500) | 1:37:A:C:H6  | 1:36:A:U:H1'  | 6        | 0.12          |
| (1,453) | 1:32:A:C:H6  | 1:31:A:G:H8   | 9        | 0.12          |
| (1,412) | 1:29:A:G:H1  | 1:28:A:C:H6   | 5        | 0.12          |
| (1,410) | 1:29:A:G:H1  | 1:28:A:C:H1'  | 1        | 0.12          |
| (1,385) | 1:28:A:C:H6  | 1:26:A:U:H2'  | 2        | 0.12          |
| (1,336) | 1:25:A:C:H6  | 1:24:A:C:H2'  | 6        | 0.12          |
| (1,323) | 1:24:A:C:H6  | 1:23:A:G:H2'  | 2        | 0.12          |
| (1,321) | 1:24:A:C:H5  | 1:24:A:C:H2'  | 10       | 0.12          |
| (1,307) | 1:23:A:G:H8  | 1:22:A:C:H2'  | 6        | 0.12          |
| (1,305) | 1:23:A:G:H1' | 1:23:A:G:H4'  | 3        | 0.12          |
| (1,305) | 1:23:A:G:H1' | 1:23:A:G:H4'  | 7        | 0.12          |
| (1,305) | 1:23:A:G:H1' | 1:23:A:G:H4'  | 8        | 0.12          |
| (1,301) | 1:23:A:G:H8  | 1:23:A:G:H2'  | 2        | 0.12          |
| (1,301) | 1:23:A:G:H8  | 1:23:A:G:H2'  | 3        | 0.12          |
| (1,301) | 1:23:A:G:H8  | 1:23:A:G:H2'  | 5        | 0.12          |
| (1,301) | 1:23:A:G:H8  | 1:23:A:G:H2'  | 6        | 0.12          |
| (1,293) | 1:21:A:U:H3  | 1:22:A:C:H42  | 10       | 0.12          |
| (1,282) | 1:20:A:A:H2  | 1:37:A:C:H1'  | 2        | 0.12          |
| (1,282) | 1:20:A:A:H2  | 1:37:A:C:H1'  | 4        | 0.12          |
| (1,267) | 1:19:A:G:H8  | 1:17:A:U:H4'  | 7        | 0.12          |
| (1,249) | 1:17:A:U:H6  | 1:16:A:A:H2'  | 7        | 0.12          |
| (1,211) | 1:12:A:C:H41 | 1:13:A:C:H5   | 9        | 0.12          |
| (1,208) | 1:13:A:C:H6  | 1:12:A:C:H6   | 7        | 0.12          |
| (1,69)  | 1:5:A:U:H6   | 1:4:A:A:H1'   | 6        | 0.12          |
| (1,69)  | 1:5:A:U:H6   | 1:4:A:A:H1'   | 9        | 0.12          |
| (1,655) | 1:51:A:G:H3' | 1:50:A:C:H2'  | 1        | 0.11          |
| (1,655) | 1:51:A:G:H3' | 1:50:A:C:H2'  | 3        | 0.11          |
| (1,655) | 1:51:A:G:H3' | 1:50:A:C:H2'  | 5        | 0.11          |
| (1,655) | 1:51:A:G:H3' | 1:50:A:C:H2'  | 7        | 0.11          |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,655) | 1:51:A:G:H3' | 1:50:A:C:H2'  | 9        | 0.11          |
| (1,655) | 1:51:A:G:H3' | 1:50:A:C:H2'  | 10       | 0.11          |
| (1,601) | 1:47:A:A:H2  | 1:48:A:G:H8   | 7        | 0.11          |
| (1,600) | 1:47:A:A:H2  | 1:48:A:G:H1'  | 8        | 0.11          |
| (1,563) | 1:43:A:G:H1  | 1:12:A:C:H41  | 3        | 0.11          |
| (1,563) | 1:43:A:G:H1  | 1:12:A:C:H41  | 7        | 0.11          |
| (1,529) | 1:40:A:G:H8  | 1:39:A:G:H8   | 3        | 0.11          |
| (1,485) | 1:35:A:A:H2  | 1:22:A:C:H1'  | 7        | 0.11          |
| (1,483) | 1:35:A:A:H8  | 1:34:A:G:H8   | 9        | 0.11          |
| (1,477) | 1:35:A:A:H8  | 1:35:A:A:H5'' | 3        | 0.11          |
| (1,477) | 1:35:A:A:H8  | 1:35:A:A:H5'' | 5        | 0.11          |
| (1,477) | 1:35:A:A:H8  | 1:35:A:A:H5'' | 9        | 0.11          |
| (1,434) | 1:31:A:G:H8  | 1:30:A:G:H8   | 9        | 0.11          |
| (1,424) | 1:30:A:G:H1  | 1:25:A:C:H5   | 6        | 0.11          |
| (1,410) | 1:29:A:G:H1  | 1:28:A:C:H1'  | 4        | 0.11          |
| (1,410) | 1:29:A:G:H1  | 1:28:A:C:H1'  | 8        | 0.11          |
| (1,397) | 1:29:A:G:H8  | 1:29:A:G:H2'  | 5        | 0.11          |
| (1,372) | 1:28:A:C:H6  | 1:28:A:C:H3'  | 9        | 0.11          |
| (1,372) | 1:28:A:C:H6  | 1:28:A:C:H3'  | 10       | 0.11          |
| (1,352) | 1:26:A:U:H5  | 1:25:A:C:H5   | 7        | 0.11          |
| (1,305) | 1:23:A:G:H1' | 1:23:A:G:H4'  | 1        | 0.11          |
| (1,305) | 1:23:A:G:H1' | 1:23:A:G:H4'  | 2        | 0.11          |
| (1,305) | 1:23:A:G:H1' | 1:23:A:G:H4'  | 4        | 0.11          |
| (1,301) | 1:23:A:G:H8  | 1:23:A:G:H2'  | 7        | 0.11          |
| (1,282) | 1:20:A:A:H2  | 1:37:A:C:H1'  | 8        | 0.11          |
| (1,279) | 1:20:A:A:H8  | 1:19:A:G:H3'  | 1        | 0.11          |
| (1,279) | 1:20:A:A:H8  | 1:19:A:G:H3'  | 2        | 0.11          |
