



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 01:33 PM UTC

PDB ID : 2M58 / pdb\_00002m58  
BMRB ID : 19040  
Title : Structure of 2'-5' AG1 lariat forming ribozyme in its inactive state  
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Deposited on : 2013-02-18

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  
Mogul : 2022.3.0, CSD as543be (2022)  
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

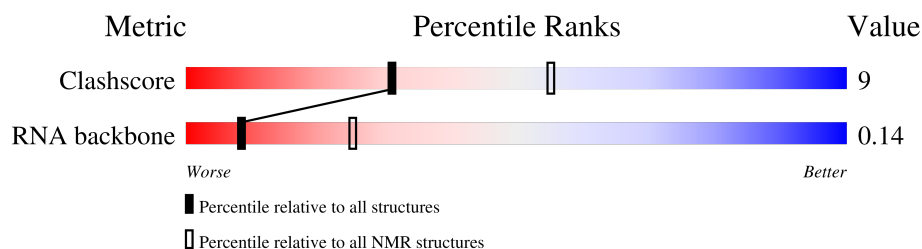
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

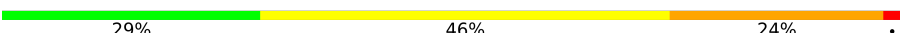
The overall completeness of chemical shifts assignment is 69%.

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     | 59     | <br>29%                      46%                      24%                      . |

## 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 [i](#)

There is only 1 type of molecule in this entry. The entry contains 1911 atoms, of which 641 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (59-MER).

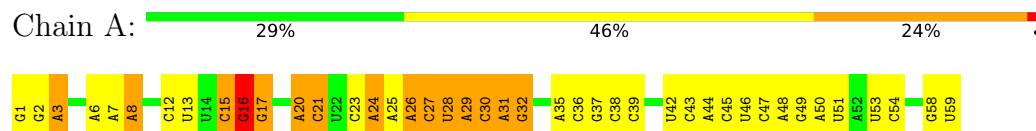
| Mol | Chain | Residues | Atoms |     |     |     |     |    | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|-------|
| 1   | A     | 59       | Total | C   | H   | N   | O   | P  | 0     |
|     |       |          | 1911  | 564 | 641 | 233 | 412 | 61 |       |

## 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: RNA (59-MER)

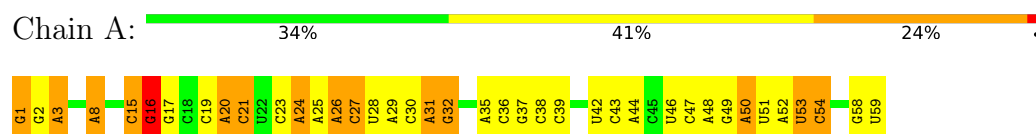


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

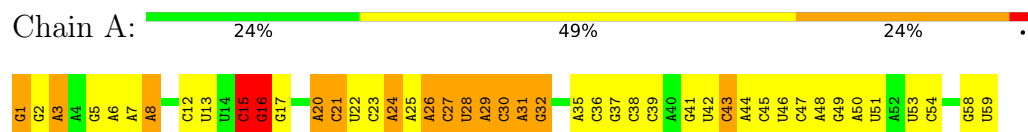
#### 4.2.1 Score per residue for model 1

- Molecule 1: RNA (59-MER)



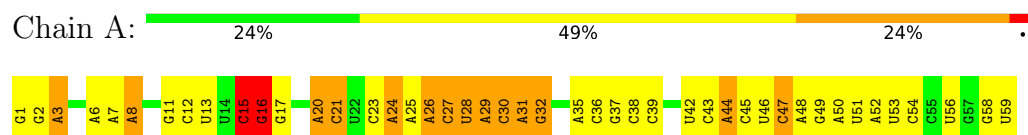
#### 4.2.2 Score per residue for model 2

- Molecule 1: RNA (59-MER)



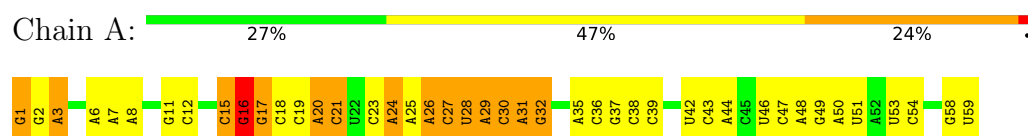
### 4.2.3 Score per residue for model 3

- Molecule 1: RNA (59-MER)



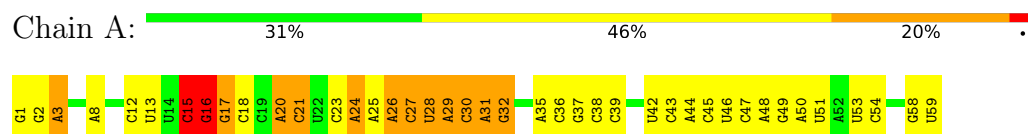
### 4.2.4 Score per residue for model 4

- Molecule 1: RNA (59-MER)



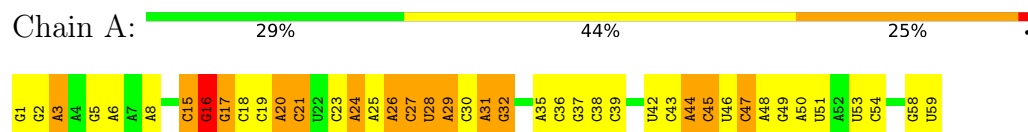
### 4.2.5 Score per residue for model 5

- Molecule 1: RNA (59-MER)



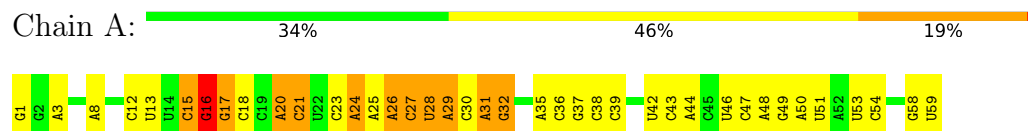
### 4.2.6 Score per residue for model 6

- Molecule 1: RNA (59-MER)



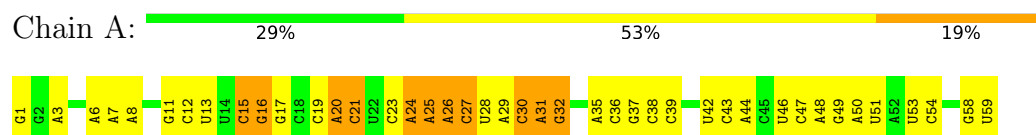
### 4.2.7 Score per residue for model 7

- Molecule 1: RNA (59-MER)



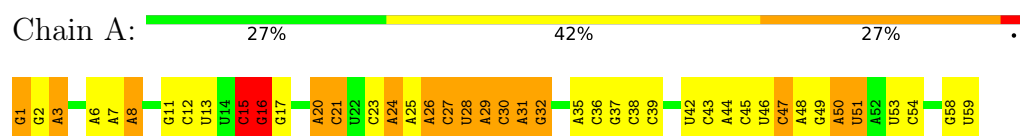
### 4.2.8 Score per residue for model 8

- Molecule 1: RNA (59-MER)



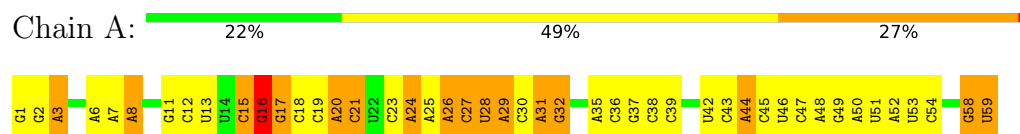
### 4.2.9 Score per residue for model 9

- Molecule 1: RNA (59-MER)



### 4.2.10 Score per residue for model 10

- Molecule 1: RNA (59-MER)



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| ARIA          | structure solution |         |
| ARIA          | 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                       | 789            |
| Number of shifts mapped to atoms             | 789            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 69%            |



## 6 Model quality

### 6.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                       | Bond angles |                       |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                  | RMSZ        | #Z>5                  |
| 1   | A     | 0.30±0.00    | 0±0/1385 ( 0.0± 0.0%) | 0.82±0.02   | 0±0/2156 ( 0.0± 0.0%) |
| All | All   | 0.30         | 0/13850 ( 0.0%)       | 0.82        | 3/21560 ( 0.0%)       |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 2.7±1.7   |
| All | All   | 0         | 27        |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 43  | C    | C1'-O4'-C4' | -5.55 | 104.35      | 109.90   | 2      | 1     |
| 1   | A     | 52  | A    | C1'-O4'-C4' | -5.37 | 104.53      | 109.90   | 1      | 1     |
| 1   | A     | 15  | C    | C3'-C2'-C1' | -5.02 | 96.48       | 101.50   | 9      | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 16  | G    | Sidechain | 9              |
| 1   | A     | 8   | A    | Sidechain | 5              |
| 1   | A     | 15  | C    | Sidechain | 4              |

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| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 45  | C    | Sidechain | 4              |
| 1   | A     | 47  | C    | Sidechain | 3              |
| 1   | A     | 41  | G    | Sidechain | 1              |
| 1   | A     | 56  | U    | Sidechain | 1              |

## 6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1270  | 641      | 640      | 17±3    |
| All | All   | 12700 | 6410     | 6400     | 169     |

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 9.

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

| Atom-1       | Atom-2        | Clash(Å) | Distance(Å) | Models |       |
|--------------|---------------|----------|-------------|--------|-------|
|              |               |          |             | Worst  | Total |
| 1:A:58:G:H2' | 1:A:59:U:C6   | 0.57     | 2.35        | 10     | 1     |
| 1:A:15:C:O4' | 1:A:16:G:C4   | 0.53     | 2.61        | 5      | 10    |
| 1:A:31:A:H2' | 1:A:32:G:O4'  | 0.53     | 2.03        | 9      | 9     |
| 1:A:50:A:H3' | 1:A:51:U:H5'' | 0.52     | 1.82        | 9      | 1     |
| 1:A:28:U:C5  | 1:A:29:A:C8   | 0.51     | 2.99        | 3      | 2     |
| 1:A:58:G:H2' | 1:A:59:U:C5   | 0.51     | 2.40        | 10     | 1     |
| 1:A:6:A:C2   | 1:A:7:A:C8    | 0.51     | 2.99        | 4      | 6     |
| 1:A:28:U:H2' | 1:A:29:A:O4'  | 0.50     | 2.06        | 5      | 6     |
| 1:A:23:C:H2' | 1:A:24:A:O4'  | 0.50     | 2.07        | 3      | 10    |
| 1:A:26:A:C2  | 1:A:27:C:C6   | 0.50     | 2.99        | 1      | 9     |
| 1:A:46:U:H2' | 1:A:47:C:O4'  | 0.49     | 2.07        | 2      | 10    |
| 1:A:31:A:H2' | 1:A:32:G:C5'  | 0.49     | 2.36        | 4      | 6     |
| 1:A:19:C:H2' | 1:A:20:A:O4'  | 0.49     | 2.07        | 8      | 5     |
| 1:A:26:A:C4  | 1:A:27:C:C5   | 0.49     | 3.00        | 10     | 5     |
| 1:A:15:C:H4' | 1:A:16:G:O4'  | 0.49     | 2.08        | 5      | 10    |
| 1:A:20:A:C5  | 1:A:21:C:C6   | 0.48     | 3.01        | 6      | 9     |
| 1:A:2:G:H2'  | 1:A:3:A:O4'   | 0.48     | 2.09        | 4      | 8     |
| 1:A:20:A:C5  | 1:A:21:C:C5   | 0.47     | 3.01        | 3      | 4     |
| 1:A:17:G:H2' | 1:A:18:C:O4'  | 0.47     | 2.10        | 6      | 5     |

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| Atom-1        | Atom-2        | Clash(Å) | Distance(Å) | Models |       |
|---------------|---------------|----------|-------------|--------|-------|
|               |               |          |             | Worst  | Total |
| 1:A:12:C:C5   | 1:A:13:U:C4   | 0.47     | 3.02        | 2      | 2     |
| 1:A:44:A:C2'  | 1:A:45:C:H5'  | 0.47     | 2.40        | 3      | 3     |
| 1:A:30:C:C3'  | 1:A:31:A:H5'' | 0.47     | 2.40        | 2      | 4     |
| 1:A:20:A:C4   | 1:A:21:C:C6   | 0.46     | 3.04        | 2      | 6     |
| 1:A:23:C:C3'  | 1:A:24:A:H5'' | 0.45     | 2.41        | 4      | 4     |
| 1:A:1:GTP:O2G | 1:A:1:GTP:O1B | 0.45     | 2.34        | 2      | 2     |
| 1:A:26:A:C5   | 1:A:27:C:C5   | 0.44     | 3.05        | 10     | 1     |
| 1:A:50:A:C3'  | 1:A:51:U:H5'' | 0.44     | 2.42        | 9      | 1     |
| 1:A:25:A:H2'  | 1:A:26:A:C8   | 0.44     | 2.48        | 8      | 1     |
| 1:A:1:GTP:O5' | 1:A:1:GTP:O2B | 0.43     | 2.35        | 1      | 1     |
| 1:A:1:GTP:O2A | 1:A:1:GTP:O1B | 0.43     | 2.36        | 9      | 1     |
| 1:A:12:C:C4   | 1:A:13:U:C4   | 0.43     | 3.07        | 10     | 5     |
| 1:A:5:G:C4    | 1:A:6:A:C8    | 0.42     | 3.08        | 2      | 2     |
| 1:A:1:GTP:O3B | 1:A:1:GTP:O2A | 0.42     | 2.37        | 4      | 1     |
| 1:A:32:G:N2   | 1:A:50:A:H62  | 0.41     | 2.13        | 1      | 1     |
| 1:A:11:G:H2'  | 1:A:12:C:O4'  | 0.41     | 2.15        | 4      | 4     |
| 1:A:53:U:H5'  | 1:A:54:C:C6   | 0.41     | 2.50        | 1      | 1     |
| 1:A:30:C:O2'  | 1:A:31:A:C8   | 0.41     | 2.72        | 4      | 1     |
| 1:A:12:C:C5   | 1:A:13:U:C5   | 0.41     | 3.08        | 2      | 1     |
| 1:A:53:U:O5'  | 1:A:54:C:C5   | 0.41     | 2.73        | 1      | 1     |
| 1:A:21:C:C2'  | 1:A:22:U:H5'  | 0.41     | 2.45        | 2      | 1     |
| 1:A:30:C:H3'  | 1:A:31:A:H5'  | 0.41     | 1.92        | 8      | 1     |
| 1:A:15:C:C6   | 1:A:16:G:C6   | 0.41     | 3.09        | 10     | 1     |
| 1:A:31:A:O2'  | 1:A:32:G:C5'  | 0.41     | 2.69        | 5      | 1     |
| 1:A:27:C:H3'  | 1:A:28:U:H5'' | 0.41     | 1.93        | 10     | 1     |
| 1:A:13:U:H2'  | 1:A:15:C:C5   | 0.40     | 2.51        | 2      | 2     |
| 1:A:11:G:C5   | 1:A:12:C:C4   | 0.40     | 3.10        | 3      | 1     |
| 1:A:26:A:N3   | 1:A:27:C:C6   | 0.40     | 2.89        | 8      | 1     |

## 6.3 Torsion angles [i](#)

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

There are no protein molecules in this entry.

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

There are no protein molecules in this entry.

### 6.3.3 RNA [i](#)

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers | Suiteness |
|-----|-------|---------------|-------------------|-----------------|-----------|
| 1   | A     | 57/59 (97%)   | 32±0 (56±0%)      | 5±2 (8±4%)      | 0.21±0.00 |
| All | All   | 570/590 (97%) | 320 (56%)         | 46 (8%)         | 0.21      |

The overall RNA backbone suiteness is 0.14.

All unique RNA backbone outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 3   | A    | 10             |
| 1   | A     | 8   | A    | 10             |
| 1   | A     | 15  | C    | 10             |
| 1   | A     | 16  | G    | 10             |
| 1   | A     | 17  | G    | 10             |
| 1   | A     | 20  | A    | 10             |
| 1   | A     | 21  | C    | 10             |
| 1   | A     | 24  | A    | 10             |
| 1   | A     | 25  | A    | 10             |
| 1   | A     | 26  | A    | 10             |
| 1   | A     | 27  | C    | 10             |
| 1   | A     | 28  | U    | 10             |
| 1   | A     | 29  | A    | 10             |
| 1   | A     | 30  | C    | 10             |
| 1   | A     | 31  | A    | 10             |
| 1   | A     | 32  | G    | 10             |
| 1   | A     | 35  | A    | 10             |
| 1   | A     | 36  | C    | 10             |
| 1   | A     | 37  | G    | 10             |
| 1   | A     | 38  | C    | 10             |
| 1   | A     | 39  | C    | 10             |
| 1   | A     | 42  | U    | 10             |
| 1   | A     | 43  | C    | 10             |
| 1   | A     | 44  | A    | 10             |
| 1   | A     | 48  | A    | 10             |
| 1   | A     | 49  | G    | 10             |
| 1   | A     | 50  | A    | 10             |
| 1   | A     | 51  | U    | 10             |
| 1   | A     | 53  | U    | 10             |
| 1   | A     | 54  | C    | 10             |
| 1   | A     | 58  | G    | 10             |
| 1   | A     | 59  | U    | 10             |

All unique RNA pucker outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 37  | G    | 7              |
| 1   | A     | 27  | C    | 5              |
| 1   | A     | 35  | A    | 5              |
| 1   | A     | 24  | A    | 5              |
| 1   | A     | 53  | U    | 4              |
| 1   | A     | 29  | A    | 4              |
| 1   | A     | 36  | C    | 3              |
| 1   | A     | 42  | U    | 3              |
| 1   | A     | 50  | A    | 2              |
| 1   | A     | 49  | G    | 2              |
| 1   | A     | 52  | A    | 2              |
| 1   | A     | 58  | G    | 2              |
| 1   | A     | 30  | C    | 1              |
| 1   | A     | 31  | A    | 1              |

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths |           |            |
|-----|------|-------|-----|------|--------------|-----------|------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2       |
| 1   | GTP  | A     | 1   | 1    | 33,34,34     | 0.65±0.01 | 0±0 (0±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles |           |            |
|-----|------|-------|-----|------|-------------|-----------|------------|
|     |      |       |     |      | Counts      | RMSZ      | #Z>2       |
| 1   | GTP  | A     | 1   | 1    | 50,54,54    | 0.70±0.05 | 2±1 (3±1%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings     |
|-----|------|-------|-----|------|---------|--------------|-----------|
| 1   | GTP  | A     | 1   | 1    | -       | 0±0,22,38,38 | 0±0,3,3,3 |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
|     |       |     |      |            |      |             |          | Worst  | Total |
| 1   | A     | 1   | GTP  | O3G-PG-O1G | 2.58 | 120.88      | 110.83   | 4      | 8     |
| 1   | A     | 1   | GTP  | O3G-PG-O3B | 2.55 | 113.19      | 104.64   | 9      | 3     |
| 1   | A     | 1   | GTP  | O3A-PB-O1B | 2.48 | 103.25      | 110.70   | 1      | 3     |
| 1   | A     | 1   | GTP  | O2A-PA-O3A | 2.06 | 112.85      | 107.27   | 9      | 1     |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 69% for the well-defined parts and 69% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