| (1,279) | 1:20:A:A:H8  | 1:19:A:G:H3'  | 3        | 0.11          |
| (1,279) | 1:20:A:A:H8  | 1:19:A:G:H3'  | 8        | 0.11          |
| (1,267) | 1:19:A:G:H8  | 1:17:A:U:H4'  | 8        | 0.11          |
| (1,267) | 1:19:A:G:H8  | 1:17:A:U:H4'  | 9        | 0.11          |
| (1,249) | 1:17:A:U:H6  | 1:16:A:A:H2'  | 10       | 0.11          |
| (1,237) | 1:16:A:A:H8  | 1:15:A:C:H3'  | 4        | 0.11          |
| (1,237) | 1:16:A:A:H8  | 1:15:A:C:H3'  | 5        | 0.11          |
| (1,226) | 1:15:A:C:H6  | 1:14:A:C:H6   | 6        | 0.11          |
| (1,209) | 1:13:A:C:H5  | 1:12:A:C:H5   | 10       | 0.11          |
| (1,184) | 1:11:A:A:H2  | 1:48:A:G:H1'  | 6        | 0.11          |
| (1,174) | 1:11:A:A:H8  | 1:11:A:A:H5'' | 6        | 0.11          |
| (1,69)  | 1:5:A:U:H6   | 1:4:A:A:H1'   | 3        | 0.11          |
| (1,69)  | 1:5:A:U:H6   | 1:4:A:A:H1'   | 7        | 0.11          |
| (1,69)  | 1:5:A:U:H6   | 1:4:A:A:H1'   | 10       | 0.11          |
| (1,742) | 1:56:A:C:H5  | 1:55:A:C:H3'  | 8        | 0.1           |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,742) | 1:56:A:C:H5  | 1:55:A:C:H3'  | 10       | 0.1           |
| (1,655) | 1:51:A:G:H3' | 1:50:A:C:H2'  | 4        | 0.1           |
| (1,655) | 1:51:A:G:H3' | 1:50:A:C:H2'  | 6        | 0.1           |
| (1,633) | 1:50:A:C:H6  | 1:50:A:C:H5'' | 7        | 0.1           |
| (1,633) | 1:50:A:C:H6  | 1:50:A:C:H5'' | 10       | 0.1           |
| (1,595) | 1:47:A:A:H8  | 1:47:A:A:H2'  | 8        | 0.1           |
| (1,545) | 1:41:A:C:H1' | 1:40:A:G:H2'  | 10       | 0.1           |
| (1,536) | 1:40:A:G:H1  | 1:14:A:C:H5   | 4        | 0.1           |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 4        | 0.1           |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 5        | 0.1           |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 7        | 0.1           |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 9        | 0.1           |
| (1,517) | 1:39:A:G:H1' | 1:39:A:G:H5'' | 10       | 0.1           |
| (1,500) | 1:37:A:C:H6  | 1:36:A:U:H1'  | 5        | 0.1           |
| (1,494) | 1:36:A:U:H1' | 1:35:A:A:H2'  | 6        | 0.1           |
| (1,493) | 1:36:A:U:H6  | 1:35:A:A:H8   | 6        | 0.1           |
| (1,384) | 1:28:A:C:H5  | 1:26:A:U:H1'  | 3        | 0.1           |
| (1,323) | 1:24:A:C:H6  | 1:23:A:G:H2'  | 3        | 0.1           |
| (1,279) | 1:20:A:A:H8  | 1:19:A:G:H3'  | 6        | 0.1           |
| (1,69)  | 1:5:A:U:H6   | 1:4:A:A:H1'   | 2        | 0.1           |
| (1,69)  | 1:5:A:U:H6   | 1:4:A:A:H1'   | 4        | 0.1           |
| (1,69)  | 1:5:A:U:H6   | 1:4:A:A:H1'   | 5        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

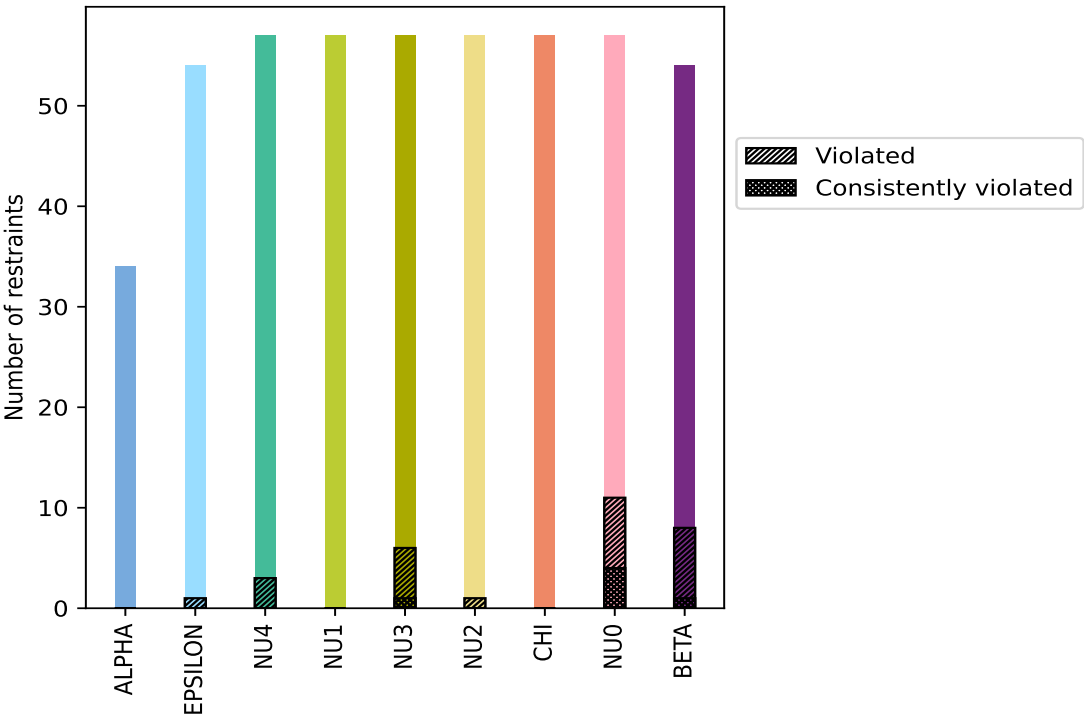
### 10.1 Summary of dihedral-angle violations ⓘ

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> |
| ALPHA      | 34    | 7.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| EPSILON    | 54    | 11.2           | 1                     | 1.9            | 0.2            | 0                                  | 0.0            | 0.0            |
| NU4        | 57    | 11.8           | 3                     | 5.3            | 0.6            | 0                                  | 0.0            | 0.0            |
| NU1        | 57    | 11.8           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| NU3        | 57    | 11.8           | 6                     | 10.5           | 1.2            | 1                                  | 1.8            | 0.2            |
| NU2        | 57    | 11.8           | 1                     | 1.8            | 0.2            | 0                                  | 0.0            | 0.0            |
| CHI        | 57    | 11.8           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| NU0        | 57    | 11.8           | 11                    | 19.3           | 2.3            | 4                                  | 7.0            | 0.8            |