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

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 789 |
| Number of shifts mapped to atoms        | 789 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

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

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

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 69%, i.e. 756 atoms were assigned a chemical shift out of a possible 1096. 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   | 548/638 (86%)  | 304/348 (87%)  | 244/290 (84%)   | 0/0 (—%)        |
| Base    | 208/458 (45%)  | 109/284 (38%)  | 87/102 (85%)    | 12/72 (17%)     |
| Overall | 756/1096 (69%) | 413/632 (65%)  | 331/392 (84%)   | 12/72 (17%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 756 atoms were assigned a chemical shift out of a possible 1096. 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   | 548/638 (86%)  | 304/348 (87%)        | 244/290 (84%)         | 0/0 (—%)              |
| Base    | 208/458 (45%)  | 109/284 (38%)        | 87/102 (85%)          | 12/72 (17%)           |
| Overall | 756/1096 (69%) | 413/632 (65%)        | 331/392 (84%)         | 12/72 (17%)           |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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

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



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 1339  |
| Intra-residue ( $ i-j =0$ )                              | 599   |
| Sequential ( $ i-j =1$ )                                 | 701   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 18    |
| Long range ( $ i-j \geq 5$ )                             | 21    |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 22.7  |
| Number of long range restraints per residue <sup>1</sup> | 0.4   |

<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)  | 90.8                                   | 0.2     |
| 0.2-0.5 (Medium) | 94.4                                   | 0.5     |
| >0.5 (Large)     | 23.9                                   | 2.7     |

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

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

## 9 Distance violation analysis ⓘ

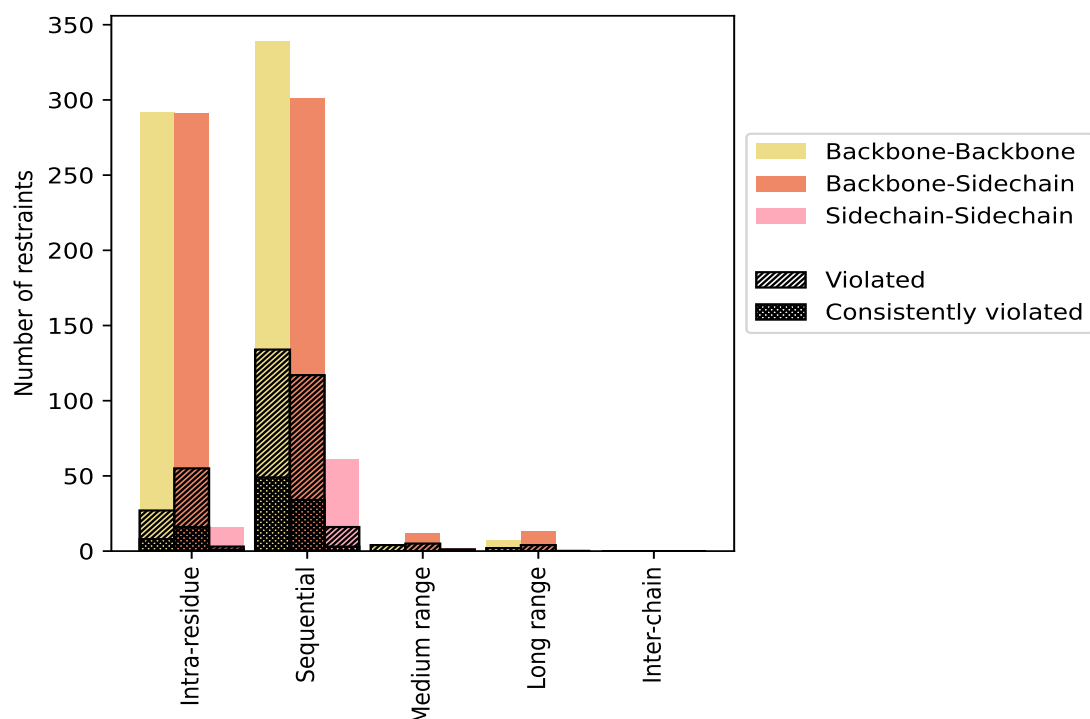
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                      |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>       | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">599</a>  | <a href="#">44.7</a>  | <a href="#">85</a>    | <a href="#">14.2</a> | <a href="#">6.3</a>  | <a href="#">25</a>                 | <a href="#">4.2</a>  | <a href="#">1.9</a> |
| Backbone-Backbone                                          | 292                  | 21.8                  | 27                    | 9.2                  | 2.0                  | 8                                  | 2.7                  | 0.6                 |
| Backbone-Sidechain                                         | 291                  | 21.7                  | 55                    | 18.9                 | 4.1                  | 16                                 | 5.5                  | 1.2                 |
| Sidechain-Sidechain                                        | 16                   | 1.2                   | 3                     | 18.8                 | 0.2                  | 1                                  | 6.2                  | 0.1                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">701</a>  | <a href="#">52.4</a>  | <a href="#">267</a>   | <a href="#">38.1</a> | <a href="#">19.9</a> | <a href="#">86</a>                 | <a href="#">12.3</a> | <a href="#">6.4</a> |
| Backbone-Backbone                                          | 339                  | 25.3                  | 134                   | 39.5                 | 10.0                 | 49                                 | 14.5                 | 3.7                 |
| Backbone-Sidechain                                         | 301                  | 22.5                  | 117                   | 38.9                 | 8.7                  | 34                                 | 11.3                 | 2.5                 |
| Sidechain-Sidechain                                        | 61                   | 4.6                   | 16                    | 26.2                 | 1.2                  | 3                                  | 4.9                  | 0.2                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">18</a>   | <a href="#">1.3</a>   | <a href="#">10</a>    | <a href="#">55.6</a> | <a href="#">0.7</a>  | <a href="#">1</a>                  | <a href="#">5.6</a>  | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 4                    | 0.3                   | 4                     | 100.0                | 0.3                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 12                   | 0.9                   | 5                     | 41.7                 | 0.4                  | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 2                    | 0.1                   | 1                     | 50.0                 | 0.1                  | 1                                  | 50.0                 | 0.1                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">21</a>   | <a href="#">1.6</a>   | <a href="#">6</a>     | <a href="#">28.6</a> | <a href="#">0.4</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 7                    | 0.5                   | 2                     | 28.6                 | 0.1                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 13                   | 1.0                   | 4                     | 30.8                 | 0.3                  | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 1                    | 0.1                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">1339</a> | <a href="#">100.0</a> | <a href="#">368</a>   | <a href="#">27.5</a> | <a href="#">27.5</a> | <a href="#">112</a>                | <a href="#">8.4</a>  | <a href="#">8.4</a> |
| Backbone-Backbone                                          | 642                  | 47.9                  | 167                   | 26.0                 | 12.5                 | 57                                 | 8.9                  | 4.3                 |
| Backbone-Sidechain                                         | 617                  | 46.1                  | 181                   | 29.3                 | 13.5                 | 50                                 | 8.1                  | 3.7                 |
| Sidechain-Sidechain                                        | 80                   | 6.0                   | 20                    | 25.0                 | 1.5                  | 5                                  | 6.2                  | 0.4                 |

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

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



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

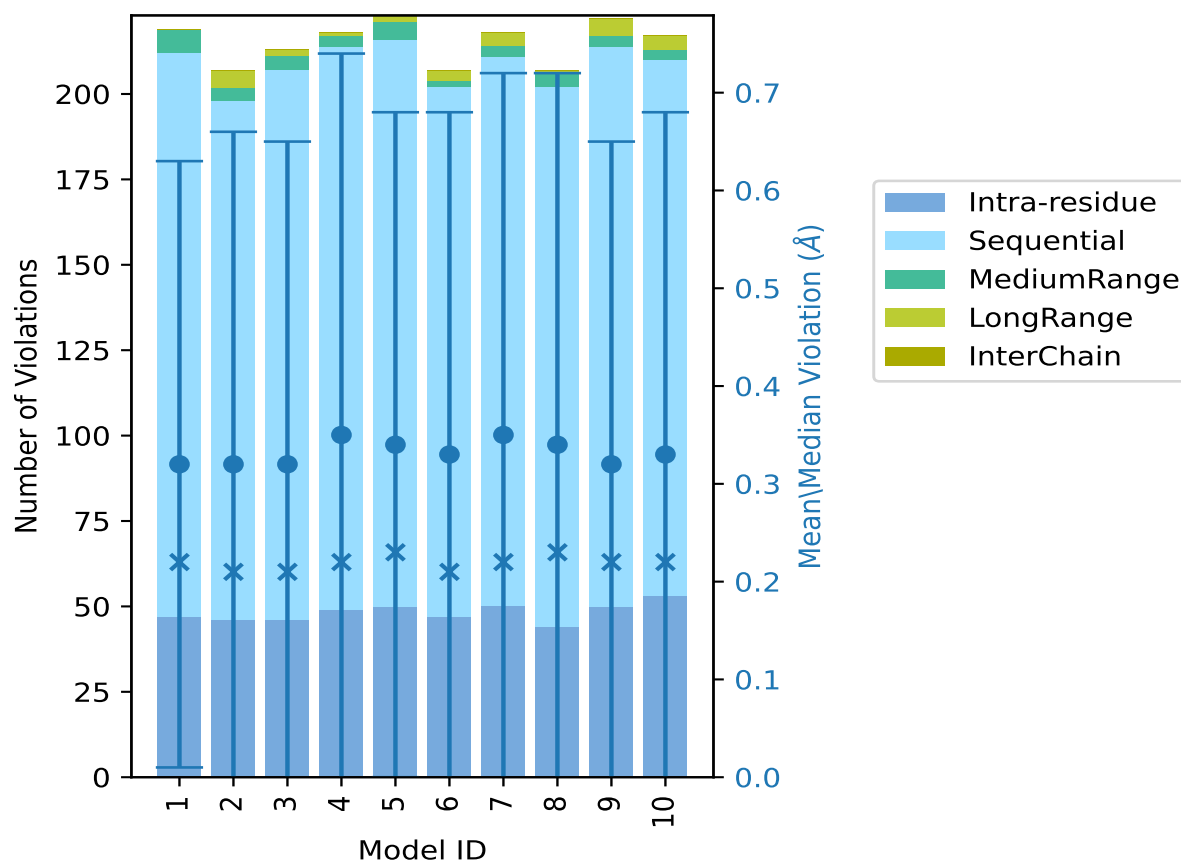
## 9.2 Distance violation statistics for each model [i](#)

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        | 47                   | 165             | 7               | 0               | 0               | 219   | 0.32     | 2.13    | 0.31                | 0.22       |
| 2        | 46                   | 152             | 4               | 5               | 0               | 207   | 0.32     | 2.12    | 0.34                | 0.21       |
| 3        | 46                   | 161             | 4               | 2               | 0               | 213   | 0.32     | 1.99    | 0.33                | 0.21       |
| 4        | 49                   | 165             | 3               | 1               | 0               | 218   | 0.35     | 2.16    | 0.39                | 0.22       |
| 5        | 50                   | 166             | 5               | 2               | 0               | 223   | 0.34     | 2.1     | 0.34                | 0.23       |
| 6        | 47                   | 155             | 2               | 3               | 0               | 207   | 0.33     | 2.16    | 0.35                | 0.21       |
| 7        | 50                   | 161             | 3               | 4               | 0               | 218   | 0.35     | 2.12    | 0.37                | 0.22       |
| 8        | 44                   | 158             | 4               | 1               | 0               | 207   | 0.34     | 2.7     | 0.38                | 0.23       |
| 9        | 50                   | 164             | 3               | 5               | 0               | 222   | 0.32     | 2.09    | 0.33                | 0.22       |
| 10       | 53                   | 157             | 3               | 4               | 0               | 217   | 0.33     | 2.11    | 0.35                | 0.22       |

<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, 971(IR:514, SQ:434, MR:8, LR:15, 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>       | %    |
| 17                            | 40              | 2               | 0               | 0               | 59    | 1                        | 10.0 |
| 9                             | 33              | 2               | 1               | 0               | 45    | 2                        | 20.0 |
| 6                             | 14              | 2               | 0               | 0               | 22    | 3                        | 30.0 |

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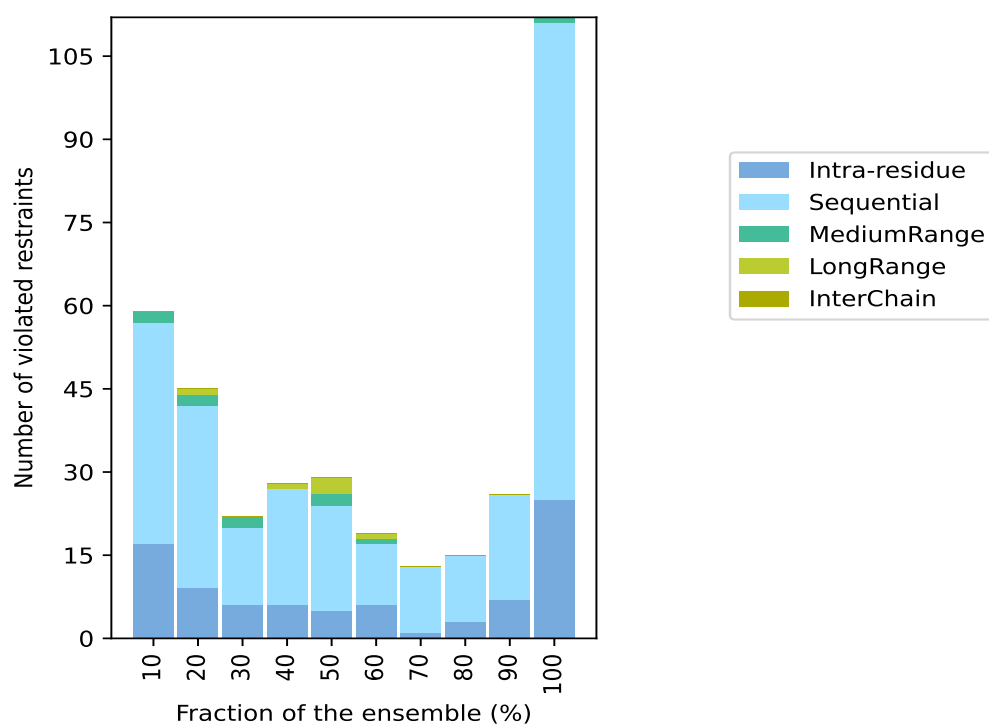
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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>       | %     |
| 6                             | 21              | 0               | 1               | 0               | 28    | 4                        | 40.0  |
| 5                             | 19              | 2               | 3               | 0               | 29    | 5                        | 50.0  |
| 6                             | 11              | 1               | 1               | 0               | 19    | 6                        | 60.0  |
| 1                             | 12              | 0               | 0               | 0               | 13    | 7                        | 70.0  |
| 3                             | 12              | 0               | 0               | 0               | 15    | 8                        | 80.0  |
| 7                             | 19              | 0               | 0               | 0               | 26    | 9                        | 90.0  |
| 25                            | 86              | 1               | 0               | 0               | 112   | 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 ⓘ