| BETA       | 54    | 11.2           | 8                     | 14.8           | 1.7            | 1                                  | 1.9            | 0.2            |
| Total      | 484   | 100.0          | 30                    | 6.2            | 6.2            | 6                                  | 1.2            | 1.2            |

<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 ⓘ



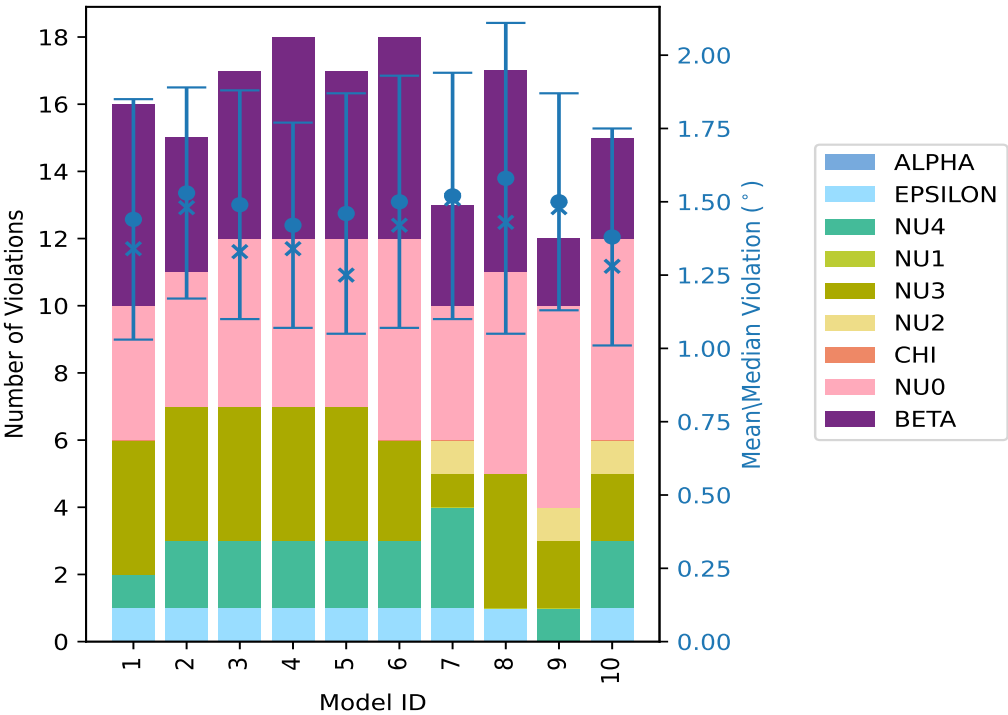
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 |         |     |     |     |     |     |     |      | Total | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|---------|-----|-----|-----|-----|-----|-----|------|-------|----------|---------|--------|------------|
|          | ALPHA                | EPSILON | NU4 | NU1 | NU3 | NU2 | CHI | NU0 | BETA |       |          |         |        |            |
| 1        | 0                    | 1       | 1   | 0   | 4   | 0   | 0   | 4   | 6    | 16    | 1.44     | 2.57    | 0.41   | 1.34       |
| 2        | 0                    | 1       | 2   | 0   | 4   | 0   | 0   | 4   | 4    | 15    | 1.53     | 2.4     | 0.36   | 1.48       |
| 3        | 0                    | 1       | 2   | 0   | 4   | 0   | 0   | 5   | 5    | 17    | 1.49     | 2.27    | 0.39   | 1.33       |
| 4        | 0                    | 1       | 2   | 0   | 4   | 0   | 0   | 5   | 6    | 18    | 1.42     | 2.41    | 0.35   | 1.34       |
| 5        | 0                    | 1       | 2   | 0   | 4   | 0   | 0   | 5   | 5    | 17    | 1.46     | 2.35    | 0.41   | 1.25       |
| 6        | 0                    | 1       | 2   | 0   | 3   | 0   | 0   | 6   | 6    | 18    | 1.5      | 2.57    | 0.43   | 1.42       |
| 7        | 0                    | 1       | 3   | 0   | 1   | 1   | 0   | 4   | 3    | 13    | 1.52     | 2.66    | 0.42   | 1.51       |
| 8        | 0                    | 1       | 0   | 0   | 4   | 0   | 0   | 6   | 6    | 17    | 1.58     | 2.88    | 0.53   | 1.43       |
| 9        | 0                    | 0       | 1   | 0   | 2   | 1   | 0   | 6   | 2    | 12    | 1.5      | 2.36    | 0.37   | 1.48       |
| 10       | 0                    | 1       | 2   | 0   | 2   | 1   | 0   | 6   | 3    | 15    | 1.38     | 2.52    | 0.37   | 1.28       |

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

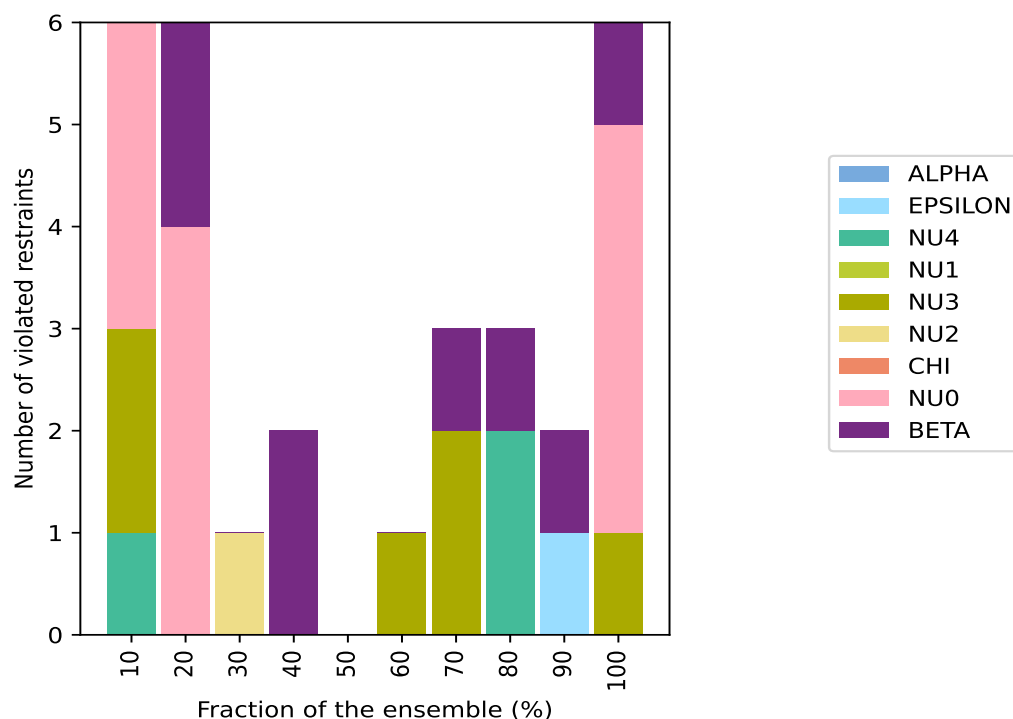
10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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 |       |
|-------------------------------|---------|-----|-----|-----|-----|-----|-----|------|-------|--------------------------|-------|
| ALPHA                         | EPSILON | NU4 | NU1 | NU3 | NU2 | CHI | NU0 | BETA | Total | Count <sup>1</sup>       | %     |
| 0                             | 0       | 1   | 0   | 2   | 0   | 0   | 3   | 0    | 6     | 1                        | 10.0  |
| 0                             | 0       | 0   | 0   | 0   | 0   | 0   | 4   | 2    | 6     | 2                        | 20.0  |
| 0                             | 0       | 0   | 0   | 0   | 1   | 0   | 0   | 0    | 1     | 3                        | 30.0  |
| 0                             | 0       | 0   | 0   | 0   | 0   | 0   | 0   | 2    | 2     | 4                        | 40.0  |
| 0                             | 0       | 0   | 0   | 0   | 0   | 0   | 0   | 0    | 0     | 5                        | 50.0  |
| 0                             | 0       | 0   | 0   | 1   | 0   | 0   | 0   | 0    | 1     | 6                        | 60.0  |
| 0                             | 0       | 0   | 0   | 2   | 0   | 0   | 0   | 1    | 3     | 7                        | 70.0  |
| 0                             | 0       | 2   | 0   | 0   | 0   | 0   | 0   | 1    | 3     | 8                        | 80.0  |
| 0                             | 1       | 0   | 0   | 0   | 0   | 0   | 0   | 1    | 2     | 9                        | 90.0  |