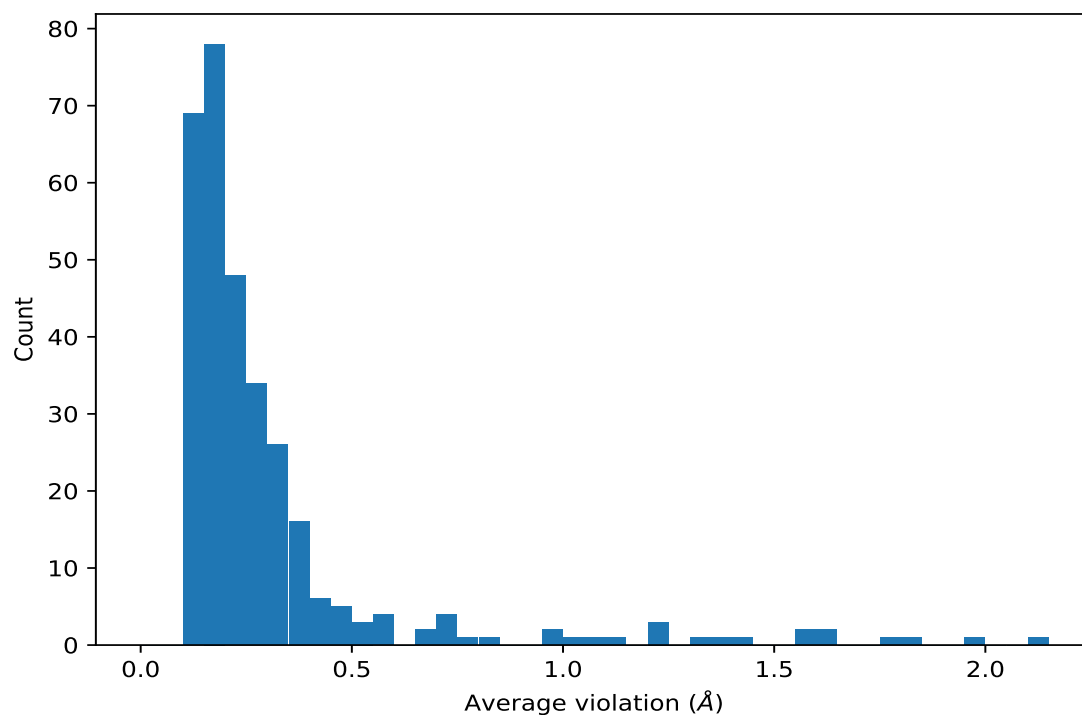


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 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) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 10                  | 2.1      | 0.04                | 2.1        |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 10                  | 1.83     | 0.2                 | 1.77       |
| (1,660)  | 1:50:A:A:H5'  | 1:51:A:U:H4'  | 10                  | 1.6      | 0.57                | 1.52       |
| (1,1285) | 1:15:A:C:H2'  | 1:16:A:G:H5'  | 10                  | 1.6      | 0.01                | 1.6        |
| (1,438)  | 1:30:A:C:H4'  | 1:31:A:A:H5'  | 10                  | 1.58     | 0.39                | 1.64       |
| (1,1038) | 1:20:A:A:H1'  | 1:21:A:C:H5'  | 10                  | 1.34     | 0.06                | 1.36       |
| (1,112)  | 1:2:A:G:H1'   | 1:3:A:A:H3'   | 10                  | 1.23     | 0.22                | 1.09       |
| (1,112)  | 1:2:A:G:H1'   | 1:3:A:A:H2'   | 10                  | 1.23     | 0.22                | 1.09       |
| (1,440)  | 1:5:A:G:H5''  | 1:4:A:A:H1'   | 10                  | 1.13     | 0.2                 | 1.08       |
| (1,650)  | 1:45:A:C:H3'  | 1:46:A:U:H5'' | 10                  | 1.07     | 0.08                | 1.1        |
| (1,1302) | 1:56:A:U:H1'  | 1:57:A:G:H5'' | 10                  | 1.04     | 0.23                | 1.14       |
| (1,406)  | 1:5:A:G:H1'   | 1:6:A:A:H5''  | 10                  | 0.98     | 0.06                | 0.99       |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 10                  | 0.78     | 0.07                | 0.74       |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 10                  | 0.72     | 0.16                | 0.78       |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 10                  | 0.7      | 0.1                 | 0.74       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 10                  | 0.7      | 0.15                | 0.7        |
| (1,176)  | 1:25:A:A:H5'  | 1:25:A:A:H8   | 10                  | 0.67     | 0.36                | 0.76       |
| (1,515)  | 1:22:A:U:H5'  | 1:22:A:U:H3'  | 10                  | 0.59     | 0.13                | 0.64       |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 10                  | 0.57     | 0.05                | 0.6        |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 10                  | 0.56     | 0.07                | 0.59       |
| (1,369)  | 1:9:A:G:H2'   | 1:8:A:A:H3'   | 10                  | 0.52     | 0.29                | 0.38       |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4'  | 10                  | 0.52     | 0.16                | 0.46       |
| (1,236)  | 1:8:A:A:H5''  | 1:8:A:A:H1'   | 10                  | 0.51     | 0.34                | 0.38       |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1'  | 10                  | 0.49     | 0.16                | 0.42       |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 10                  | 0.45     | 0.02                | 0.45       |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 10                  | 0.43     | 0.01                | 0.43       |
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 10                  | 0.43     | 0.07                | 0.47       |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1'  | 10                  | 0.41     | 0.02                | 0.4        |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8   | 10                  | 0.4      | 0.01                | 0.4        |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1'  | 10                  | 0.4      | 0.03                | 0.39       |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1'  | 10                  | 0.39     | 0.02                | 0.38       |
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4'  | 10                  | 0.39     | 0.01                | 0.38       |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5'  | 10                  | 0.38     | 0.01                | 0.38       |
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8   | 10                  | 0.38     | 0.03                | 0.38       |
| (1,1298) | 1:8:A:A:H1'   | 1:9:A:G:H5''  | 10                  | 0.37     | 0.04                | 0.37       |
| (1,942)  | 1:20:A:A:H1'  | 1:19:A:C:H3'  | 10                  | 0.37     | 0.03                | 0.38       |
| (1,1203) | 1:59:A:U:H3'  | 1:58:A:G:H1'  | 10                  | 0.36     | 0.4                 | 0.24       |
| (1,394)  | 1:9:A:G:H2'   | 1:8:A:A:H2    | 10                  | 0.36     | 0.29                | 0.27       |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2'  | 10                  | 0.36     | 0.04                | 0.36       |
| (1,198)  | 1:26:A:A:H8   | 1:26:A:A:H2'  | 10                  | 0.35     | 0.02                | 0.36       |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4'  | 10                  | 0.35     | 0.06                | 0.36       |
| (1,836)  | 1:22:A:U:H1'  | 1:23:A:C:H6   | 10                  | 0.34     | 0.01                | 0.34       |
| (1,1196) | 1:12:A:C:H6   | 1:11:A:G:H1'  | 10                  | 0.34     | 0.03                | 0.33       |
| (1,820)  | 1:50:A:A:H8   | 1:47:A:C:H6   | 10                  | 0.34     | 0.09                | 0.34       |
| (1,1290) | 1:31:A:A:H1'  | 1:32:A:G:H5'' | 10                  | 0.33     | 0.04                | 0.32       |
| (1,852)  | 1:20:A:A:H2'  | 1:21:A:C:H6   | 10                  | 0.32     | 0.03                | 0.32       |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4'  | 10                  | 0.32     | 0.03                | 0.32       |
| (1,180)  | 1:25:A:A:H1'  | 1:26:A:A:H8   | 10                  | 0.32     | 0.07                | 0.34       |
| (1,170)  | 1:3:A:A:H1'   | 1:4:A:A:H8    | 10                  | 0.32     | 0.06                | 0.3        |
| (1,332)  | 1:2:A:G:H3'   | 1:3:A:A:H8    | 10                  | 0.31     | 0.03                | 0.31       |
| (1,1206) | 1:8:A:A:H1'   | 1:9:A:G:H1'   | 10                  | 0.31     | 0.05                | 0.31       |
| (1,1000) | 1:20:A:A:H8   | 1:19:A:C:H1'  | 10                  | 0.3      | 0.02                | 0.29       |
| (1,956)  | 1:14:A:U:H1'  | 1:15:A:C:H5'' | 10                  | 0.3      | 0.03                | 0.32       |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 10                  | 0.3      | 0.01                | 0.3        |
| (1,1108) | 1:2:A:G:H8    | 1:2:A:G:H2'   | 10                  | 0.29     | 0.05                | 0.28       |
| (1,1297) | 1:8:A:A:H4'   | 1:9:A:G:H5''  | 10                  | 0.29     | 0.04                | 0.28       |
| (1,352)  | 1:27:A:C:H5   | 1:26:A:A:H2'  | 10                  | 0.29     | 0.03                | 0.28       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,682)  | 1:55:A:C:H2'  | 1:55:A:C:H6   | 10                  | 0.28     | 0.05                | 0.27       |
| (1,1308) | 1:18:A:C:H5   | 1:17:A:G:H5'  | 10                  | 0.28     | 0.04                | 0.29       |
| (1,989)  | 1:20:A:A:H2'  | 1:21:A:C:H5   | 10                  | 0.28     | 0.05                | 0.28       |
| (1,434)  | 1:51:A:U:H5   | 1:52:A:A:H8   | 10                  | 0.27     | 0.04                | 0.28       |
| (1,104)  | 1:21:A:C:H5   | 1:20:A:A:H4'  | 10                  | 0.27     | 0.1                 | 0.26       |
| (1,391)  | 1:27:A:C:H5   | 1:26:A:A:H2   | 10                  | 0.27     | 0.03                | 0.26       |
| (1,373)  | 1:23:A:C:H3'  | 1:24:A:A:H1'  | 10                  | 0.27     | 0.02                | 0.28       |
| (1,882)  | 1:11:A:G:H1'  | 1:12:A:C:H4'  | 10                  | 0.26     | 0.02                | 0.26       |
| (1,419)  | 1:19:A:C:H2'  | 1:20:A:A:H3'  | 10                  | 0.26     | 0.08                | 0.26       |
| (1,213)  | 1:26:A:A:H8   | 1:26:A:A:H3'  | 10                  | 0.26     | 0.07                | 0.26       |
| (1,1052) | 1:46:A:U:H2'  | 1:47:A:C:H3'  | 10                  | 0.26     | 0.06                | 0.23       |
| (1,825)  | 1:16:A:G:H5'  | 1:15:A:C:H1'  | 10                  | 0.25     | 0.02                | 0.25       |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5   | 10                  | 0.25     | 0.07                | 0.25       |
| (1,209)  | 1:24:A:A:H8   | 1:24:A:A:H2'  | 10                  | 0.25     | 0.04                | 0.24       |
| (1,1013) | 1:24:A:A:H8   | 1:23:A:C:H1'  | 10                  | 0.25     | 0.06                | 0.24       |
| (1,1161) | 1:15:A:C:H3'  | 1:16:A:G:H8   | 10                  | 0.25     | 0.01                | 0.24       |
| (1,868)  | 1:24:A:A:H8   | 1:23:A:C:H4'  | 10                  | 0.24     | 0.04                | 0.26       |
| (1,913)  | 1:40:A:A:H8   | 1:39:A:C:H2'  | 10                  | 0.24     | 0.04                | 0.26       |
| (1,425)  | 1:49:A:G:H4'  | 1:50:A:A:H4'  | 10                  | 0.24     | 0.09                | 0.22       |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 10                  | 0.24     | 0.01                | 0.24       |
| (1,1098) | 1:16:A:G:H8   | 1:16:A:G:H2'  | 10                  | 0.24     | 0.02                | 0.24       |
| (1,901)  | 1:22:A:U:H3'  | 1:21:A:C:H2'  | 10                  | 0.23     | 0.05                | 0.22       |
| (1,770)  | 1:21:A:C:H6   | 1:21:A:C:H5'' | 10                  | 0.22     | 0.02                | 0.22       |
| (1,962)  | 1:44:A:A:H8   | 1:45:A:C:H5'  | 10                  | 0.22     | 0.03                | 0.22       |
| (1,848)  | 1:20:A:A:H1'  | 1:21:A:C:H6   | 10                  | 0.22     | 0.01                | 0.22       |
| (1,908)  | 1:20:A:A:H8   | 1:19:A:C:H2'  | 10                  | 0.22     | 0.04                | 0.21       |
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 10                  | 0.22     | 0.04                | 0.22       |
| (1,678)  | 1:54:A:C:H4'  | 1:54:A:C:H6   | 10                  | 0.21     | 0.04                | 0.2        |
| (1,161)  | 1:24:A:A:H4'  | 1:23:A:C:H1'  | 10                  | 0.21     | 0.1                 | 0.19       |
| (1,346)  | 1:23:A:C:H1'  | 1:24:A:A:H4'  | 10                  | 0.21     | 0.1                 | 0.19       |
| (1,883)  | 1:13:A:U:H5   | 1:12:A:C:H4'  | 10                  | 0.21     | 0.02                | 0.22       |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 10                  | 0.21     | 0.03                | 0.22       |
| (1,999)  | 1:14:A:U:H1'  | 1:15:A:C:H5   | 10                  | 0.2      | 0.02                | 0.2        |
| (1,257)  | 1:7:A:A:H3'   | 1:6:A:A:H2    | 10                  | 0.2      | 0.03                | 0.21       |
| (1,473)  | 1:14:A:U:H6   | 1:14:A:U:H3'  | 10                  | 0.2      | 0.02                | 0.2        |
| (1,1288) | 1:15:A:C:H5'  | 1:16:A:G:H5'' | 10                  | 0.2      | 0.02                | 0.2        |
| (1,1055) | 1:56:A:U:H4'  | 1:55:A:C:H3'  | 10                  | 0.2      | 0.03                | 0.2        |
| (1,1269) | 1:18:A:C:H6   | 1:17:A:G:H3'  | 10                  | 0.2      | 0.02                | 0.2        |
| (1,321)  | 1:26:A:A:H3'  | 1:26:A:A:H2   | 10                  | 0.2      | 0.05                | 0.18       |
| (1,664)  | 1:58:A:G:H4'  | 1:59:A:U:H4'  | 10                  | 0.19     | 0.07                | 0.16       |
| (1,1046) | 1:22:A:U:H6   | 1:21:A:C:H5   | 10                  | 0.19     | 0.02                | 0.19       |
| (1,91)   | 1:21:A:C:H2'  | 1:21:A:C:H5   | 10                  | 0.19     | 0.01                | 0.19       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,1146) | 1:5:A:G:H8    | 1:5:A:G:H2'   | 10                  | 0.18     | 0.02                | 0.18       |
| (1,503)  | 1:14:A:U:H5   | 1:14:A:U:H2'  | 10                  | 0.18     | 0.01                | 0.18       |
| (1,537)  | 1:14:A:U:H4'  | 1:14:A:U:H5'  | 10                  | 0.18     | 0.01                | 0.18       |
| (1,824)  | 1:16:A:G:H1'  | 1:15:A:C:H1'  | 10                  | 0.18     | 0.01                | 0.18       |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 10                  | 0.18     | 0.02                | 0.18       |
| (1,893)  | 1:22:A:U:H6   | 1:21:A:C:H2'  | 10                  | 0.17     | 0.02                | 0.16       |
| (1,201)  | 1:20:A:A:H8   | 1:20:A:A:H2'  | 10                  | 0.16     | 0.03                | 0.17       |
| (1,478)  | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 10                  | 0.16     | 0.02                | 0.16       |
| (1,706)  | 1:15:A:C:H5'' | 1:15:A:C:H3'  | 10                  | 0.16     | 0.01                | 0.16       |
| (1,574)  | 1:56:A:U:H5'' | 1:56:A:U:H4'  | 10                  | 0.15     | 0.02                | 0.15       |
| (1,1163) | 1:15:A:C:H5'  | 1:16:A:G:H8   | 10                  | 0.15     | 0.01                | 0.15       |
| (1,763)  | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 10                  | 0.14     | 0.0                 | 0.14       |
| (1,1306) | 1:40:A:A:H2'  | 1:41:A:G:H5'' | 10                  | 0.14     | 0.02                | 0.14       |
| (1,793)  | 1:27:A:C:H6   | 1:27:A:C:H5   | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,13)   | 1:18:A:C:H4'  | 1:19:A:C:H5   | 9                   | 0.48     | 0.1                 | 0.48       |
| (1,168)  | 1:50:A:A:H3'  | 1:50:A:A:H8   | 9                   | 0.46     | 0.47                | 0.21       |
| (1,381)  | 1:30:A:C:H4'  | 1:29:A:A:H1'  | 9                   | 0.33     | 0.2                 | 0.27       |
| (1,864)  | 1:46:A:U:H1'  | 1:47:A:C:H4'  | 9                   | 0.32     | 0.08                | 0.3        |
| (1,862)  | 1:53:A:U:H4'  | 1:54:A:C:H4'  | 9                   | 0.31     | 0.1                 | 0.32       |
| (1,627)  | 1:47:A:C:H6   | 1:46:A:U:H2'  | 9                   | 0.27     | 0.04                | 0.29       |
| (1,632)  | 1:29:A:A:H4'  | 1:28:A:U:H3'  | 9                   | 0.23     | 0.11                | 0.19       |
| (1,878)  | 1:26:A:A:H2'  | 1:27:A:C:H4'  | 9                   | 0.22     | 0.07                | 0.21       |
| (1,1050) | 1:31:A:A:H5'  | 1:30:A:C:H6   | 9                   | 0.2      | 0.03                | 0.2        |
| (1,1227) | 1:33:A:A:H8   | 1:32:A:G:H4'  | 9                   | 0.2      | 0.04                | 0.19       |
| (1,366)  | 1:9:A:G:H8    | 1:8:A:A:H3'   | 9                   | 0.19     | 0.02                | 0.2        |
| (1,1208) | 1:3:A:A:H8    | 1:2:A:G:H1'   | 9                   | 0.19     | 0.05                | 0.18       |
| (1,203)  | 1:40:A:A:H8   | 1:40:A:A:H2'  | 9                   | 0.19     | 0.03                | 0.2        |
| (1,668)  | 1:54:A:C:H6   | 1:53:A:U:H4'  | 9                   | 0.19     | 0.03                | 0.18       |
| (1,823)  | 1:46:A:U:H4'  | 1:47:A:C:H6   | 9                   | 0.18     | 0.03                | 0.18       |
| (1,202)  | 1:4:A:A:H8    | 1:4:A:A:H2'   | 9                   | 0.18     | 0.06                | 0.15       |
| (1,815)  | 1:39:A:C:H5   | 1:39:A:C:H5'' | 9                   | 0.18     | 0.04                | 0.19       |
| (1,1330) | 1:38:A:C:H5   | 1:37:A:G:H3'  | 9                   | 0.17     | 0.05                | 0.15       |
| (1,383)  | 1:5:A:G:H1'   | 1:4:A:A:H1'   | 9                   | 0.17     | 0.03                | 0.16       |
| (1,200)  | 1:8:A:A:H8    | 1:8:A:A:H2'   | 9                   | 0.17     | 0.02                | 0.18       |
| (1,275)  | 1:40:A:A:H5'  | 1:40:A:A:H4'  | 9                   | 0.16     | 0.02                | 0.17       |
| (1,581)  | 1:45:A:C:H4'  | 1:46:A:U:H6   | 9                   | 0.15     | 0.04                | 0.15       |
| (1,1238) | 1:12:A:C:H5   | 1:11:A:G:H4'  | 9                   | 0.14     | 0.03                | 0.14       |
| (1,874)  | 1:22:A:U:H5   | 1:21:A:C:H4'  | 9                   | 0.14     | 0.03                | 0.15       |
| (1,1301) | 1:8:A:A:H2'   | 1:9:A:G:H5'   | 9                   | 0.14     | 0.02                | 0.15       |
| (1,524)  | 1:59:A:U:H2'  | 1:59:A:U:H3'  | 9                   | 0.12     | 0.01                | 0.12       |
| (1,645)  | 1:50:A:A:H4'  | 1:51:A:U:H5'  | 8                   | 1.77     | 0.17                | 1.83       |
| (1,604)  | 1:29:A:A:H5'  | 1:28:A:U:H1'  | 8                   | 1.36     | 0.09                | 1.35       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,445)  | 1:53:A:U:H5'' | 1:53:A:U:H6   | 8                   | 0.36     | 0.1                 | 0.38       |
| (1,395)  | 1:28:A:U:H4'  | 1:29:A:A:H8   | 8                   | 0.34     | 0.06                | 0.34       |
| (1,877)  | 1:22:A:U:H5'' | 1:21:A:C:H4'  | 8                   | 0.31     | 0.03                | 0.31       |
| (1,875)  | 1:28:A:U:H5   | 1:27:A:C:H4'  | 8                   | 0.27     | 0.09                | 0.22       |
| (1,396)  | 1:51:A:U:H3'  | 1:50:A:A:H1'  | 8                   | 0.24     | 0.06                | 0.22       |
| (1,1224) | 1:31:A:A:H1'  | 1:32:A:G:H4'  | 8                   | 0.22     | 0.11                | 0.16       |
| (1,895)  | 1:31:A:A:H8   | 1:30:A:C:H2'  | 8                   | 0.19     | 0.06                | 0.19       |
| (1,181)  | 1:8:A:A:H3'   | 1:8:A:A:H8    | 8                   | 0.18     | 0.03                | 0.2        |
| (1,1317) | 1:59:A:U:H5   | 1:58:A:G:H3'  | 8                   | 0.18     | 0.05                | 0.18       |
| (1,1042) | 1:20:A:A:H3'  | 1:21:A:C:H5'' | 8                   | 0.18     | 0.05                | 0.17       |
| (1,871)  | 1:31:A:A:H8   | 1:30:A:C:H4'  | 8                   | 0.17     | 0.03                | 0.18       |
| (1,608)  | 1:45:A:C:H3'  | 1:46:A:U:H1'  | 8                   | 0.17     | 0.03                | 0.17       |
| (1,208)  | 1:6:A:A:H8    | 1:6:A:A:H2'   | 8                   | 0.13     | 0.02                | 0.12       |
| (1,587)  | 1:29:A:A:H4'  | 1:28:A:U:H6   | 7                   | 0.33     | 0.17                | 0.31       |
| (1,1168) | 1:31:A:A:H1'  | 1:32:A:G:H8   | 7                   | 0.28     | 0.07                | 0.25       |
| (1,900)  | 1:28:A:U:H3'  | 1:27:A:C:H2'  | 7                   | 0.2      | 0.09                | 0.16       |
| (1,1027) | 1:37:A:G:H8   | 1:36:A:C:H1'  | 7                   | 0.19     | 0.05                | 0.16       |
| (1,860)  | 1:37:A:G:H4'  | 1:36:A:C:H4'  | 7                   | 0.18     | 0.04                | 0.21       |
| (1,435)  | 1:30:A:C:H2'  | 1:31:A:A:H5'' | 7                   | 0.18     | 0.05                | 0.19       |
| (1,954)  | 1:37:A:G:H3'  | 1:38:A:C:H3'  | 7                   | 0.17     | 0.04                | 0.16       |
| (1,1325) | 1:38:A:C:H5   | 1:37:A:G:H4'  | 7                   | 0.17     | 0.02                | 0.17       |
| (1,885)  | 1:37:A:G:H2'  | 1:38:A:C:H4'  | 7                   | 0.15     | 0.05                | 0.13       |
| (1,1309) | 1:33:A:A:H8   | 1:32:A:G:H2'  | 7                   | 0.14     | 0.02                | 0.13       |
| (1,1254) | 1:59:A:U:H6   | 1:58:A:G:H2'  | 7                   | 0.14     | 0.03                | 0.13       |
| (1,965)  | 1:20:A:A:H2'  | 1:21:A:C:H5'  | 7                   | 0.13     | 0.02                | 0.14       |
| (1,748)  | 1:12:A:C:H2'  | 1:12:A:C:H3'  | 7                   | 0.11     | 0.01                | 0.1        |
| (1,424)  | 1:49:A:G:H2'  | 1:50:A:A:H4'  | 6                   | 0.38     | 0.45                | 0.18       |
| (1,899)  | 1:31:A:A:H3'  | 1:30:A:C:H2'  | 6                   | 0.36     | 0.54                | 0.12       |
| (1,621)  | 1:54:A:C:H6   | 1:53:A:U:H2'  | 6                   | 0.32     | 0.11                | 0.32       |
| (1,910)  | 1:44:A:A:H1'  | 1:43:A:C:H2'  | 6                   | 0.3      | 0.05                | 0.29       |
| (1,163)  | 1:49:A:G:H2'  | 1:47:A:C:H3'  | 6                   | 0.28     | 0.15                | 0.24       |
| (1,163)  | 1:50:A:A:H3'  | 1:47:A:C:H3'  | 6                   | 0.28     | 0.15                | 0.24       |
| (1,506)  | 1:28:A:U:H6   | 1:28:A:U:H3'  | 6                   | 0.26     | 0.07                | 0.26       |
| (1,3)    | 1:41:A:G:H4'  | 1:40:A:A:H1'  | 6                   | 0.25     | 0.07                | 0.27       |
| (1,541)  | 1:53:A:U:H4'  | 1:53:A:U:H5'  | 6                   | 0.22     | 0.06                | 0.23       |
| (1,150)  | 1:46:A:U:H6   | 1:47:A:C:H5'  | 6                   | 0.18     | 0.07                | 0.16       |
| (1,150)  | 1:46:A:U:H6   | 1:47:A:C:H5'' | 6                   | 0.18     | 0.07                | 0.16       |
| (1,169)  | 1:3:A:A:H2'   | 1:3:A:A:H8    | 6                   | 0.18     | 0.05                | 0.17       |
| (1,291)  | 1:24:A:A:H8   | 1:24:A:A:H5'' | 6                   | 0.17     | 0.03                | 0.17       |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'  | 6                   | 0.17     | 0.04                | 0.16       |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'' | 6                   | 0.17     | 0.04                | 0.16       |
| (1,593)  | 1:50:A:A:H1'  | 1:51:A:U:H5   | 6                   | 0.14     | 0.02                | 0.14       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,1270) | 1:12:A:C:H3'  | 1:11:A:G:H2'  | 6                   | 0.14     | 0.01                | 0.15       |
| (1,426)  | 1:45:A:C:H1'  | 1:44:A:A:H2'  | 6                   | 0.14     | 0.01                | 0.13       |
| (1,928)  | 1:42:A:U:H3'  | 1:43:A:C:H3'  | 6                   | 0.13     | 0.04                | 0.12       |
| (1,310)  | 1:31:A:A:H4'  | 1:31:A:A:H8   | 6                   | 0.13     | 0.03                | 0.13       |
| (1,629)  | 1:57:A:G:H8   | 1:56:A:U:H2'  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,446)  | 1:59:A:U:H5   | 1:59:A:U:H6   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,402)  | 1:19:A:C:H1'  | 1:20:A:A:H5'  | 5                   | 0.97     | 0.02                | 0.97       |
| (1,679)  | 1:54:A:C:H5'' | 1:54:A:C:H6   | 5                   | 0.74     | 0.11                | 0.69       |
| (1,121)  | 1:54:A:C:H3'  | 1:53:A:U:H2'  | 5                   | 0.58     | 0.15                | 0.5        |
| (1,401)  | 1:19:A:C:H1'  | 1:20:A:A:H5'' | 5                   | 0.47     | 0.01                | 0.47       |
| (1,861)  | 1:53:A:U:H3'  | 1:54:A:C:H4'  | 5                   | 0.32     | 0.09                | 0.37       |
| (1,606)  | 1:54:A:C:H5   | 1:53:A:U:H1'  | 5                   | 0.31     | 0.05                | 0.28       |
| (1,1225) | 1:47:A:C:H2'  | 1:49:A:G:H4'  | 5                   | 0.27     | 0.07                | 0.29       |
| (1,658)  | 1:27:A:C:H4'  | 1:28:A:U:H5'' | 5                   | 0.27     | 0.05                | 0.26       |
| (1,109)  | 1:27:A:C:H3'  | 1:26:A:A:H3'  | 5                   | 0.25     | 0.06                | 0.25       |
| (1,109)  | 1:27:A:C:H4'  | 1:26:A:A:H3'  | 5                   | 0.25     | 0.06                | 0.25       |
| (1,410)  | 1:2:A:G:H3'   | 1:3:A:A:H5'   | 5                   | 0.21     | 0.08                | 0.24       |
| (1,146)  | 1:24:A:A:H3'  | 1:23:A:C:H3'  | 5                   | 0.19     | 0.04                | 0.2        |
| (1,665)  | 1:54:A:C:H6   | 1:53:A:U:H6   | 5                   | 0.19     | 0.04                | 0.2        |
| (1,1048) | 1:44:A:A:H1'  | 1:54:A:C:H5   | 5                   | 0.18     | 0.05                | 0.16       |
| (1,340)  | 1:19:A:C:H4'  | 1:20:A:A:H8   | 5                   | 0.18     | 0.02                | 0.17       |
| (1,1211) | 1:50:A:A:H8   | 1:49:A:G:H1'  | 5                   | 0.17     | 0.04                | 0.15       |
| (1,951)  | 1:37:A:G:H1'  | 1:38:A:C:H3'  | 5                   | 0.16     | 0.08                | 0.13       |
| (1,304)  | 1:29:A:A:H8   | 1:29:A:A:H5'' | 5                   | 0.16     | 0.05                | 0.12       |
| (1,329)  | 1:31:A:A:H8   | 1:31:A:A:H5'' | 5                   | 0.15     | 0.04                | 0.17       |
| (1,412)  | 1:2:A:G:H2'   | 1:3:A:A:H5''  | 5                   | 0.14     | 0.02                | 0.15       |
| (1,348)  | 1:46:A:U:H5'' | 1:52:A:A:H4'  | 5                   | 0.14     | 0.03                | 0.13       |
| (1,921)  | 1:13:A:U:H3'  | 1:12:A:C:H2'  | 5                   | 0.14     | 0.03                | 0.13       |
| (1,713)  | 1:36:A:C:H2'  | 1:36:A:C:H3'  | 5                   | 0.13     | 0.02                | 0.14       |
| (1,378)  | 1:5:A:G:H1'   | 1:6:A:A:H1'   | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1006) | 1:44:A:A:H2   | 1:55:A:C:H1'  | 5                   | 0.12     | 0.01                | 0.13       |
| (1,1328) | 1:12:A:C:H6   | 1:11:A:G:H5'' | 5                   | 0.12     | 0.01                | 0.12       |
| (1,829)  | 1:13:A:U:H1'  | 1:15:A:C:H6   | 5                   | 0.12     | 0.01                | 0.12       |
| (1,872)  | 1:26:A:A:H2   | 1:27:A:C:H4'  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,528)  | 1:56:A:U:H2'  | 1:56:A:U:H3'  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,912)  | 1:13:A:U:H6   | 1:12:A:C:H2'  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,2)    | 1:28:A:U:H5'  | 1:27:A:C:H2'  | 4                   | 1.95     | 0.14                | 1.93       |
| (1,382)  | 1:30:A:C:H5'  | 1:29:A:A:H1'  | 4                   | 1.44     | 0.21                | 1.42       |
| (1,194)  | 1:52:A:A:H5'  | 1:52:A:A:H4'  | 4                   | 0.21     | 0.03                | 0.22       |
| (1,830)  | 1:42:A:U:H2'  | 1:43:A:C:H6   | 4                   | 0.21     | 0.05                | 0.22       |
| (1,107)  | 1:34:A:G:H2'  | 1:35:A:A:H2'  | 4                   | 0.21     | 0.08                | 0.2        |
| (1,1235) | 1:59:A:U:H5   | 1:58:A:G:H4'  | 4                   | 0.21     | 0.12                | 0.15       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,1218) | 1:31:A:A:H3'  | 1:32:A:G:H8   | 4                   | 0.2      | 0.02                | 0.2        |
| (1,444)  | 1:53:A:U:H4'  | 1:53:A:U:H6   | 4                   | 0.18     | 0.02                | 0.18       |
| (1,992)  | 1:28:A:U:H6   | 1:27:A:C:H5   | 4                   | 0.18     | 0.06                | 0.16       |
| (1,938)  | 1:28:A:U:H2'  | 1:27:A:C:H3'  | 4                   | 0.18     | 0.04                | 0.18       |
| (1,1039) | 1:29:A:A:H3'  | 1:30:A:C:H5'  | 4                   | 0.18     | 0.04                | 0.17       |
| (1,851)  | 1:29:A:A:H4'  | 1:30:A:C:H6   | 4                   | 0.17     | 0.03                | 0.18       |
| (1,1106) | 1:49:A:G:H8   | 1:49:A:G:H3'  | 4                   | 0.16     | 0.02                | 0.16       |
| (1,981)  | 1:53:A:U:H6   | 1:54:A:C:H5   | 4                   | 0.16     | 0.04                | 0.16       |
| (1,497)  | 1:42:A:U:H6   | 1:42:A:U:H2'  | 4                   | 0.15     | 0.04                | 0.14       |
| (1,902)  | 1:22:A:U:H4'  | 1:21:A:C:H2'  | 4                   | 0.15     | 0.02                | 0.15       |
| (1,195)  | 1:52:A:A:H5'' | 1:52:A:A:H4'  | 4                   | 0.14     | 0.02                | 0.14       |
| (1,418)  | 1:19:A:C:H3'  | 1:20:A:A:H3'  | 4                   | 0.14     | 0.03                | 0.12       |
| (1,1197) | 1:56:A:U:H1'  | 1:57:A:G:H1'  | 4                   | 0.14     | 0.02                | 0.13       |
| (1,946)  | 1:40:A:A:H4'  | 1:39:A:C:H3'  | 4                   | 0.13     | 0.03                | 0.12       |
| (1,1316) | 1:59:A:U:H6   | 1:58:A:G:H3'  | 4                   | 0.13     | 0.02                | 0.12       |
| (1,128)  | 1:4:A:A:H3'   | 1:5:A:G:H1'   | 4                   | 0.12     | 0.02                | 0.12       |
| (1,886)  | 1:14:A:U:H4'  | 1:15:A:C:H2'  | 4                   | 0.12     | 0.03                | 0.12       |
| (1,905)  | 1:56:A:U:H6   | 1:55:A:C:H2'  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1212) | 1:29:A:A:H2   | 1:49:A:G:H1'  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,481)  | 1:51:A:U:H2'  | 1:51:A:U:H3'  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,681)  | 1:54:A:C:H2'  | 1:55:A:C:H6   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1160) | 1:15:A:C:H1'  | 1:16:A:G:H8   | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,221)  | 1:29:A:A:H8   | 1:29:A:A:H3'  | 3                   | 0.26     | 0.11                | 0.31       |
| (1,819)  | 1:43:A:C:H6   | 1:43:A:C:H1'  | 3                   | 0.24     | 0.0                 | 0.24       |
| (1,929)  | 1:31:A:A:H8   | 1:30:A:C:H3'  | 3                   | 0.23     | 0.15                | 0.15       |
| (1,634)  | 1:29:A:A:H5'' | 1:28:A:U:H3'  | 3                   | 0.22     | 0.01                | 0.22       |
| (1,431)  | 1:28:A:U:H2'  | 1:29:A:A:H5'  | 3                   | 0.22     | 0.1                 | 0.18       |
| (1,139)  | 1:42:A:U:H3'  | 1:43:A:C:H6   | 3                   | 0.22     | 0.06                | 0.2        |
| (1,551)  | 1:28:A:U:H3'  | 1:28:A:U:H5'' | 3                   | 0.17     | 0.03                | 0.19       |
| (1,1026) | 1:50:A:A:H4'  | 1:47:A:C:H1'  | 3                   | 0.17     | 0.07                | 0.12       |
| (1,1178) | 1:38:A:C:H5   | 1:37:A:G:H8   | 3                   | 0.17     | 0.01                | 0.17       |
| (1,927)  | 1:44:A:A:H8   | 1:43:A:C:H3'  | 3                   | 0.16     | 0.05                | 0.14       |
| (1,1021) | 1:44:A:A:H2   | 1:45:A:C:H1'  | 3                   | 0.15     | 0.01                | 0.15       |
| (1,997)  | 1:37:A:G:H2'  | 1:38:A:C:H5   | 3                   | 0.15     | 0.04                | 0.14       |
| (1,1318) | 1:59:A:U:H3'  | 1:58:A:G:H3'  | 3                   | 0.14     | 0.04                | 0.13       |
| (1,283)  | 1:20:A:A:H8   | 1:20:A:A:H5'' | 3                   | 0.14     | 0.02                | 0.14       |
| (1,620)  | 1:44:A:A:H8   | 1:42:A:U:H2'  | 3                   | 0.14     | 0.03                | 0.12       |
| (1,482)  | 1:51:A:U:H5'' | 1:51:A:U:H3'  | 3                   | 0.14     | 0.02                | 0.14       |
| (1,617)  | 1:47:A:C:H3'  | 1:46:A:U:H3'  | 3                   | 0.14     | 0.04                | 0.11       |
| (1,628)  | 1:29:A:A:H8   | 1:28:A:U:H2'  | 3                   | 0.14     | 0.02                | 0.14       |
| (1,939)  | 1:28:A:U:H6   | 1:27:A:C:H3'  | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,1216) | 1:33:A:A:H2   | 1:34:A:G:H1'  | 3                   | 0.14     | 0.01                | 0.14       |