| 0                             | 0       | 0   | 0   | 1   | 0   | 0   | 4   | 1    | 6     | 10                       | 100.0 |

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

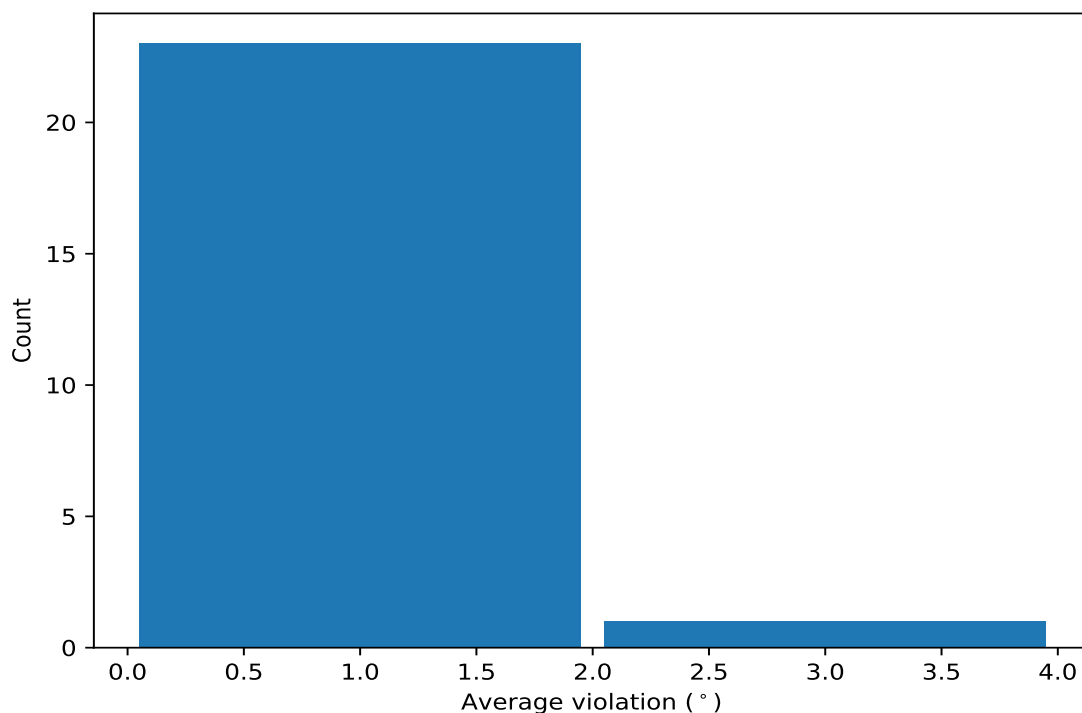
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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 |
|---------|--------------|--------------|--------------|--------------|---------------------|------|-----------------|--------|
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 10                  | 2.46 | 0.12            | 2.46   |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 10                  | 1.76 | 0.25            | 1.74   |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 10                  | 1.75 | 0.13            | 1.74   |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 10                  | 1.73 | 0.24            | 1.72   |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 10                  | 1.48 | 0.17            | 1.48   |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 10                  | 1.27 | 0.14            | 1.26   |
| (1,156) | 1:19:A:G:C4' | 1:19:A:G:C3' | 1:19:A:G:O3' | 1:20:A:A:P   | 9                   | 1.81 | 0.16            | 1.8    |
| (1,155) | 1:19:A:G:P   | 1:19:A:G:O5' | 1:19:A:G:C5' | 1:19:A:G:C4' | 9                   | 1.33 | 0.13            | 1.33   |
| (1,396) | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 1:47:A:A:C1' | 8                   | 1.26 | 0.14            | 1.26   |
| (1,356) | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 1:42:A:U:C1' | 8                   | 1.24 | 0.21            | 1.14   |
| (1,89)  | 1:11:A:A:P   | 1:11:A:A:O5' | 1:11:A:A:C5' | 1:11:A:A:C4' | 8                   | 1.09 | 0.08            | 1.07   |
| (1,355) | 1:42:A:U:C2' | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 7                   | 1.78 | 0.12            | 1.79   |
| (1,382) | 1:46:A:U:P   | 1:46:A:U:O5' | 1:46:A:U:C5' | 1:46:A:U:C4' | 7                   | 1.33 | 0.17            | 1.38   |
| (1,380) | 1:45:A:C:C2' | 1:45:A:C:C3' | 1:45:A:C:C4' | 1:45:A:C:O4' | 7                   | 1.12 | 0.07            | 1.16   |
| (1,395) | 1:47:A:A:C2' | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 6                   | 1.45 | 0.65            | 1.23   |
| (1,315) | 1:38:A:U:P   | 1:38:A:U:O5' | 1:38:A:U:C5' | 1:38:A:U:C4' | 4                   | 1.25 | 0.14            | 1.26   |
| (1,231) | 1:28:A:C:P   | 1:28:A:C:O5' | 1:28:A:C:C5' | 1:28:A:C:C4' | 4                   | 1.1  | 0.06            | 1.11   |
| (1,346) | 1:41:A:C:C1' | 1:41:A:C:C2' | 1:41:A:C:C3' | 1:41:A:C:C4' | 3                   | 1.59 | 0.24            | 1.65   |
| (1,267) | 1:32:A:C:C4' | 1:32:A:C:O4' | 1:32:A:C:C1' | 1:32:A:C:C2' | 2                   | 1.14 | 0.08            | 1.14   |
| (1,272) | 1:33:A:U:P   | 1:33:A:U:O5' | 1:33:A:U:C5' | 1:33:A:U:C4' | 2                   | 1.14 | 0.05            | 1.14   |
| (1,327) | 1:39:A:G:C4' | 1:39:A:G:O4' | 1:39:A:G:C1' | 1:39:A:G:C2' | 2                   | 1.09 | 0.04            | 1.09   |

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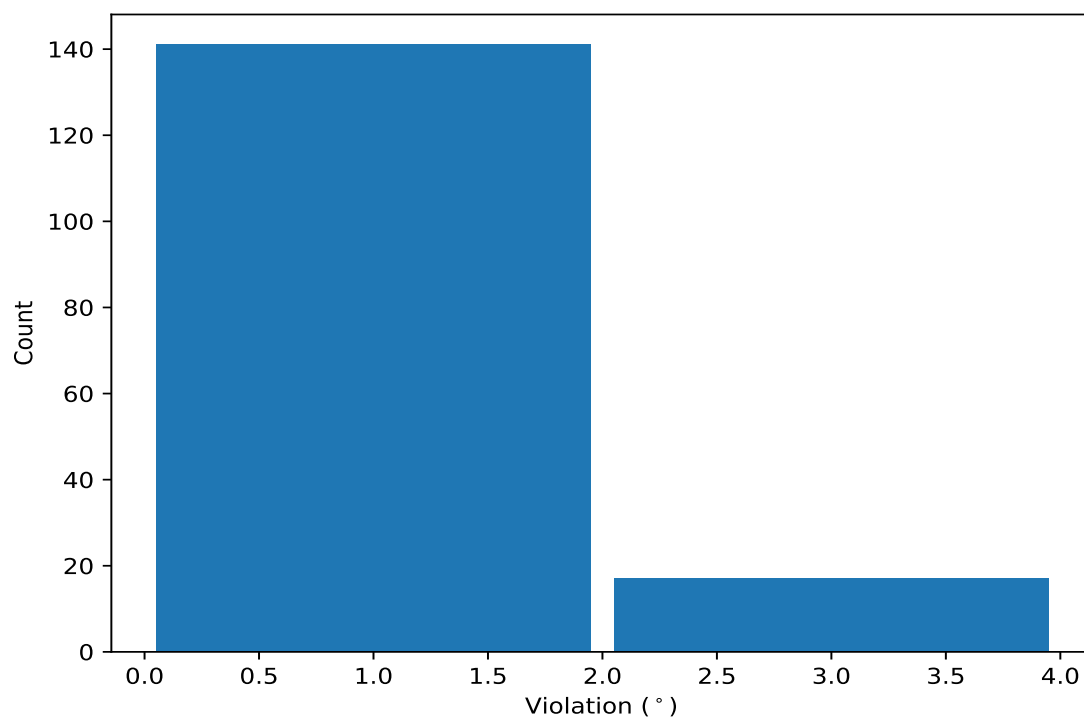
| Key     | Atom-1       | Atom-2       | Atom-3       | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|--------------|--------------|--------------|---------------------|------|-----------------|--------|
| (1,215) | 1:26:A:U:P   | 1:26:A:U:O5' | 1:26:A:U:C5' | 1:26:A:U:C4' | 2                   | 1.06 | 0.02            | 1.06   |
| (1,369) | 1:44:A:G:C4' | 1:44:A:G:O4' | 1:44:A:G:C1' | 1:44:A:G:C2' | 2                   | 1.06 | 0.06            | 1.06   |
| (1,201) | 1:24:A:C:C4' | 1:24:A:C:O4' | 1:24:A:C:C1' | 1:24:A:C:C2' | 2                   | 1.02 | 0.0             | 1.02   |

<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 (°) |
|---------|--------------|--------------|--------------|--------------|----------|---------------|