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| Key      | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,940)  | 1:22:A:U:H6   | 1:21:A:C:H3'  | 3                   | 0.13     | 0.01                | 0.13       |
| (1,456)  | 1:56:A:U:H6   | 1:56:A:U:H5   | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,672)  | 1:50:A:A:H4'  | 1:51:A:U:H5   | 2                   | 1.56     | 0.06                | 1.56       |
| (1,1240) | 1:59:A:U:H3'  | 1:58:A:G:H4'  | 2                   | 1.2      | 0.71                | 1.2        |
| (1,889)  | 1:50:A:A:H8   | 1:47:A:C:H3'  | 2                   | 0.8      | 0.1                 | 0.8        |
| (1,197)  | 1:52:A:A:H8   | 1:52:A:A:H3'  | 2                   | 0.68     | 0.5                 | 0.68       |
| (1,123)  | 1:54:A:C:H3'  | 1:53:A:U:H3'  | 2                   | 0.42     | 0.11                | 0.42       |
| (1,583)  | 1:50:A:A:H2'  | 1:51:A:U:H6   | 2                   | 0.35     | 0.01                | 0.35       |
| (1,595)  | 1:27:A:C:H2'  | 1:28:A:U:H5   | 2                   | 0.35     | 0.0                 | 0.35       |
| (1,196)  | 1:52:A:A:H8   | 1:52:A:A:H2'  | 2                   | 0.32     | 0.18                | 0.32       |
| (1,870)  | 1:28:A:U:H6   | 1:27:A:C:H4'  | 2                   | 0.3      | 0.02                | 0.3        |
| (1,603)  | 1:29:A:A:H8   | 1:28:A:U:H1'  | 2                   | 0.3      | 0.13                | 0.3        |
| (1,149)  | 1:50:A:A:H8   | 1:47:A:C:H5'  | 2                   | 0.28     | 0.02                | 0.28       |
| (1,149)  | 1:50:A:A:H8   | 1:47:A:C:H5'' | 2                   | 0.28     | 0.02                | 0.28       |
| (1,1249) | 1:50:A:A:H5'' | 1:49:A:G:H3'  | 2                   | 0.25     | 0.13                | 0.25       |
| (1,635)  | 1:54:A:C:H6   | 1:53:A:U:H3'  | 2                   | 0.24     | 0.04                | 0.24       |
| (1,420)  | 1:51:A:U:H2'  | 1:50:A:A:H2   | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,859)  | 1:37:A:G:H8   | 1:36:A:C:H4'  | 2                   | 0.22     | 0.02                | 0.22       |
| (1,134)  | 1:50:A:A:H8   | 1:49:A:G:H5'  | 2                   | 0.2      | 0.03                | 0.2        |
| (1,134)  | 1:50:A:A:H8   | 1:49:A:G:H5'' | 2                   | 0.2      | 0.03                | 0.2        |
| (1,659)  | 1:50:A:A:H2'  | 1:51:A:U:H4'  | 2                   | 0.2      | 0.05                | 0.2        |
| (1,932)  | 1:28:A:U:H5   | 1:27:A:C:H3'  | 2                   | 0.19     | 0.01                | 0.19       |
| (1,850)  | 1:29:A:A:H1'  | 1:30:A:C:H6   | 2                   | 0.18     | 0.02                | 0.18       |
| (1,1268) | 1:42:A:U:H6   | 1:41:A:G:H3'  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,443)  | 1:46:A:U:H4'  | 1:46:A:U:H6   | 2                   | 0.18     | 0.03                | 0.18       |
| (1,338)  | 1:30:A:C:H6   | 1:29:A:A:H8   | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1326) | 1:36:A:C:H2'  | 1:37:A:G:H4'  | 2                   | 0.18     | 0.03                | 0.18       |
| (1,898)  | 1:31:A:A:H1'  | 1:30:A:C:H2'  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1264) | 1:38:A:C:H6   | 1:37:A:G:H2'  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,307)  | 1:48:A:A:H3'  | 1:48:A:A:H5'  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,662)  | 1:27:A:C:H2'  | 1:28:A:U:H4'  | 2                   | 0.15     | 0.01                | 0.15       |
| (1,500)  | 1:59:A:U:H6   | 1:59:A:U:H2'  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,172)  | 1:29:A:A:H2'  | 1:29:A:A:H8   | 2                   | 0.14     | 0.03                | 0.14       |
| (1,280)  | 1:52:A:A:H5'' | 1:52:A:A:H3'  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,335)  | 1:23:A:C:H5   | 1:24:A:A:H8   | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1259) | 1:59:A:U:H5   | 1:58:A:G:H2'  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,409)  | 1:2:A:G:H2'   | 1:3:A:A:H5'   | 2                   | 0.13     | 0.02                | 0.13       |
| (1,649)  | 1:45:A:C:H4'  | 1:46:A:U:H5'' | 2                   | 0.13     | 0.01                | 0.13       |
| (1,960)  | 1:35:A:A:H2'  | 1:36:A:C:H5'' | 2                   | 0.13     | 0.03                | 0.13       |
| (1,1008) | 1:42:A:U:H3'  | 1:43:A:C:H1'  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,1179) | 1:38:A:C:H6   | 1:37:A:G:H8   | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,105)  | 1:27:A:C:H5   | 1:26:A:A:H4'  | 2                   | 0.12     | 0.01                | 0.12       |