| (1,395) | 1:47:A:A:C2' | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 8        | 2.88          |
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 7        | 2.66          |
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 1        | 2.57          |
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 6        | 2.57          |

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| Key     | Atom-1       | Atom-2       | Atom-3       | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|--------------|--------------|----------|---------------|
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 8        | 2.52          |
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 10       | 2.52          |
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 4        | 2.41          |
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 2        | 2.4           |
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 9        | 2.36          |
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 5        | 2.35          |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 8        | 2.31          |
| (1,148) | 1:18:A:U:P   | 1:18:A:U:O5' | 1:18:A:U:C5' | 1:18:A:U:C4' | 3        | 2.27          |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 6        | 2.23          |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 3        | 2.06          |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 5        | 2.04          |
| (1,156) | 1:19:A:G:C4' | 1:19:A:G:C3' | 1:19:A:G:O3' | 1:20:A:A:P   | 3        | 2.03          |
| (1,156) | 1:19:A:G:C4' | 1:19:A:G:C3' | 1:19:A:G:O3' | 1:20:A:A:P   | 5        | 2.01          |
| (1,156) | 1:19:A:G:C4' | 1:19:A:G:C3' | 1:19:A:G:O3' | 1:20:A:A:P   | 6        | 1.99          |
| (1,355) | 1:42:A:U:C2' | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 2        | 1.96          |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 5        | 1.93          |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 2        | 1.85          |
| (1,355) | 1:42:A:U:C2' | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 1        | 1.85          |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 4        | 1.84          |
| (1,346) | 1:41:A:C:C1' | 1:41:A:C:C2' | 1:41:A:C:C3' | 1:41:A:C:C4' | 9        | 1.84          |
| (1,355) | 1:42:A:U:C2' | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 8        | 1.83          |
| (1,156) | 1:19:A:G:C4' | 1:19:A:G:C3' | 1:19:A:G:O3' | 1:20:A:A:P   | 8        | 1.83          |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 2        | 1.82          |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 6        | 1.82          |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 5        | 1.8           |
| (1,156) | 1:19:A:G:C4' | 1:19:A:G:C3' | 1:19:A:G:O3' | 1:20:A:A:P   | 7        | 1.8           |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 3        | 1.79          |
| (1,355) | 1:42:A:U:C2' | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 5        | 1.79          |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 1        | 1.78          |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 8        | 1.77          |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 7        | 1.76          |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 4        | 1.76          |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 6        | 1.75          |
| (1,355) | 1:42:A:U:C2' | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 3        | 1.75          |
| (1,156) | 1:19:A:G:C4' | 1:19:A:G:C3' | 1:19:A:G:O3' | 1:20:A:A:P   | 2        | 1.74          |
| (1,153) | 1:18:A:U:C2' | 1:18:A:U:C3' | 1:18:A:U:C4' | 1:18:A:U:O4' | 9        | 1.74          |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 4        | 1.73          |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 3        | 1.73          |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 1        | 1.72          |