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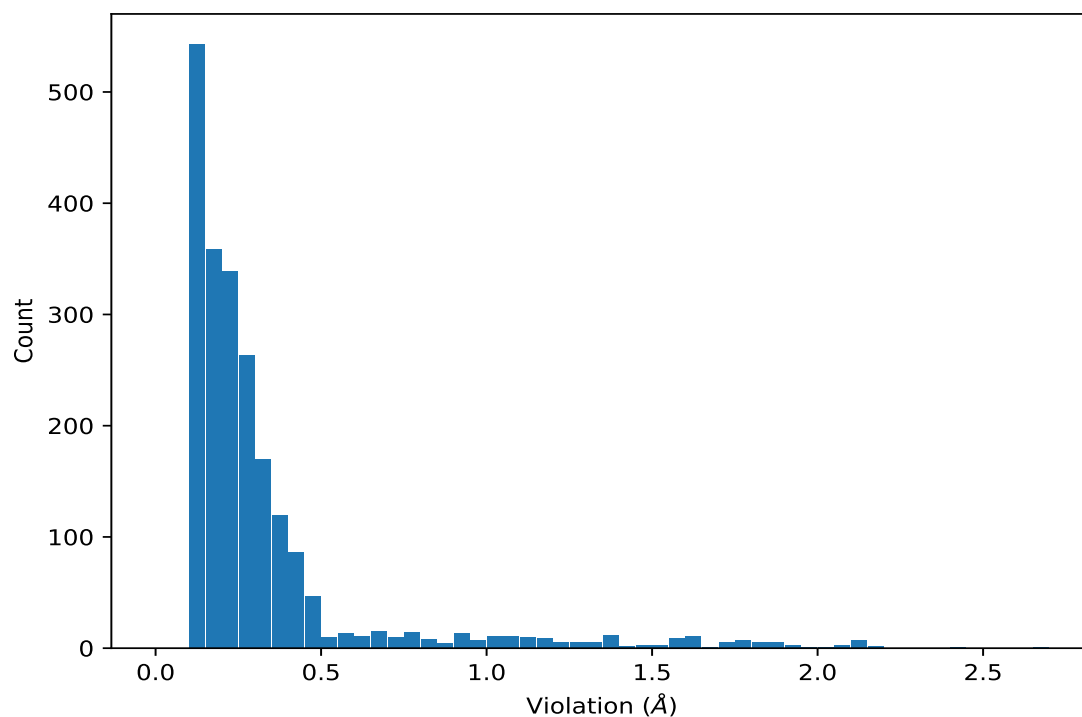
| Key      | Atom-1        | Atom-2       | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|---------------|--------------|---------------------|----------|---------------------|------------|
| (1,296)  | 1:3:A:A:H3'   | 1:3:A:A:H5'  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1314) | 1:12:A:C:H4'  | 1:11:A:G:H3' | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1220) | 1:3:A:A:H8    | 1:2:A:G:H4'  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,299)  | 1:3:A:A:H8    | 1:3:A:A:H5'' | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1053) | 1:46:A:U:H4'  | 1:45:A:C:H3' | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,414)  | 1:53:A:U:H4'  | 1:35:A:A:H2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1060) | 1:1:A:GTP:H1' | 1:2:A:G:H8   | 2                   | 0.11     | 0.0                 | 0.11       |

<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) |
|----------|---------------|---------------|----------|---------------|
| (1,660)  | 1:50:A:A:H5'  | 1:51:A:U:H4'  | 8        | 2.7           |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 8        | 2.44          |
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 6        | 2.16          |
| (1,2)    | 1:28:A:U:H5'  | 1:27:A:C:H2'  | 4        | 2.16          |
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 1        | 2.13          |
| (1,660)  | 1:50:A:A:H5'  | 1:51:A:U:H4'  | 6        | 2.13          |
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 2        | 2.12          |
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 7        | 2.12          |
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 10       | 2.11          |
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 5        | 2.1           |
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 8        | 2.1           |
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 9        | 2.09          |
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 4        | 2.08          |
| (1,660)  | 1:50:A:A:H5'  | 1:51:A:U:H4'  | 4        | 2.06          |
| (1,2)    | 1:28:A:U:H5'  | 1:27:A:C:H2'  | 10       | 2.0           |
| (1,1004) | 1:56:A:U:H5'' | 1:55:A:C:H1'  | 3        | 1.99          |
| (1,660)  | 1:50:A:A:H5'  | 1:51:A:U:H4'  | 3        | 1.94          |
| (1,645)  | 1:50:A:A:H4'  | 1:51:A:U:H5'  | 7        | 1.92          |
| (1,1240) | 1:59:A:U:H3'  | 1:58:A:G:H4'  | 4        | 1.91          |
| (1,645)  | 1:50:A:A:H4'  | 1:51:A:U:H5'  | 2        | 1.89          |
| (1,645)  | 1:50:A:A:H4'  | 1:51:A:U:H5'  | 10       | 1.87          |
| (1,645)  | 1:50:A:A:H4'  | 1:51:A:U:H5'  | 6        | 1.86          |
| (1,438)  | 1:30:A:C:H4'  | 1:31:A:A:H5'  | 7        | 1.86          |
| (1,2)    | 1:28:A:U:H5'  | 1:27:A:C:H2'  | 7        | 1.86          |
| (1,438)  | 1:30:A:C:H4'  | 1:31:A:A:H5'  | 4        | 1.84          |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 4        | 1.83          |
| (1,438)  | 1:30:A:C:H4'  | 1:31:A:A:H5'  | 2        | 1.82          |
| (1,438)  | 1:30:A:C:H4'  | 1:31:A:A:H5'  | 9        | 1.81          |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 10       | 1.8           |
| (1,645)  | 1:50:A:A:H4'  | 1:51:A:U:H5'  | 4        | 1.79          |
| (1,2)    | 1:28:A:U:H5'  | 1:27:A:C:H2'  | 5        | 1.79          |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 3        | 1.78          |
| (1,645)  | 1:50:A:A:H4'  | 1:51:A:U:H5'  | 8        | 1.78          |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 6        | 1.77          |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 9        | 1.77          |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 2        | 1.76          |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 1        | 1.74          |
| (1,382)  | 1:30:A:C:H5'  | 1:29:A:A:H1'  | 7        | 1.74          |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 7        | 1.73          |
| (1,645)  | 1:50:A:A:H4'  | 1:51:A:U:H5'  | 3        | 1.73          |
| (1,1300) | 1:31:A:A:H4'  | 1:32:A:G:H5'' | 5        | 1.72          |
| (1,438)  | 1:30:A:C:H4'  | 1:31:A:A:H5'  | 3        | 1.69          |
| (1,672)  | 1:50:A:A:H4'  | 1:51:A:U:H5   | 5        | 1.62          |

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| Key      | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|----------|--------------|--------------|----------|---------------|
| (1,112)  | 1:2:A:G:H1'  | 1:3:A:A:H2'  | 6        | 1.62          |
| (1,1285) | 1:15:A:C:H2' | 1:16:A:G:H5' | 2        | 1.61          |
| (1,1285) | 1:15:A:C:H2' | 1:16:A:G:H5' | 3        | 1.61          |
| (1,1285) | 1:15:A:C:H2' | 1:16:A:G:H5' | 7        | 1.61          |
| (1,1285) | 1:15:A:C:H2' | 1:16:A:G:H5' | 9        | 1.61          |
| (1,1285) | 1:15:A:C:H2' | 1:16:A:G:H5' | 1        | 1.6           |
| (1,1285) | 1:15:A:C:H2' | 1:16:A:G:H5' | 4        | 1.6           |
| (1,1285) | 1:15:A:C:H2' | 1:16:A:G:H5' | 6        | 1.6           |
| (1,1285) | 1:15:A:C:H2' | 1:16:A:G:H5' | 8        | 1.6           |
| (1,1285) | 1:15:A:C:H2' | 1:16:A:G:H5' | 10       | 1.6           |
| (1,1285) | 1:15:A:C:H2' | 1:16:A:G:H5' | 5        | 1.59          |
| (1,438)  | 1:30:A:C:H4' | 1:31:A:A:H5' | 1        | 1.59          |
| (1,438)  | 1:30:A:C:H4' | 1:31:A:A:H5' | 5        | 1.59          |
| (1,438)  | 1:30:A:C:H4' | 1:31:A:A:H5' | 10       | 1.57          |
| (1,899)  | 1:31:A:A:H3' | 1:30:A:C:H2' | 8        | 1.56          |
| (1,660)  | 1:50:A:A:H5' | 1:51:A:U:H4' | 9        | 1.56          |
| (1,604)  | 1:29:A:A:H5' | 1:28:A:U:H1' | 5        | 1.56          |
| (1,1203) | 1:59:A:U:H3' | 1:58:A:G:H1' | 4        | 1.55          |
| (1,438)  | 1:30:A:C:H4' | 1:31:A:A:H5' | 6        | 1.55          |
| (1,382)  | 1:30:A:C:H5' | 1:29:A:A:H1' | 3        | 1.52          |
| (1,112)  | 1:2:A:G:H1'  | 1:3:A:A:H2'  | 9        | 1.51          |
| (1,672)  | 1:50:A:A:H4' | 1:51:A:U:H5' | 1        | 1.5           |
| (1,660)  | 1:50:A:A:H5' | 1:51:A:U:H4' | 2        | 1.49          |
| (1,112)  | 1:2:A:G:H1'  | 1:3:A:A:H3'  | 7        | 1.49          |
| (1,440)  | 1:5:A:G:H5'' | 1:4:A:A:H1'  | 5        | 1.48          |
| (1,440)  | 1:5:A:G:H5'' | 1:4:A:A:H1'  | 10       | 1.45          |
| (1,168)  | 1:50:A:A:H3' | 1:50:A:A:H8  | 5        | 1.45          |
| (1,1038) | 1:20:A:A:H1' | 1:21:A:C:H5' | 7        | 1.4           |
| (1,604)  | 1:29:A:A:H5' | 1:28:A:U:H1' | 10       | 1.4           |
| (1,1038) | 1:20:A:A:H1' | 1:21:A:C:H5' | 6        | 1.39          |
| (1,604)  | 1:29:A:A:H5' | 1:28:A:U:H1' | 4        | 1.39          |
| (1,1038) | 1:20:A:A:H1' | 1:21:A:C:H5' | 8        | 1.38          |
| (1,424)  | 1:49:A:G:H2' | 1:50:A:A:H4' | 8        | 1.38          |
| (1,1038) | 1:20:A:A:H1' | 1:21:A:C:H5' | 9        | 1.37          |
| (1,1038) | 1:20:A:A:H1' | 1:21:A:C:H5' | 4        | 1.36          |
| (1,1038) | 1:20:A:A:H1' | 1:21:A:C:H5' | 5        | 1.36          |
| (1,645)  | 1:50:A:A:H4' | 1:51:A:U:H5' | 9        | 1.35          |
| (1,604)  | 1:29:A:A:H5' | 1:28:A:U:H1' | 3        | 1.35          |
| (1,604)  | 1:29:A:A:H5' | 1:28:A:U:H1' | 6        | 1.35          |
| (1,112)  | 1:2:A:G:H1'  | 1:3:A:A:H3'  | 8        | 1.34          |
| (1,1038) | 1:20:A:A:H1' | 1:21:A:C:H5' | 3        | 1.33          |
| (1,1038) | 1:20:A:A:H1' | 1:21:A:C:H5' | 1        | 1.32          |