| (1,355) | 1:42:A:U:C2' | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 6        | 1.72          |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 7        | 1.72          |
| (1,156) | 1:19:A:G:C4' | 1:19:A:G:C3' | 1:19:A:G:O3' | 1:20:A:A:P   | 10       | 1.71          |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 9        | 1.69          |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 10       | 1.68          |
| (1,346) | 1:41:A:C:C1' | 1:41:A:C:C2' | 1:41:A:C:C3' | 1:41:A:C:C4' | 7        | 1.65          |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 2        | 1.65          |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 3        | 1.64          |
| (1,156) | 1:19:A:G:C4' | 1:19:A:G:C3' | 1:19:A:G:O3' | 1:20:A:A:P   | 1        | 1.62          |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 1        | 1.6           |
| (1,356) | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 1:42:A:U:C1' | 9        | 1.6           |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 4        | 1.6           |

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| Key     | Atom-1       | Atom-2       | Atom-3       | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|--------------|--------------|----------|---------------|
| (1,356) | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 1:42:A:U:C1' | 7        | 1.58          |
| (1,156) | 1:19:A:G:C4' | 1:19:A:G:C3' | 1:19:A:G:O3' | 1:20:A:A:P   | 4        | 1.58          |
| (1,382) | 1:46:A:U:P   | 1:46:A:U:O5' | 1:46:A:U:C5' | 1:46:A:U:C4' | 8        | 1.56          |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 3        | 1.56          |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 2        | 1.56          |
| (1,355) | 1:42:A:U:C2' | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 4        | 1.55          |
| (1,396) | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 1:47:A:A:C1' | 6        | 1.54          |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 6        | 1.54          |
| (1,155) | 1:19:A:G:P   | 1:19:A:G:O5' | 1:19:A:G:C5' | 1:19:A:G:C4' | 4        | 1.53          |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 1        | 1.52          |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 7        | 1.51          |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 10       | 1.51          |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 9        | 1.51          |
| (1,400) | 1:48:A:G:C4' | 1:48:A:G:O4' | 1:48:A:G:C1' | 1:48:A:G:C2' | 8        | 1.49          |
| (1,382) | 1:46:A:U:P   | 1:46:A:U:O5' | 1:46:A:U:C5' | 1:46:A:U:C4' | 2        | 1.48          |
| (1,155) | 1:19:A:G:P   | 1:19:A:G:O5' | 1:19:A:G:C5' | 1:19:A:G:C4' | 6        | 1.47          |
| (1,388) | 1:46:A:U:C2' | 1:46:A:U:C3' | 1:46:A:U:C4' | 1:46:A:U:O4' | 9        | 1.44          |
| (1,315) | 1:38:A:U:P   | 1:38:A:U:O5' | 1:38:A:U:C5' | 1:38:A:U:C4' | 1        | 1.44          |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 10       | 1.44          |
| (1,382) | 1:46:A:U:P   | 1:46:A:U:O5' | 1:46:A:U:C5' | 1:46:A:U:C4' | 4        | 1.43          |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 8        | 1.43          |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 9        | 1.42          |
| (1,155) | 1:19:A:G:P   | 1:19:A:G:O5' | 1:19:A:G:C5' | 1:19:A:G:C4' | 10       | 1.42          |
| (1,382) | 1:46:A:U:P   | 1:46:A:U:O5' | 1:46:A:U:C5' | 1:46:A:U:C4' | 6        | 1.38          |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 8        | 1.37          |
| (1,155) | 1:19:A:G:P   | 1:19:A:G:O5' | 1:19:A:G:C5' | 1:19:A:G:C4' | 8        | 1.37          |
| (1,184) | 1:22:A:C:C4' | 1:22:A:C:O4' | 1:22:A:C:C1' | 1:22:A:C:C2' | 10       | 1.36          |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 5        | 1.36          |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 7        | 1.34          |
| (1,315) | 1:38:A:U:P   | 1:38:A:U:O5' | 1:38:A:U:C5' | 1:38:A:U:C4' | 2        | 1.33          |
| (1,155) | 1:19:A:G:P   | 1:19:A:G:O5' | 1:19:A:G:C5' | 1:19:A:G:C4' | 3        | 1.33          |
| (1,396) | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 1:47:A:A:C1' | 5        | 1.31          |
| (1,396) | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 1:47:A:A:C1' | 2        | 1.29          |
| (1,396) | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 1:47:A:A:C1' | 3        | 1.28          |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 2        | 1.28          |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 10       | 1.28          |
| (1,155) | 1:19:A:G:P   | 1:19:A:G:O5' | 1:19:A:G:C5' | 1:19:A:G:C4' | 2        | 1.28          |
| (1,155) | 1:19:A:G:P   | 1:19:A:G:O5' | 1:19:A:G:C5' | 1:19:A:G:C4' | 7        | 1.28          |
| (1,346) | 1:41:A:C:C1' | 1:41:A:C:C2' | 1:41:A:C:C3' | 1:41:A:C:C4' | 10       | 1.27          |
| (1,395) | 1:47:A:A:C2' | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 3        | 1.26          |
| (1,395) | 1:47:A:A:C2' | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 1        | 1.25          |
| (1,382) | 1:46:A:U:P   | 1:46:A:U:O5' | 1:46:A:U:C5' | 1:46:A:U:C4' | 5        | 1.25          |
| (1,396) | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 1:47:A:A:C1' | 1        | 1.24          |
| (1,396) | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 1:47:A:A:C1' | 4        | 1.24          |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 5        | 1.24          |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 7        | 1.24          |
| (1,395) | 1:47:A:A:C2' | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 5        | 1.22          |
| (1,267) | 1:32:A:C:C4' | 1:32:A:C:O4' | 1:32:A:C:C1' | 1:32:A:C:C2' | 6        | 1.22          |
| (1,89)  | 1:11:A:A:P   | 1:11:A:A:O5' | 1:11:A:A:C5' | 1:11:A:A:C4' | 8        | 1.22          |
| (1,315) | 1:38:A:U:P   | 1:38:A:U:O5' | 1:38:A:U:C5' | 1:38:A:U:C4' | 6        | 1.19          |
| (1,272) | 1:33:A:U:P   | 1:33:A:U:O5' | 1:33:A:U:C5' | 1:33:A:U:C4' | 3        | 1.19          |

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| Key     | Atom-1       | Atom-2       | Atom-3       | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|--------------|--------------|----------|---------------|
| (1,380) | 1:45:A:C:C2' | 1:45:A:C:C3' | 1:45:A:C:C4' | 1:45:A:C:O4' | 2        | 1.18          |
| (1,380) | 1:45:A:C:C2' | 1:45:A:C:C3' | 1:45:A:C:C4' | 1:45:A:C:O4' | 4        | 1.18          |
| (1,380) | 1:45:A:C:C2' | 1:45:A:C:C3' | 1:45:A:C:C4' | 1:45:A:C:O4' | 6        | 1.18          |
| (1,356) | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 1:42:A:U:C1' | 3        | 1.18          |
| (1,356) | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 1:42:A:U:C1' | 4        | 1.18          |
| (1,231) | 1:28:A:C:P   | 1:28:A:C:O5' | 1:28:A:C:C5' | 1:28:A:C:C4' | 4        | 1.17          |
| (1,380) | 1:45:A:C:C2' | 1:45:A:C:C3' | 1:45:A:C:C4' | 1:45:A:C:O4' | 8        | 1.16          |
| (1,89)  | 1:11:A:A:P   | 1:11:A:A:O5' | 1:11:A:A:C5' | 1:11:A:A:C4' | 9        | 1.16          |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 6        | 1.15          |
| (1,89)  | 1:11:A:A:P   | 1:11:A:A:O5' | 1:11:A:A:C5' | 1:11:A:A:C4' | 7        | 1.15          |
| (1,382) | 1:46:A:U:P   | 1:46:A:U:O5' | 1:46:A:U:C5' | 1:46:A:U:C4' | 3        | 1.14          |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 4        | 1.14          |
| (1,109) | 1:13:A:C:C4' | 1:13:A:C:O4' | 1:13:A:C:C1' | 1:13:A:C:C2' | 9        | 1.14          |
| (1,369) | 1:44:A:G:C4' | 1:44:A:G:O4' | 1:44:A:G:C1' | 1:44:A:G:C2' | 4        | 1.13          |
| (1,327) | 1:39:A:G:C4' | 1:39:A:G:O4' | 1:39:A:G:C1' | 1:39:A:G:C2' | 5        | 1.13          |