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| Key      | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,382)  | 1:30:A:C:H5' | 1:29:A:A:H1'  | 9        | 1.31          |
| (1,440)  | 1:5:A:G:H5'' | 1:4:A:A:H1'   | 2        | 1.3           |
| (1,1038) | 1:20:A:A:H1' | 1:21:A:C:H5'  | 10       | 1.29          |
| (1,604)  | 1:29:A:A:H5' | 1:28:A:U:H1'  | 2        | 1.29          |
| (1,1302) | 1:56:A:U:H1' | 1:57:A:G:H5'' | 1        | 1.28          |
| (1,604)  | 1:29:A:A:H5' | 1:28:A:U:H1'  | 9        | 1.27          |
| (1,660)  | 1:50:A:A:H5' | 1:51:A:U:H4'  | 10       | 1.25          |
| (1,604)  | 1:29:A:A:H5' | 1:28:A:U:H1'  | 7        | 1.24          |
| (1,1302) | 1:56:A:U:H1' | 1:57:A:G:H5'' | 8        | 1.22          |
| (1,394)  | 1:9:A:G:H2'  | 1:8:A:A:H2    | 2        | 1.22          |
| (1,168)  | 1:50:A:A:H3' | 1:50:A:A:H8   | 1        | 1.22          |
| (1,1302) | 1:56:A:U:H1' | 1:57:A:G:H5'' | 9        | 1.21          |
| (1,660)  | 1:50:A:A:H5' | 1:51:A:U:H4'  | 7        | 1.2           |
| (1,382)  | 1:30:A:C:H5' | 1:29:A:A:H1'  | 4        | 1.2           |
| (1,236)  | 1:8:A:A:H5'' | 1:8:A:A:H1'   | 7        | 1.2           |
| (1,1302) | 1:56:A:U:H1' | 1:57:A:G:H5'' | 6        | 1.19          |
| (1,1302) | 1:56:A:U:H1' | 1:57:A:G:H5'' | 7        | 1.19          |
| (1,197)  | 1:52:A:A:H8  | 1:52:A:A:H3'  | 7        | 1.19          |
| (1,650)  | 1:45:A:C:H3' | 1:46:A:U:H5'' | 10       | 1.18          |
| (1,236)  | 1:8:A:A:H5'' | 1:8:A:A:H1'   | 6        | 1.18          |
| (1,1038) | 1:20:A:A:H1' | 1:21:A:C:H5'  | 2        | 1.17          |
| (1,369)  | 1:9:A:G:H2'  | 1:8:A:A:H3'   | 8        | 1.14          |
| (1,650)  | 1:45:A:C:H3' | 1:46:A:U:H5'' | 4        | 1.13          |
| (1,440)  | 1:5:A:G:H5'' | 1:4:A:A:H1'   | 9        | 1.13          |
| (1,650)  | 1:45:A:C:H3' | 1:46:A:U:H5'' | 2        | 1.11          |
| (1,650)  | 1:45:A:C:H3' | 1:46:A:U:H5'' | 5        | 1.11          |
| (1,650)  | 1:45:A:C:H3' | 1:46:A:U:H5'' | 8        | 1.11          |
| (1,176)  | 1:25:A:A:H5' | 1:25:A:A:H8   | 10       | 1.11          |
| (1,650)  | 1:45:A:C:H3' | 1:46:A:U:H5'' | 9        | 1.1           |
| (1,440)  | 1:5:A:G:H5'' | 1:4:A:A:H1'   | 4        | 1.1           |
| (1,112)  | 1:2:A:G:H1'  | 1:3:A:A:H3'   | 4        | 1.1           |
| (1,1302) | 1:56:A:U:H1' | 1:57:A:G:H5'' | 2        | 1.09          |
| (1,112)  | 1:2:A:G:H1'  | 1:3:A:A:H3'   | 1        | 1.08          |
| (1,112)  | 1:2:A:G:H1'  | 1:3:A:A:H2'   | 3        | 1.07          |
| (1,1302) | 1:56:A:U:H1' | 1:57:A:G:H5'' | 5        | 1.06          |
| (1,650)  | 1:45:A:C:H3' | 1:46:A:U:H5'' | 3        | 1.06          |
| (1,440)  | 1:5:A:G:H5'' | 1:4:A:A:H1'   | 7        | 1.06          |
| (1,406)  | 1:5:A:G:H1'  | 1:6:A:A:H5''  | 6        | 1.06          |
| (1,406)  | 1:5:A:G:H1'  | 1:6:A:A:H5''  | 9        | 1.06          |
| (1,176)  | 1:25:A:A:H5' | 1:25:A:A:H8   | 5        | 1.06          |
| (1,440)  | 1:5:A:G:H5'' | 1:4:A:A:H1'   | 8        | 1.05          |
| (1,369)  | 1:9:A:G:H2'  | 1:8:A:A:H3'   | 7        | 1.05          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,406)  | 1:5:A:G:H1'   | 1:6:A:A:H5''  | 5        | 1.04          |
| (1,112)  | 1:2:A:G:H1'   | 1:3:A:A:H3'   | 2        | 1.04          |
| (1,112)  | 1:2:A:G:H1'   | 1:3:A:A:H3'   | 10       | 1.04          |
| (1,112)  | 1:2:A:G:H1'   | 1:3:A:A:H3'   | 5        | 1.03          |
| (1,650)  | 1:45:A:C:H3'  | 1:46:A:U:H5'' | 6        | 1.02          |
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 2        | 1.01          |
| (1,650)  | 1:45:A:C:H3'  | 1:46:A:U:H5'' | 1        | 1.01          |
| (1,406)  | 1:5:A:G:H1'   | 1:6:A:A:H5''  | 1        | 1.01          |
| (1,406)  | 1:5:A:G:H1'   | 1:6:A:A:H5''  | 10       | 1.01          |
| (1,440)  | 1:5:A:G:H5''  | 1:4:A:A:H1'   | 3        | 1.0           |
| (1,176)  | 1:25:A:A:H5'  | 1:25:A:A:H8   | 1        | 1.0           |
| (1,402)  | 1:19:A:C:H1'  | 1:20:A:A:H5'  | 8        | 0.99          |
| (1,402)  | 1:19:A:C:H1'  | 1:20:A:A:H5'  | 10       | 0.98          |
| (1,176)  | 1:25:A:A:H5'  | 1:25:A:A:H8   | 7        | 0.98          |
| (1,406)  | 1:5:A:G:H1'   | 1:6:A:A:H5''  | 2        | 0.97          |
| (1,402)  | 1:19:A:C:H1'  | 1:20:A:A:H5'  | 4        | 0.97          |
| (1,402)  | 1:19:A:C:H1'  | 1:20:A:A:H5'  | 6        | 0.97          |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 7        | 0.96          |
| (1,440)  | 1:5:A:G:H5''  | 1:4:A:A:H1'   | 6        | 0.95          |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4'  | 2        | 0.93          |
| (1,679)  | 1:54:A:C:H5'' | 1:54:A:C:H6   | 4        | 0.93          |
| (1,406)  | 1:5:A:G:H1'   | 1:6:A:A:H5''  | 3        | 0.93          |
| (1,402)  | 1:19:A:C:H1'  | 1:20:A:A:H5'  | 1        | 0.93          |
| (1,176)  | 1:25:A:A:H5'  | 1:25:A:A:H8   | 9        | 0.93          |
| (1,660)  | 1:50:A:A:H5'  | 1:51:A:U:H4'  | 5        | 0.91          |
| (1,1302) | 1:56:A:U:H1'  | 1:57:A:G:H5'' | 10       | 0.9           |
| (1,889)  | 1:50:A:A:H8   | 1:47:A:C:H3'  | 1        | 0.9           |
| (1,650)  | 1:45:A:C:H3'  | 1:46:A:U:H5'' | 7        | 0.9           |
| (1,406)  | 1:5:A:G:H1'   | 1:6:A:A:H5''  | 4        | 0.9           |
| (1,406)  | 1:5:A:G:H1'   | 1:6:A:A:H5''  | 7        | 0.9           |
| (1,406)  | 1:5:A:G:H1'   | 1:6:A:A:H5''  | 8        | 0.9           |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 9        | 0.89          |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 5        | 0.88          |
| (1,381)  | 1:30:A:C:H4'  | 1:29:A:A:H1'  | 7        | 0.88          |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1'  | 4        | 0.86          |
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 1        | 0.84          |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 4        | 0.84          |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 5        | 0.83          |
| (1,1302) | 1:56:A:U:H1'  | 1:57:A:G:H5'' | 4        | 0.82          |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 8        | 0.82          |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 7        | 0.82          |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 8        | 0.81          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,440)  | 1:5:A:G:H5''  | 1:4:A:A:H1'   | 1        | 0.81          |
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 3        | 0.79          |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 1        | 0.79          |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 6        | 0.79          |
| (1,660)  | 1:50:A:A:H5'  | 1:51:A:U:H4'  | 1        | 0.79          |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 10       | 0.79          |
| (1,428)  | 1:5:A:G:H8    | 1:4:A:A:H5''  | 1        | 0.79          |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 6        | 0.78          |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 10       | 0.78          |
| (1,121)  | 1:54:A:C:H3'  | 1:53:A:U:H2'  | 4        | 0.78          |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 9        | 0.77          |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 10       | 0.77          |
| (1,679)  | 1:54:A:C:H5'' | 1:54:A:C:H6   | 1        | 0.76          |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1'  | 3        | 0.75          |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 9        | 0.75          |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 2        | 0.74          |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 6        | 0.74          |
| (1,121)  | 1:54:A:C:H3'  | 1:53:A:U:H2'  | 1        | 0.74          |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 1        | 0.73          |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 7        | 0.72          |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 3        | 0.72          |
| (1,653)  | 1:12:A:C:H1'  | 1:13:A:U:H5'' | 4        | 0.72          |
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 5        | 0.71          |
| (1,889)  | 1:50:A:A:H8   | 1:47:A:C:H3'  | 5        | 0.71          |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 3        | 0.71          |
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 10       | 0.7           |
| (1,587)  | 1:29:A:A:H4'  | 1:28:A:U:H6   | 10       | 0.7           |
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 8        | 0.69          |
| (1,679)  | 1:54:A:C:H5'' | 1:54:A:C:H6   | 5        | 0.69          |
| (1,515)  | 1:22:A:U:H5'  | 1:22:A:U:H3'  | 7        | 0.69          |
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 9        | 0.68          |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4'  | 10       | 0.68          |
| (1,515)  | 1:22:A:U:H5'  | 1:22:A:U:H3'  | 10       | 0.68          |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 2        | 0.66          |
| (1,679)  | 1:54:A:C:H5'' | 1:54:A:C:H6   | 8        | 0.66          |
| (1,515)  | 1:22:A:U:H5'  | 1:22:A:U:H3'  | 5        | 0.66          |
| (1,515)  | 1:22:A:U:H5'  | 1:22:A:U:H3'  | 8        | 0.66          |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 5        | 0.65          |
| (1,515)  | 1:22:A:U:H5'  | 1:22:A:U:H3'  | 4        | 0.65          |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 10       | 0.65          |
| (1,679)  | 1:54:A:C:H5'' | 1:54:A:C:H6   | 10       | 0.64          |
| (1,515)  | 1:22:A:U:H5'  | 1:22:A:U:H3'  | 6        | 0.64          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,515)  | 1:22:A:U:H5'  | 1:22:A:U:H3'  | 1        | 0.63          |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 4        | 0.62          |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 9        | 0.62          |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 10       | 0.62          |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 9        | 0.62          |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 7        | 0.61          |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 1        | 0.61          |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 5        | 0.61          |
| (1,13)   | 1:18:A:C:H4'  | 1:19:A:C:H5   | 7        | 0.61          |
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 7        | 0.6           |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 6        | 0.6           |
| (1,515)  | 1:22:A:U:H5'  | 1:22:A:U:H3'  | 3        | 0.6           |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 7        | 0.6           |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 5        | 0.59          |
| (1,13)   | 1:18:A:C:H4'  | 1:19:A:C:H5   | 9        | 0.59          |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 1        | 0.58          |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 3        | 0.58          |
| (1,176)  | 1:25:A:A:H5'  | 1:25:A:A:H8   | 2        | 0.58          |
| (1,163)  | 1:50:A:A:H3'  | 1:47:A:C:H3'  | 2        | 0.58          |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 4        | 0.57          |
| (1,13)   | 1:18:A:C:H4'  | 1:19:A:C:H5   | 2        | 0.57          |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 2        | 0.55          |
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 6        | 0.54          |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 8        | 0.54          |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 2        | 0.53          |
| (1,123)  | 1:54:A:C:H3'  | 1:53:A:U:H3'  | 9        | 0.53          |
| (1,13)   | 1:18:A:C:H4'  | 1:19:A:C:H5   | 5        | 0.53          |
| (1,445)  | 1:53:A:U:H5'' | 1:53:A:U:H6   | 1        | 0.52          |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 1        | 0.5           |
| (1,1186) | 1:56:A:U:H5'  | 1:57:A:G:H8   | 3        | 0.5           |
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 9        | 0.5           |
| (1,121)  | 1:54:A:C:H3'  | 1:53:A:U:H2'  | 8        | 0.5           |
| (1,1240) | 1:59:A:U:H3'  | 1:58:A:G:H4'  | 10       | 0.49          |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 2        | 0.49          |
| (1,1201) | 1:12:A:C:H5'' | 1:11:A:G:H1'  | 3        | 0.49          |
| (1,864)  | 1:46:A:U:H1'  | 1:47:A:C:H4'  | 1        | 0.49          |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 8        | 0.49          |
| (1,196)  | 1:52:A:A:H8   | 1:52:A:A:H2'  | 7        | 0.49          |
| (1,104)  | 1:21:A:C:H5   | 1:20:A:A:H4'  | 3        | 0.49          |
| (1,1302) | 1:56:A:U:H1'  | 1:57:A:G:H5'' | 3        | 0.48          |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4'  | 1        | 0.48          |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4'  | 7        | 0.48          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 1        | 0.48          |
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 7        | 0.48          |
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 10       | 0.48          |
| (1,401)  | 1:19:A:C:H1'  | 1:20:A:A:H5'' | 3        | 0.48          |
| (1,13)   | 1:18:A:C:H4'  | 1:19:A:C:H5   | 3        | 0.48          |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 10       | 0.47          |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4'  | 5        | 0.47          |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 2        | 0.47          |
| (1,632)  | 1:29:A:A:H4'  | 1:28:A:U:H3'  | 2        | 0.47          |
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 3        | 0.47          |
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 5        | 0.47          |
| (1,401)  | 1:19:A:C:H1'  | 1:20:A:A:H5'' | 5        | 0.47          |
| (1,401)  | 1:19:A:C:H1'  | 1:20:A:A:H5'' | 9        | 0.47          |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4'  | 8        | 0.46          |
| (1,862)  | 1:53:A:U:H4'  | 1:54:A:C:H4'  | 4        | 0.46          |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 4        | 0.46          |
| (1,401)  | 1:19:A:C:H1'  | 1:20:A:A:H5'' | 2        | 0.46          |
| (1,401)  | 1:19:A:C:H1'  | 1:20:A:A:H5'' | 7        | 0.46          |
| (1,13)   | 1:18:A:C:H4'  | 1:19:A:C:H5   | 8        | 0.46          |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 1        | 0.45          |
| (1,1298) | 1:8:A:A:H1'   | 1:9:A:G:H5''  | 8        | 0.45          |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 1        | 0.45          |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 4        | 0.45          |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 6        | 0.45          |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 8        | 0.45          |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 9        | 0.45          |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1'  | 1        | 0.45          |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1'  | 2        | 0.45          |
| (1,929)  | 1:31:A:A:H8   | 1:30:A:C:H3'  | 8        | 0.45          |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4'  | 4        | 0.45          |
| (1,842)  | 1:13:A:U:H1'  | 1:12:A:C:H6   | 8        | 0.45          |
| (1,621)  | 1:54:A:C:H6   | 1:53:A:U:H2'  | 5        | 0.45          |
| (1,445)  | 1:53:A:U:H5'' | 1:53:A:U:H6   | 9        | 0.45          |
| (1,445)  | 1:53:A:U:H5'' | 1:53:A:U:H6   | 10       | 0.45          |
| (1,438)  | 1:30:A:C:H4'  | 1:31:A:A:H5'  | 8        | 0.45          |
| (1,121)  | 1:54:A:C:H3'  | 1:53:A:U:H2'  | 5        | 0.45          |
| (1,121)  | 1:54:A:C:H3'  | 1:53:A:U:H2'  | 10       | 0.45          |
| (1,1332) | 1:18:A:C:H4'  | 1:17:A:G:H4'  | 4        | 0.44          |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 5        | 0.44          |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 6        | 0.44          |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 8        | 0.44          |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 3        | 0.44          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1224) | 1:31:A:A:H1'  | 1:32:A:G:H4'  | 5        | 0.44          |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1'  | 7        | 0.44          |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1'  | 8        | 0.44          |
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8   | 7        | 0.44          |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4'  | 6        | 0.44          |
| (1,875)  | 1:28:A:U:H5   | 1:27:A:C:H4'  | 5        | 0.44          |
| (1,621)  | 1:54:A:C:H6   | 1:53:A:U:H2'  | 8        | 0.44          |
| (1,408)  | 1:23:A:C:H1'  | 1:24:A:A:H5'  | 6        | 0.44          |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1'  | 1        | 0.44          |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1'  | 7        | 0.44          |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1'  | 9        | 0.44          |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 2        | 0.43          |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 3        | 0.43          |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 9        | 0.43          |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 10       | 0.43          |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 5        | 0.43          |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1'  | 9        | 0.43          |
| (1,820)  | 1:50:A:A:H8   | 1:47:A:C:H6   | 7        | 0.43          |
| (1,820)  | 1:50:A:A:H8   | 1:47:A:C:H6   | 9        | 0.43          |
| (1,603)  | 1:29:A:A:H8   | 1:28:A:U:H1'  | 1        | 0.43          |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1'  | 5        | 0.43          |
| (1,369)  | 1:9:A:G:H2'   | 1:8:A:A:H3'   | 4        | 0.43          |
| (1,346)  | 1:23:A:C:H1'  | 1:24:A:A:H4'  | 4        | 0.43          |
| (1,161)  | 1:24:A:A:H4'  | 1:23:A:C:H1'  | 4        | 0.43          |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 4        | 0.42          |
| (1,1321) | 1:18:A:C:H6   | 1:17:A:G:H5'  | 7        | 0.42          |
| (1,1298) | 1:8:A:A:H1'   | 1:9:A:G:H5''  | 5        | 0.42          |
| (1,1290) | 1:31:A:A:H1'  | 1:32:A:G:H5'' | 8        | 0.42          |
| (1,1229) | 1:15:A:C:H1'  | 1:16:A:G:H4'  | 7        | 0.42          |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1'  | 4        | 0.42          |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1'  | 5        | 0.42          |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8   | 7        | 0.42          |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1'  | 5        | 0.42          |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2'  | 9        | 0.42          |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4'  | 9        | 0.42          |
| (1,862)  | 1:53:A:U:H4'  | 1:54:A:C:H4'  | 1        | 0.42          |
| (1,820)  | 1:50:A:A:H8   | 1:47:A:C:H6   | 8        | 0.42          |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4'  | 7        | 0.42          |
| (1,425)  | 1:49:A:G:H4'  | 1:50:A:A:H4'  | 1        | 0.42          |
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 2        | 0.42          |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1'  | 7        | 0.42          |
| (1,369)  | 1:9:A:G:H2'   | 1:8:A:A:H3'   | 5        | 0.42          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,236)  | 1:8:A:A:H5''  | 1:8:A:A:H1'   | 5        | 0.42          |
| (1,180)  | 1:25:A:A:H1'  | 1:26:A:A:H8   | 7        | 0.42          |
| (1,13)   | 1:18:A:C:H4'  | 1:19:A:C:H5   | 6        | 0.42          |
| (1,1235) | 1:59:A:U:H5   | 1:58:A:G:H4'  | 10       | 0.41          |
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4'  | 7        | 0.41          |
| (1,1196) | 1:12:A:C:H6   | 1:11:A:G:H1'  | 8        | 0.41          |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1'  | 6        | 0.41          |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8   | 4        | 0.41          |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8   | 5        | 0.41          |
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8   | 6        | 0.41          |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1'  | 7        | 0.41          |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5'  | 3        | 0.41          |
| (1,942)  | 1:20:A:A:H1'  | 1:19:A:C:H3'  | 6        | 0.41          |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2'  | 7        | 0.41          |
| (1,861)  | 1:53:A:U:H3'  | 1:54:A:C:H4'  | 6        | 0.41          |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4'  | 3        | 0.41          |
| (1,395)  | 1:28:A:U:H4'  | 1:29:A:A:H8   | 6        | 0.41          |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1'  | 2        | 0.41          |
| (1,236)  | 1:8:A:A:H5''  | 1:8:A:A:H1'   | 2        | 0.41          |
| (1,180)  | 1:25:A:A:H1'  | 1:26:A:A:H8   | 2        | 0.41          |
| (1,170)  | 1:3:A:A:H1'   | 1:4:A:A:H8    | 1        | 0.41          |
| (1,1298) | 1:8:A:A:H1'   | 1:9:A:G:H5''  | 7        | 0.4           |
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4'  | 3        | 0.4           |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1'  | 9        | 0.4           |
| (1,1168) | 1:31:A:A:H1'  | 1:32:A:G:H8   | 3        | 0.4           |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8   | 3        | 0.4           |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8   | 8        | 0.4           |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8   | 9        | 0.4           |
| (1,1052) | 1:46:A:U:H2'  | 1:47:A:C:H3'  | 5        | 0.4           |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1'  | 8        | 0.4           |
| (1,942)  | 1:20:A:A:H1'  | 1:19:A:C:H3'  | 3        | 0.4           |
| (1,862)  | 1:53:A:U:H4'  | 1:54:A:C:H4'  | 10       | 0.4           |
| (1,515)  | 1:22:A:U:H5'  | 1:22:A:U:H3'  | 9        | 0.4           |
| (1,445)  | 1:53:A:U:H5'' | 1:53:A:U:H6   | 5        | 0.4           |
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 8        | 0.4           |
| (1,395)  | 1:28:A:U:H4'  | 1:29:A:A:H8   | 3        | 0.4           |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1'  | 6        | 0.4           |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1'  | 6        | 0.4           |
| (1,170)  | 1:3:A:A:H1'   | 1:4:A:A:H8    | 8        | 0.4           |
| (1,1298) | 1:8:A:A:H1'   | 1:9:A:G:H5''  | 2        | 0.39          |
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4'  | 4        | 0.39          |
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4'  | 5        | 0.39          |

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| Key      | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|----------|---------------|--------------|----------|---------------|
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4' | 6        | 0.39          |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1' | 1        | 0.39          |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1' | 3        | 0.39          |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1' | 10       | 0.39          |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8  | 1        | 0.39          |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8  | 10       | 0.39          |
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8  | 3        | 0.39          |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1' | 6        | 0.39          |
| (1,1005) | 1:40:A:A:H8   | 1:39:A:C:H1' | 10       | 0.39          |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5' | 4        | 0.39          |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5' | 7        | 0.39          |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5' | 10       | 0.39          |
| (1,942)  | 1:20:A:A:H1'  | 1:19:A:C:H3' | 1        | 0.39          |
| (1,942)  | 1:20:A:A:H1'  | 1:19:A:C:H3' | 8        | 0.39          |
| (1,942)  | 1:20:A:A:H1'  | 1:19:A:C:H3' | 10       | 0.39          |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2' | 3        | 0.39          |
| (1,875)  | 1:28:A:U:H5   | 1:27:A:C:H4' | 7        | 0.39          |
| (1,861)  | 1:53:A:U:H3'  | 1:54:A:C:H4' | 7        | 0.39          |
| (1,682)  | 1:55:A:C:H2'  | 1:55:A:C:H6  | 10       | 0.39          |
| (1,621)  | 1:54:A:C:H6   | 1:53:A:U:H2' | 10       | 0.39          |
| (1,606)  | 1:54:A:C:H5   | 1:53:A:U:H1' | 1        | 0.39          |
| (1,395)  | 1:28:A:U:H4'  | 1:29:A:A:H8  | 7        | 0.39          |
| (1,393)  | 1:5:A:G:H2'   | 1:4:A:A:H2   | 4        | 0.39          |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1' | 10       | 0.39          |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1' | 5        | 0.39          |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1' | 10       | 0.39          |
| (1,236)  | 1:8:A:A:H5''  | 1:8:A:A:H1'  | 1        | 0.39          |
| (1,177)  | 1:25:A:A:H5'' | 1:25:A:A:H8  | 2        | 0.39          |
| (1,170)  | 1:3:A:A:H1'   | 1:4:A:A:H8   | 4        | 0.39          |
| (1,1298) | 1:8:A:A:H1'   | 1:9:A:G:H5'' | 4        | 0.38          |
| (1,1297) | 1:8:A:A:H4'   | 1:9:A:G:H5'' | 6        | 0.38          |
| (1,1249) | 1:50:A:A:H5'' | 1:49:A:G:H3' | 8        | 0.38          |
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4' | 1        | 0.38          |
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4' | 8        | 0.38          |
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4' | 9        | 0.38          |
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4' | 10       | 0.38          |
| (1,1224) | 1:31:A:A:H1'  | 1:32:A:G:H4' | 1        | 0.38          |
| (1,1192) | 1:15:A:C:H3'  | 1:16:A:G:H1' | 2        | 0.38          |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8  | 2        | 0.38          |
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8  | 1        | 0.38          |
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8  | 2        | 0.38          |
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8  | 4        | 0.38          |