| (1,231) | 1:28:A:C:P   | 1:28:A:C:O5' | 1:28:A:C:C5' | 1:28:A:C:C4' | 8        | 1.13          |
| (1,155) | 1:19:A:G:P   | 1:19:A:G:O5' | 1:19:A:G:C5' | 1:19:A:G:C4' | 1        | 1.13          |
| (1,155) | 1:19:A:G:P   | 1:19:A:G:O5' | 1:19:A:G:C5' | 1:19:A:G:C4' | 5        | 1.13          |
| (1,396) | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 1:47:A:A:C1' | 10       | 1.12          |
| (1,380) | 1:45:A:C:C2' | 1:45:A:C:C3' | 1:45:A:C:C4' | 1:45:A:C:O4' | 1        | 1.11          |
| (1,347) | 1:41:A:C:C2' | 1:41:A:C:C3' | 1:41:A:C:C4' | 1:41:A:C:O4' | 10       | 1.11          |
| (1,356) | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 1:42:A:U:C1' | 6        | 1.1           |
| (1,356) | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 1:42:A:U:C1' | 10       | 1.1           |
| (1,395) | 1:47:A:A:C2' | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 2        | 1.09          |
| (1,356) | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 1:42:A:U:C1' | 5        | 1.09          |
| (1,231) | 1:28:A:C:P   | 1:28:A:C:O5' | 1:28:A:C:C5' | 1:28:A:C:C4' | 5        | 1.09          |
| (1,382) | 1:46:A:U:P   | 1:46:A:U:O5' | 1:46:A:U:C5' | 1:46:A:U:C4' | 1        | 1.08          |
| (1,272) | 1:33:A:U:P   | 1:33:A:U:O5' | 1:33:A:U:C5' | 1:33:A:U:C4' | 4        | 1.08          |
| (1,215) | 1:26:A:U:P   | 1:26:A:U:O5' | 1:26:A:U:C5' | 1:26:A:U:C4' | 5        | 1.08          |
| (1,356) | 1:42:A:U:C3' | 1:42:A:U:C4' | 1:42:A:U:O4' | 1:42:A:U:C1' | 2        | 1.07          |
| (1,89)  | 1:11:A:A:P   | 1:11:A:A:O5' | 1:11:A:A:C5' | 1:11:A:A:C4' | 4        | 1.07          |
| (1,89)  | 1:11:A:A:P   | 1:11:A:A:O5' | 1:11:A:A:C5' | 1:11:A:A:C4' | 10       | 1.07          |
| (1,381) | 1:45:A:C:C3' | 1:45:A:C:C4' | 1:45:A:C:O4' | 1:45:A:C:C1' | 7        | 1.06          |
| (1,315) | 1:38:A:U:P   | 1:38:A:U:O5' | 1:38:A:U:C5' | 1:38:A:U:C4' | 8        | 1.06          |
| (1,292) | 1:35:A:A:C4' | 1:35:A:A:O4' | 1:35:A:A:C1' | 1:35:A:A:C2' | 1        | 1.06          |
| (1,84)  | 1:10:A:C:C4' | 1:10:A:C:O4' | 1:10:A:C:C1' | 1:10:A:C:C2' | 3        | 1.06          |
| (1,327) | 1:39:A:G:C4' | 1:39:A:G:O4' | 1:39:A:G:C1' | 1:39:A:G:C2' | 9        | 1.05          |
| (1,267) | 1:32:A:C:C4' | 1:32:A:C:O4' | 1:32:A:C:C1' | 1:32:A:C:C2' | 10       | 1.05          |
| (1,215) | 1:26:A:U:P   | 1:26:A:U:O5' | 1:26:A:U:C5' | 1:26:A:U:C4' | 6        | 1.05          |
| (1,396) | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 1:47:A:A:C1' | 7        | 1.04          |
| (1,380) | 1:45:A:C:C2' | 1:45:A:C:C3' | 1:45:A:C:C4' | 1:45:A:C:O4' | 5        | 1.03          |
| (1,275) | 1:33:A:U:C4' | 1:33:A:U:O4' | 1:33:A:U:C1' | 1:33:A:U:C2' | 9        | 1.02          |
| (1,201) | 1:24:A:C:C4' | 1:24:A:C:O4' | 1:24:A:C:C1' | 1:24:A:C:C2' | 6        | 1.02          |
| (1,201) | 1:24:A:C:C4' | 1:24:A:C:O4' | 1:24:A:C:C1' | 1:24:A:C:C2' | 10       | 1.02          |
| (1,395) | 1:47:A:A:C2' | 1:47:A:A:C3' | 1:47:A:A:C4' | 1:47:A:A:O4' | 4        | 1.01          |
| (1,336) | 1:40:A:G:C4' | 1:40:A:G:O4' | 1:40:A:G:C1' | 1:40:A:G:C2' | 8        | 1.01          |
| (1,89)  | 1:11:A:A:P   | 1:11:A:A:O5' | 1:11:A:A:C5' | 1:11:A:A:C4' | 1        | 1.01          |
| (1,89)  | 1:11:A:A:P   | 1:11:A:A:O5' | 1:11:A:A:C5' | 1:11:A:A:C4' | 6        | 1.01          |
| (1,380) | 1:45:A:C:C2' | 1:45:A:C:C3' | 1:45:A:C:C4' | 1:45:A:C:O4' | 3        | 1.0           |
| (1,369) | 1:44:A:G:C4' | 1:44:A:G:O4' | 1:44:A:G:C1' | 1:44:A:G:C2' | 8        | 1.0           |
| (1,231) | 1:28:A:C:P   | 1:28:A:C:O5' | 1:28:A:C:C5' | 1:28:A:C:C4' | 1        | 1.0           |

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| Key    | Atom-1     | Atom-2       | Atom-3       | Atom-4       | Model ID | Violation (°) |
|--------|------------|--------------|--------------|--------------|----------|---------------|
| (1,89) | 1:11:A:A:P | 1:11:A:A:O5' | 1:11:A:A:C5' | 1:11:A:A:C4' | 3        | 1.0           |