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| Key      | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|----------|---------------|--------------|----------|---------------|
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8  | 8        | 0.38          |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5' | 1        | 0.38          |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5' | 5        | 0.38          |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5' | 9        | 0.38          |
| (1,910)  | 1:44:A:A:H1'  | 1:43:A:C:H2' | 6        | 0.38          |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2' | 1        | 0.38          |
| (1,852)  | 1:20:A:A:H2'  | 1:21:A:C:H6  | 3        | 0.38          |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4' | 2        | 0.38          |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4' | 9        | 0.38          |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1' | 1        | 0.38          |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1' | 3        | 0.38          |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1' | 8        | 0.38          |
| (1,369)  | 1:9:A:G:H2'   | 1:8:A:A:H3'  | 9        | 0.38          |
| (1,236)  | 1:8:A:A:H5''  | 1:8:A:A:H1'  | 4        | 0.38          |
| (1,213)  | 1:26:A:A:H8   | 1:26:A:A:H3' | 7        | 0.38          |
| (1,198)  | 1:26:A:A:H8   | 1:26:A:A:H2' | 1        | 0.38          |
| (1,104)  | 1:21:A:C:H5   | 1:20:A:A:H4' | 2        | 0.38          |
| (1,13)   | 1:18:A:C:H4'  | 1:19:A:C:H5  | 1        | 0.38          |
| (1,1225) | 1:47:A:C:H2'  | 1:49:A:G:H4' | 1        | 0.37          |
| (1,1206) | 1:8:A:A:H1'   | 1:9:A:G:H1'  | 10       | 0.37          |
| (1,1165) | 1:15:A:C:H2'  | 1:16:A:G:H8  | 6        | 0.37          |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5  | 5        | 0.37          |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5' | 6        | 0.37          |
| (1,942)  | 1:20:A:A:H1'  | 1:19:A:C:H3' | 4        | 0.37          |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2' | 8        | 0.37          |
| (1,879)  | 1:20:A:A:H3'  | 1:21:A:C:H4' | 3        | 0.37          |
| (1,878)  | 1:26:A:A:H2'  | 1:27:A:C:H4' | 7        | 0.37          |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4' | 2        | 0.37          |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4' | 3        | 0.37          |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4' | 7        | 0.37          |
| (1,864)  | 1:46:A:U:H1'  | 1:47:A:C:H4' | 5        | 0.37          |
| (1,861)  | 1:53:A:U:H3'  | 1:54:A:C:H4' | 2        | 0.37          |
| (1,852)  | 1:20:A:A:H2'  | 1:21:A:C:H6  | 2        | 0.37          |
| (1,836)  | 1:22:A:U:H1'  | 1:23:A:C:H6  | 9        | 0.37          |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4' | 6        | 0.37          |
| (1,506)  | 1:28:A:U:H6   | 1:28:A:U:H3' | 4        | 0.37          |
| (1,395)  | 1:28:A:U:H4'  | 1:29:A:A:H8  | 4        | 0.37          |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1' | 4        | 0.37          |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1' | 9        | 0.37          |
| (1,369)  | 1:9:A:G:H2'   | 1:8:A:A:H3'  | 1        | 0.37          |
| (1,369)  | 1:9:A:G:H2'   | 1:8:A:A:H3'  | 3        | 0.37          |
| (1,346)  | 1:23:A:C:H1'  | 1:24:A:A:H4' | 6        | 0.37          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,198)  | 1:26:A:A:H8   | 1:26:A:A:H2'  | 2        | 0.37          |
| (1,198)  | 1:26:A:A:H8   | 1:26:A:A:H2'  | 6        | 0.37          |
| (1,180)  | 1:25:A:A:H1'  | 1:26:A:A:H8   | 9        | 0.37          |
| (1,161)  | 1:24:A:A:H4'  | 1:23:A:C:H1'  | 6        | 0.37          |
| (1,1298) | 1:8:A:A:H1'   | 1:9:A:G:H5''  | 3        | 0.36          |
| (1,1298) | 1:8:A:A:H1'   | 1:9:A:G:H5''  | 9        | 0.36          |
| (1,1290) | 1:31:A:A:H1'  | 1:32:A:G:H5'' | 7        | 0.36          |
| (1,1231) | 1:15:A:C:H3'  | 1:16:A:G:H4'  | 2        | 0.36          |
| (1,1196) | 1:12:A:C:H6   | 1:11:A:G:H1'  | 2        | 0.36          |
| (1,1168) | 1:31:A:A:H1'  | 1:32:A:G:H8   | 10       | 0.36          |
| (1,1108) | 1:2:A:G:H8    | 1:2:A:G:H2'   | 1        | 0.36          |
| (1,1108) | 1:2:A:G:H8    | 1:2:A:G:H2'   | 8        | 0.36          |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5'  | 2        | 0.36          |
| (1,958)  | 1:16:A:G:H5'  | 1:15:A:C:H5'  | 8        | 0.36          |
| (1,942)  | 1:20:A:A:H1'  | 1:19:A:C:H3'  | 7        | 0.36          |
| (1,900)  | 1:28:A:U:H3'  | 1:27:A:C:H2'  | 10       | 0.36          |
| (1,877)  | 1:22:A:U:H5'' | 1:21:A:C:H4'  | 7        | 0.36          |
| (1,836)  | 1:22:A:U:H1'  | 1:23:A:C:H6   | 3        | 0.36          |
| (1,820)  | 1:50:A:A:H8   | 1:47:A:C:H6   | 2        | 0.36          |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4'  | 1        | 0.36          |
| (1,583)  | 1:50:A:A:H2'  | 1:51:A:U:H6   | 5        | 0.36          |
| (1,434)  | 1:51:A:U:H5   | 1:52:A:A:H8   | 10       | 0.36          |
| (1,431)  | 1:28:A:U:H2'  | 1:29:A:A:H5'  | 5        | 0.36          |
| (1,419)  | 1:19:A:C:H2'  | 1:20:A:A:H3'  | 8        | 0.36          |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1'  | 3        | 0.36          |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1'  | 4        | 0.36          |
| (1,369)  | 1:9:A:G:H2'   | 1:8:A:A:H3'   | 10       | 0.36          |
| (1,332)  | 1:2:A:G:H3'   | 1:3:A:A:H8    | 1        | 0.36          |
| (1,221)  | 1:29:A:A:H8   | 1:29:A:A:H3'  | 3        | 0.36          |
| (1,198)  | 1:26:A:A:H8   | 1:26:A:A:H2'  | 3        | 0.36          |
| (1,198)  | 1:26:A:A:H8   | 1:26:A:A:H2'  | 9        | 0.36          |
| (1,180)  | 1:25:A:A:H1'  | 1:26:A:A:H8   | 6        | 0.36          |
| (1,1290) | 1:31:A:A:H1'  | 1:32:A:G:H5'' | 2        | 0.35          |
| (1,1206) | 1:8:A:A:H1'   | 1:9:A:G:H1'   | 1        | 0.35          |
| (1,1203) | 1:59:A:U:H3'  | 1:58:A:G:H1'  | 10       | 0.35          |
| (1,1196) | 1:12:A:C:H6   | 1:11:A:G:H1'  | 1        | 0.35          |
| (1,1196) | 1:12:A:C:H6   | 1:11:A:G:H1'  | 6        | 0.35          |
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8   | 9        | 0.35          |
| (1,864)  | 1:46:A:U:H1'  | 1:47:A:C:H4'  | 6        | 0.35          |
| (1,862)  | 1:53:A:U:H4'  | 1:54:A:C:H4'  | 8        | 0.35          |
| (1,852)  | 1:20:A:A:H2'  | 1:21:A:C:H6   | 9        | 0.35          |
| (1,836)  | 1:22:A:U:H1'  | 1:23:A:C:H6   | 6        | 0.35          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,836)  | 1:22:A:U:H1'  | 1:23:A:C:H6   | 8        | 0.35          |
| (1,836)  | 1:22:A:U:H1'  | 1:23:A:C:H6   | 10       | 0.35          |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4'  | 4        | 0.35          |
| (1,606)  | 1:54:A:C:H5   | 1:53:A:U:H1'  | 5        | 0.35          |
| (1,595)  | 1:27:A:C:H2'  | 1:28:A:U:H5   | 5        | 0.35          |
| (1,595)  | 1:27:A:C:H2'  | 1:28:A:U:H5   | 7        | 0.35          |
| (1,445)  | 1:53:A:U:H5'' | 1:53:A:U:H6   | 8        | 0.35          |
| (1,419)  | 1:19:A:C:H2'  | 1:20:A:A:H3'  | 4        | 0.35          |
| (1,381)  | 1:30:A:C:H4'  | 1:29:A:A:H1'  | 2        | 0.35          |
| (1,381)  | 1:30:A:C:H4'  | 1:29:A:A:H1'  | 3        | 0.35          |
| (1,374)  | 1:27:A:C:H6   | 1:26:A:A:H1'  | 8        | 0.35          |
| (1,372)  | 1:45:A:C:H5'' | 1:44:A:A:H1'  | 2        | 0.35          |
| (1,369)  | 1:9:A:G:H2'   | 1:8:A:A:H3'   | 2        | 0.35          |
| (1,198)  | 1:26:A:A:H8   | 1:26:A:A:H2'  | 7        | 0.35          |
| (1,180)  | 1:25:A:A:H1'  | 1:26:A:A:H8   | 1        | 0.35          |
| (1,109)  | 1:27:A:C:H3'  | 1:26:A:A:H3'  | 9        | 0.35          |
| (1,1298) | 1:8:A:A:H1'   | 1:9:A:G:H5''  | 10       | 0.34          |
| (1,1290) | 1:31:A:A:H1'  | 1:32:A:G:H5'' | 9        | 0.34          |
| (1,1167) | 1:50:A:A:H8   | 1:49:A:G:H8   | 8        | 0.34          |
| (1,1108) | 1:2:A:G:H8    | 1:2:A:G:H2'   | 9        | 0.34          |
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8   | 10       | 0.34          |
| (1,1052) | 1:46:A:U:H2'  | 1:47:A:C:H3'  | 1        | 0.34          |
| (1,1013) | 1:24:A:A:H8   | 1:23:A:C:H1'  | 10       | 0.34          |
| (1,1000) | 1:20:A:A:H8   | 1:19:A:C:H1'  | 2        | 0.34          |
| (1,989)  | 1:20:A:A:H2'  | 1:21:A:C:H5   | 6        | 0.34          |
| (1,989)  | 1:20:A:A:H2'  | 1:21:A:C:H5   | 8        | 0.34          |
| (1,956)  | 1:14:A:U:H1'  | 1:15:A:C:H5'' | 6        | 0.34          |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2'  | 5        | 0.34          |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2'  | 10       | 0.34          |
| (1,877)  | 1:22:A:U:H5'' | 1:21:A:C:H4'  | 8        | 0.34          |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4'  | 8        | 0.34          |
| (1,864)  | 1:46:A:U:H1'  | 1:47:A:C:H4'  | 3        | 0.34          |
| (1,836)  | 1:22:A:U:H1'  | 1:23:A:C:H6   | 2        | 0.34          |
| (1,836)  | 1:22:A:U:H1'  | 1:23:A:C:H6   | 4        | 0.34          |
| (1,820)  | 1:50:A:A:H8   | 1:47:A:C:H6   | 3        | 0.34          |
| (1,820)  | 1:50:A:A:H8   | 1:47:A:C:H6   | 4        | 0.34          |
| (1,820)  | 1:50:A:A:H8   | 1:47:A:C:H6   | 6        | 0.34          |
| (1,820)  | 1:50:A:A:H8   | 1:47:A:C:H6   | 10       | 0.34          |
| (1,664)  | 1:58:A:G:H4'  | 1:59:A:U:H4'  | 8        | 0.34          |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4'  | 8        | 0.34          |
| (1,632)  | 1:29:A:A:H4'  | 1:28:A:U:H3'  | 9        | 0.34          |
| (1,587)  | 1:29:A:A:H4'  | 1:28:A:U:H6   | 5        | 0.34          |

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| Key      | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,583)  | 1:50:A:A:H2' | 1:51:A:U:H6   | 1        | 0.34          |
| (1,425)  | 1:49:A:G:H4' | 1:50:A:A:H4'  | 2        | 0.34          |
| (1,419)  | 1:19:A:C:H2' | 1:20:A:A:H3'  | 1        | 0.34          |
| (1,419)  | 1:19:A:C:H2' | 1:20:A:A:H3'  | 10       | 0.34          |
| (1,396)  | 1:51:A:U:H3' | 1:50:A:A:H1'  | 9        | 0.34          |
| (1,391)  | 1:27:A:C:H5  | 1:26:A:A:H2   | 4        | 0.34          |
| (1,352)  | 1:27:A:C:H5  | 1:26:A:A:H2'  | 4        | 0.34          |
| (1,332)  | 1:2:A:G:H3'  | 1:3:A:A:H8    | 7        | 0.34          |
| (1,213)  | 1:26:A:A:H8  | 1:26:A:A:H3'  | 6        | 0.34          |
| (1,198)  | 1:26:A:A:H8  | 1:26:A:A:H2'  | 5        | 0.34          |
| (1,1308) | 1:18:A:C:H5  | 1:17:A:G:H5'  | 6        | 0.33          |
| (1,1298) | 1:8:A:A:H1'  | 1:9:A:G:H5''  | 1        | 0.33          |
| (1,1290) | 1:31:A:A:H1' | 1:32:A:G:H5'' | 5        | 0.33          |
| (1,1206) | 1:8:A:A:H1'  | 1:9:A:G:H1'   | 9        | 0.33          |
| (1,1196) | 1:12:A:C:H6  | 1:11:A:G:H1'  | 7        | 0.33          |
| (1,1196) | 1:12:A:C:H6  | 1:11:A:G:H1'  | 9        | 0.33          |
| (1,1196) | 1:12:A:C:H6  | 1:11:A:G:H1'  | 10       | 0.33          |
| (1,1108) | 1:2:A:G:H8   | 1:2:A:G:H2'   | 7        | 0.33          |
| (1,1019) | 1:31:A:A:H8  | 1:30:A:C:H1'  | 8        | 0.33          |
| (1,1013) | 1:24:A:A:H8  | 1:23:A:C:H1'  | 5        | 0.33          |
| (1,1000) | 1:20:A:A:H8  | 1:19:A:C:H1'  | 3        | 0.33          |
| (1,1000) | 1:20:A:A:H8  | 1:19:A:C:H1'  | 9        | 0.33          |
| (1,942)  | 1:20:A:A:H1' | 1:19:A:C:H3'  | 2        | 0.33          |
| (1,942)  | 1:20:A:A:H1' | 1:19:A:C:H3'  | 5        | 0.33          |
| (1,910)  | 1:44:A:A:H1' | 1:43:A:C:H2'  | 2        | 0.33          |
| (1,901)  | 1:22:A:U:H3' | 1:21:A:C:H2'  | 2        | 0.33          |
| (1,852)  | 1:20:A:A:H2' | 1:21:A:C:H6   | 10       | 0.33          |
| (1,836)  | 1:22:A:U:H1' | 1:23:A:C:H6   | 1        | 0.33          |
| (1,836)  | 1:22:A:U:H1' | 1:23:A:C:H6   | 5        | 0.33          |
| (1,836)  | 1:22:A:U:H1' | 1:23:A:C:H6   | 7        | 0.33          |
| (1,682)  | 1:55:A:C:H2' | 1:55:A:C:H6   | 3        | 0.33          |
| (1,658)  | 1:27:A:C:H4' | 1:28:A:U:H5'' | 8        | 0.33          |
| (1,410)  | 1:2:A:G:H3'  | 1:3:A:A:H5'   | 3        | 0.33          |
| (1,369)  | 1:9:A:G:H2'  | 1:8:A:A:H3'   | 6        | 0.33          |
| (1,332)  | 1:2:A:G:H3'  | 1:3:A:A:H8    | 5        | 0.33          |
| (1,198)  | 1:26:A:A:H8  | 1:26:A:A:H2'  | 4        | 0.33          |
| (1,180)  | 1:25:A:A:H1' | 1:26:A:A:H8   | 3        | 0.33          |
| (1,176)  | 1:25:A:A:H5' | 1:25:A:A:H8   | 3        | 0.33          |
| (1,104)  | 1:21:A:C:H5  | 1:20:A:A:H4'  | 9        | 0.33          |
| (1,1308) | 1:18:A:C:H5  | 1:17:A:G:H5'  | 4        | 0.32          |
| (1,1308) | 1:18:A:C:H5  | 1:17:A:G:H5'  | 7        | 0.32          |
| (1,1290) | 1:31:A:A:H1' | 1:32:A:G:H5'' | 6        | 0.32          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1208) | 1:3:A:A:H8    | 1:2:A:G:H1'   | 8        | 0.32          |
| (1,1206) | 1:8:A:A:H1'   | 1:9:A:G:H1'   | 2        | 0.32          |
| (1,1196) | 1:12:A:C:H6   | 1:11:A:G:H1'  | 4        | 0.32          |
| (1,1168) | 1:31:A:A:H1'  | 1:32:A:G:H8   | 4        | 0.32          |
| (1,1013) | 1:24:A:A:H8   | 1:23:A:C:H1'  | 2        | 0.32          |
| (1,1000) | 1:20:A:A:H8   | 1:19:A:C:H1'  | 4        | 0.32          |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5   | 1        | 0.32          |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5   | 10       | 0.32          |
| (1,956)  | 1:14:A:U:H1'  | 1:15:A:C:H5'' | 2        | 0.32          |
| (1,956)  | 1:14:A:U:H1'  | 1:15:A:C:H5'' | 4        | 0.32          |
| (1,956)  | 1:14:A:U:H1'  | 1:15:A:C:H5'' | 5        | 0.32          |
| (1,956)  | 1:14:A:U:H1'  | 1:15:A:C:H5'' | 10       | 0.32          |
| (1,951)  | 1:37:A:G:H1'  | 1:38:A:C:H3'  | 9        | 0.32          |
| (1,942)  | 1:20:A:A:H1'  | 1:19:A:C:H3'  | 9        | 0.32          |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2'  | 4        | 0.32          |
| (1,877)  | 1:22:A:U:H5'' | 1:21:A:C:H4'  | 4        | 0.32          |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4'  | 6        | 0.32          |
| (1,870)  | 1:28:A:U:H6   | 1:27:A:C:H4'  | 7        | 0.32          |
| (1,862)  | 1:53:A:U:H4'  | 1:54:A:C:H4'  | 5        | 0.32          |
| (1,852)  | 1:20:A:A:H2'  | 1:21:A:C:H6   | 4        | 0.32          |
| (1,852)  | 1:20:A:A:H2'  | 1:21:A:C:H6   | 7        | 0.32          |
| (1,395)  | 1:28:A:U:H4'  | 1:29:A:A:H8   | 5        | 0.32          |
| (1,394)  | 1:9:A:G:H2'   | 1:8:A:A:H2    | 6        | 0.32          |
| (1,332)  | 1:2:A:G:H3'   | 1:3:A:A:H8    | 6        | 0.32          |
| (1,236)  | 1:8:A:A:H5''  | 1:8:A:A:H1'   | 8        | 0.32          |
| (1,209)  | 1:24:A:A:H8   | 1:24:A:A:H2'  | 8        | 0.32          |
| (1,198)  | 1:26:A:A:H8   | 1:26:A:A:H2'  | 8        | 0.32          |
| (1,198)  | 1:26:A:A:H8   | 1:26:A:A:H2'  | 10       | 0.32          |
| (1,107)  | 1:34:A:G:H2'  | 1:35:A:A:H2'  | 5        | 0.32          |
| (1,1308) | 1:18:A:C:H5   | 1:17:A:G:H5'  | 9        | 0.31          |
| (1,1298) | 1:8:A:A:H1'   | 1:9:A:G:H5''  | 6        | 0.31          |
| (1,1297) | 1:8:A:A:H4'   | 1:9:A:G:H5''  | 1        | 0.31          |
| (1,1290) | 1:31:A:A:H1'  | 1:32:A:G:H5'' | 1        | 0.31          |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 8        | 0.31          |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 9        | 0.31          |
| (1,1206) | 1:8:A:A:H1'   | 1:9:A:G:H1'   | 4        | 0.31          |
| (1,1206) | 1:8:A:A:H1'   | 1:9:A:G:H1'   | 5        | 0.31          |
| (1,1206) | 1:8:A:A:H1'   | 1:9:A:G:H1'   | 6        | 0.31          |
| (1,1196) | 1:12:A:C:H6   | 1:11:A:G:H1'  | 3        | 0.31          |
| (1,1196) | 1:12:A:C:H6   | 1:11:A:G:H1'  | 5        | 0.31          |
| (1,1064) | 1:41:A:G:H4'  | 1:41:A:G:H8   | 5        | 0.31          |
| (1,989)  | 1:20:A:A:H2'  | 1:21:A:C:H5   | 5        | 0.31          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,956)  | 1:14:A:U:H1'  | 1:15:A:C:H5'' | 3        | 0.31          |
| (1,882)  | 1:11:A:G:H1'  | 1:12:A:C:H4'  | 1        | 0.31          |
| (1,877)  | 1:22:A:U:H5'' | 1:21:A:C:H4'  | 5        | 0.31          |
| (1,877)  | 1:22:A:U:H5'' | 1:21:A:C:H4'  | 6        | 0.31          |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4'  | 10       | 0.31          |
| (1,852)  | 1:20:A:A:H2'  | 1:21:A:C:H6   | 1        | 0.31          |
| (1,682)  | 1:55:A:C:H2'  | 1:55:A:C:H6   | 5        | 0.31          |
| (1,682)  | 1:55:A:C:H2'  | 1:55:A:C:H6   | 8        | 0.31          |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4'  | 5        | 0.31          |
| (1,658)  | 1:27:A:C:H4'  | 1:28:A:U:H5'' | 1        | 0.31          |
| (1,627)  | 1:47:A:C:H6   | 1:46:A:U:H2'  | 7        | 0.31          |
| (1,627)  | 1:47:A:C:H6   | 1:46:A:U:H2'  | 10       | 0.31          |
| (1,587)  | 1:29:A:A:H4'  | 1:28:A:U:H6   | 4        | 0.31          |
| (1,587)  | 1:29:A:A:H4'  | 1:28:A:U:H6   | 7        | 0.31          |
| (1,566)  | 1:59:A:U:H5'  | 1:59:A:U:H4'  | 7        | 0.31          |
| (1,541)  | 1:53:A:U:H4'  | 1:53:A:U:H5'  | 7        | 0.31          |
| (1,506)  | 1:28:A:U:H6   | 1:28:A:U:H3'  | 7        | 0.31          |
| (1,445)  | 1:53:A:U:H5'' | 1:53:A:U:H6   | 6        | 0.31          |
| (1,395)  | 1:28:A:U:H4'  | 1:29:A:A:H8   | 9        | 0.31          |
| (1,395)  | 1:28:A:U:H4'  | 1:29:A:A:H8   | 10       | 0.31          |
| (1,391)  | 1:27:A:C:H5   | 1:26:A:A:H2   | 8        | 0.31          |
| (1,352)  | 1:27:A:C:H5   | 1:26:A:A:H2'  | 1        | 0.31          |
| (1,352)  | 1:27:A:C:H5   | 1:26:A:A:H2'  | 8        | 0.31          |
| (1,332)  | 1:2:A:G:H3'   | 1:3:A:A:H8    | 2        | 0.31          |
| (1,332)  | 1:2:A:G:H3'   | 1:3:A:A:H8    | 9        | 0.31          |
| (1,221)  | 1:29:A:A:H8   | 1:29:A:A:H3'  | 7        | 0.31          |
| (1,170)  | 1:3:A:A:H1'   | 1:4:A:A:H8    | 7        | 0.31          |
| (1,163)  | 1:49:A:G:H2'  | 1:47:A:C:H3'  | 6        | 0.31          |
| (1,150)  | 1:46:A:U:H6   | 1:47:A:C:H5'  | 8        | 0.31          |
| (1,150)  | 1:46:A:U:H6   | 1:47:A:C:H5'' | 8        | 0.31          |
| (1,123)  | 1:54:A:C:H3'  | 1:53:A:U:H3'  | 3        | 0.31          |
| (1,13)   | 1:18:A:C:H4'  | 1:19:A:C:H5   | 10       | 0.31          |
| (1,3)    | 1:41:A:G:H4'  | 1:40:A:A:H1'  | 4        | 0.31          |
| (1,3)    | 1:41:A:G:H4'  | 1:40:A:A:H1'  | 5        | 0.31          |
| (1,1297) | 1:8:A:A:H4'   | 1:9:A:G:H5''  | 7        | 0.3           |
| (1,1225) | 1:47:A:C:H2'  | 1:49:A:G:H4'  | 8        | 0.3           |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 1        | 0.3           |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 2        | 0.3           |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 4        | 0.3           |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 10       | 0.3           |
| (1,1206) | 1:8:A:A:H1'   | 1:9:A:G:H1'   | 3        | 0.3           |
| (1,1203) | 1:59:A:U:H3'  | 1:58:A:G:H1'  | 1        | 0.3           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1042) | 1:20:A:A:H3'  | 1:21:A:C:H5'' | 3        | 0.3           |
| (1,989)  | 1:20:A:A:H2'  | 1:21:A:C:H5   | 7        | 0.3           |
| (1,956)  | 1:14:A:U:H1'  | 1:15:A:C:H5'' | 1        | 0.3           |
| (1,877)  | 1:22:A:U:H5'' | 1:21:A:C:H4'  | 10       | 0.3           |
| (1,875)  | 1:28:A:U:H5   | 1:27:A:C:H4'  | 10       | 0.3           |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4'  | 4        | 0.3           |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4'  | 5        | 0.3           |
| (1,864)  | 1:46:A:U:H1'  | 1:47:A:C:H4'  | 2        | 0.3           |
| (1,864)  | 1:46:A:U:H1'  | 1:47:A:C:H4'  | 10       | 0.3           |
| (1,852)  | 1:20:A:A:H2'  | 1:21:A:C:H6   | 5        | 0.3           |
| (1,678)  | 1:54:A:C:H4'  | 1:54:A:C:H6   | 2        | 0.3           |
| (1,664)  | 1:58:A:G:H4'  | 1:59:A:U:H4'  | 5        | 0.3           |
| (1,632)  | 1:29:A:A:H4'  | 1:28:A:U:H3'  | 7        | 0.3           |
| (1,627)  | 1:47:A:C:H6   | 1:46:A:U:H2'  | 2        | 0.3           |
| (1,419)  | 1:19:A:C:H2'  | 1:20:A:A:H3'  | 6        | 0.3           |
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 4        | 0.3           |
| (1,394)  | 1:9:A:G:H2'   | 1:8:A:A:H2    | 10       | 0.3           |
| (1,373)  | 1:23:A:C:H3'  | 1:24:A:A:H1'  | 8        | 0.3           |
| (1,321)  | 1:26:A:A:H3'  | 1:26:A:A:H2   | 7        | 0.3           |
| (1,213)  | 1:26:A:A:H8   | 1:26:A:A:H3'  | 2        | 0.3           |
| (1,213)  | 1:26:A:A:H8   | 1:26:A:A:H3'  | 5        | 0.3           |
| (1,176)  | 1:25:A:A:H5'  | 1:25:A:A:H8   | 6        | 0.3           |
| (1,170)  | 1:3:A:A:H1'   | 1:4:A:A:H8    | 3        | 0.3           |
| (1,170)  | 1:3:A:A:H1'   | 1:4:A:A:H8    | 5        | 0.3           |
| (1,170)  | 1:3:A:A:H1'   | 1:4:A:A:H8    | 9        | 0.3           |
| (1,149)  | 1:50:A:A:H8   | 1:47:A:C:H5'  | 5        | 0.3           |
| (1,149)  | 1:50:A:A:H8   | 1:47:A:C:H5'' | 5        | 0.3           |
| (1,139)  | 1:42:A:U:H3'  | 1:43:A:C:H6   | 6        | 0.3           |
| (1,3)    | 1:41:A:G:H4'  | 1:40:A:A:H1'  | 1        | 0.3           |
| (1,1308) | 1:18:A:C:H5   | 1:17:A:G:H5'  | 5        | 0.29          |
| (1,1297) | 1:8:A:A:H4'   | 1:9:A:G:H5''  | 8        | 0.29          |
| (1,1225) | 1:47:A:C:H2'  | 1:49:A:G:H4'  | 5        | 0.29          |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 3        | 0.29          |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 5        | 0.29          |
| (1,1206) | 1:8:A:A:H1'   | 1:9:A:G:H1'   | 8        | 0.29          |
| (1,1052) | 1:46:A:U:H2'  | 1:47:A:C:H3'  | 10       | 0.29          |
| (1,1027) | 1:37:A:G:H8   | 1:36:A:C:H1'  | 6        | 0.29          |
| (1,1000) | 1:20:A:A:H8   | 1:19:A:C:H1'  | 1        | 0.29          |
| (1,1000) | 1:20:A:A:H8   | 1:19:A:C:H1'  | 5        | 0.29          |
| (1,1000) | 1:20:A:A:H8   | 1:19:A:C:H1'  | 7        | 0.29          |
| (1,1000) | 1:20:A:A:H8   | 1:19:A:C:H1'  | 8        | 0.29          |
| (1,1000) | 1:20:A:A:H8   | 1:19:A:C:H1'  | 10       | 0.29          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,913)  | 1:40:A:A:H8   | 1:39:A:C:H2'  | 5        | 0.29          |
| (1,910)  | 1:44:A:A:H1'  | 1:43:A:C:H2'  | 9        | 0.29          |
| (1,908)  | 1:20:A:A:H8   | 1:19:A:C:H2'  | 8        | 0.29          |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2'  | 2        | 0.29          |
| (1,906)  | 1:24:A:A:H8   | 1:23:A:C:H2'  | 6        | 0.29          |
| (1,882)  | 1:11:A:G:H1'  | 1:12:A:C:H4'  | 5        | 0.29          |
| (1,877)  | 1:22:A:U:H5'' | 1:21:A:C:H4'  | 1        | 0.29          |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4'  | 9        | 0.29          |
| (1,868)  | 1:24:A:A:H8   | 1:23:A:C:H4'  | 1        | 0.29          |
| (1,864)  | 1:46:A:U:H1'  | 1:47:A:C:H4'  | 4        | 0.29          |
| (1,852)  | 1:20:A:A:H2'  | 1:21:A:C:H6   | 8        | 0.29          |
| (1,627)  | 1:47:A:C:H6   | 1:46:A:U:H2'  | 3        | 0.29          |
| (1,627)  | 1:47:A:C:H6   | 1:46:A:U:H2'  | 6        | 0.29          |
| (1,627)  | 1:47:A:C:H6   | 1:46:A:U:H2'  | 9        | 0.29          |
| (1,434)  | 1:51:A:U:H5   | 1:52:A:A:H8   | 5        | 0.29          |
| (1,434)  | 1:51:A:U:H5   | 1:52:A:A:H8   | 6        | 0.29          |
| (1,434)  | 1:51:A:U:H5   | 1:52:A:A:H8   | 7        | 0.29          |
| (1,425)  | 1:49:A:G:H4'  | 1:50:A:A:H4'  | 7        | 0.29          |
| (1,407)  | 1:23:A:C:H1'  | 1:24:A:A:H5'' | 6        | 0.29          |
| (1,396)  | 1:51:A:U:H3'  | 1:50:A:A:H1'  | 8        | 0.29          |
| (1,394)  | 1:9:A:G:H2'   | 1:8:A:A:H2    | 3        | 0.29          |
| (1,236)  | 1:8:A:A:H5''  | 1:8:A:A:H1'   | 10       | 0.29          |
| (1,213)  | 1:26:A:A:H8   | 1:26:A:A:H3'  | 9        | 0.29          |
| (1,209)  | 1:24:A:A:H8   | 1:24:A:A:H2'  | 3        | 0.29          |
| (1,170)  | 1:3:A:A:H1'   | 1:4:A:A:H8    | 2        | 0.29          |
| (1,168)  | 1:50:A:A:H3'  | 1:50:A:A:H8   | 8        | 0.29          |
| (1,163)  | 1:49:A:G:H2'  | 1:47:A:C:H3'  | 4        | 0.29          |
| (1,104)  | 1:21:A:C:H5   | 1:20:A:A:H4'  | 7        | 0.29          |
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 7        | 0.28          |
| (1,1308) | 1:18:A:C:H5   | 1:17:A:G:H5'  | 8        | 0.28          |
| (1,1308) | 1:18:A:C:H5   | 1:17:A:G:H5'  | 10       | 0.28          |
| (1,1297) | 1:8:A:A:H4'   | 1:9:A:G:H5''  | 4        | 0.28          |
| (1,1290) | 1:31:A:A:H1'  | 1:32:A:G:H5'' | 3        | 0.28          |
| (1,1290) | 1:31:A:A:H1'  | 1:32:A:G:H5'' | 10       | 0.28          |
| (1,1223) | 1:50:A:A:H8   | 1:49:A:G:H4'  | 8        | 0.28          |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 6        | 0.28          |
| (1,1213) | 1:6:A:A:H8    | 1:5:A:G:H1'   | 7        | 0.28          |
| (1,1203) | 1:59:A:U:H3'  | 1:58:A:G:H1'  | 7        | 0.28          |
| (1,1108) | 1:2:A:G:H8    | 1:2:A:G:H2'   | 5        | 0.28          |
| (1,1000) | 1:20:A:A:H8   | 1:19:A:C:H1'  | 6        | 0.28          |
| (1,992)  | 1:28:A:U:H6   | 1:27:A:C:H5   | 5        | 0.28          |
| (1,989)  | 1:20:A:A:H2'  | 1:21:A:C:H5   | 4        | 0.28          |

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| Key      | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,956)  | 1:14:A:U:H1' | 1:15:A:C:H5'' | 7        | 0.28          |
| (1,913)  | 1:40:A:A:H8  | 1:39:A:C:H2'  | 2        | 0.28          |
| (1,910)  | 1:44:A:A:H1' | 1:43:A:C:H2'  | 8        | 0.28          |
| (1,900)  | 1:28:A:U:H3' | 1:27:A:C:H2'  | 4        | 0.28          |
| (1,870)  | 1:28:A:U:H6  | 1:27:A:C:H4'  | 5        | 0.28          |
| (1,868)  | 1:24:A:A:H8  | 1:23:A:C:H4'  | 6        | 0.28          |
| (1,825)  | 1:16:A:G:H5' | 1:15:A:C:H1'  | 8        | 0.28          |
| (1,682)  | 1:55:A:C:H2' | 1:55:A:C:H6   | 2        | 0.28          |
| (1,635)  | 1:54:A:C:H6  | 1:53:A:U:H3'  | 4        | 0.28          |
| (1,606)  | 1:54:A:C:H5  | 1:53:A:U:H1'  | 8        | 0.28          |
| (1,606)  | 1:54:A:C:H5  | 1:53:A:U:H1'  | 10       | 0.28          |
| (1,587)  | 1:29:A:A:H4' | 1:28:A:U:H6   | 2        | 0.28          |
| (1,515)  | 1:22:A:U:H5' | 1:22:A:U:H3'  | 2        | 0.28          |
| (1,434)  | 1:51:A:U:H5  | 1:52:A:A:H8   | 4        | 0.28          |
| (1,434)  | 1:51:A:U:H5  | 1:52:A:A:H8   | 8        | 0.28          |
| (1,425)  | 1:49:A:G:H4' | 1:50:A:A:H4'  | 5        | 0.28          |
| (1,391)  | 1:27:A:C:H5  | 1:26:A:A:H2   | 2        | 0.28          |
| (1,391)  | 1:27:A:C:H5  | 1:26:A:A:H2   | 3        | 0.28          |
| (1,381)  | 1:30:A:C:H4' | 1:29:A:A:H1'  | 8        | 0.28          |
| (1,373)  | 1:23:A:C:H3' | 1:24:A:A:H1'  | 2        | 0.28          |
| (1,373)  | 1:23:A:C:H3' | 1:24:A:A:H1'  | 7        | 0.28          |
| (1,373)  | 1:23:A:C:H3' | 1:24:A:A:H1'  | 9        | 0.28          |
| (1,373)  | 1:23:A:C:H3' | 1:24:A:A:H1'  | 10       | 0.28          |
| (1,352)  | 1:27:A:C:H5  | 1:26:A:A:H2'  | 2        | 0.28          |
| (1,352)  | 1:27:A:C:H5  | 1:26:A:A:H2'  | 9        | 0.28          |
| (1,332)  | 1:2:A:G:H3'  | 1:3:A:A:H8    | 3        | 0.28          |
| (1,332)  | 1:2:A:G:H3'  | 1:3:A:A:H8    | 4        | 0.28          |
| (1,309)  | 1:50:A:A:H2' | 1:50:A:A:H8   | 9        | 0.28          |
| (1,209)  | 1:24:A:A:H8  | 1:24:A:A:H2'  | 4        | 0.28          |
| (1,202)  | 1:4:A:A:H8   | 1:4:A:A:H2'   | 2        | 0.28          |
| (1,180)  | 1:25:A:A:H1' | 1:26:A:A:H8   | 5        | 0.28          |
| (1,1317) | 1:59:A:U:H5  | 1:58:A:G:H3'  | 8        | 0.27          |
| (1,1297) | 1:8:A:A:H4'  | 1:9:A:G:H5''  | 10       | 0.27          |
| (1,1290) | 1:31:A:A:H1' | 1:32:A:G:H5'' | 4        | 0.27          |
| (1,1203) | 1:59:A:U:H3' | 1:58:A:G:H1'  | 5        | 0.27          |
| (1,1108) | 1:2:A:G:H8   | 1:2:A:G:H2'   | 4        | 0.27          |
| (1,1108) | 1:2:A:G:H8   | 1:2:A:G:H2'   | 6        | 0.27          |
| (1,1108) | 1:2:A:G:H8   | 1:2:A:G:H2'   | 10       | 0.27          |
| (1,1098) | 1:16:A:G:H8  | 1:16:A:G:H2'  | 7        | 0.27          |
| (1,1098) | 1:16:A:G:H8  | 1:16:A:G:H2'  | 8        | 0.27          |
| (1,1052) | 1:46:A:U:H2' | 1:47:A:C:H3'  | 4        | 0.27          |
| (1,1026) | 1:50:A:A:H4' | 1:47:A:C:H1'  | 10       | 0.27          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,989)  | 1:20:A:A:H2'  | 1:21:A:C:H5   | 1        | 0.27          |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5   | 9        | 0.27          |
| (1,956)  | 1:14:A:U:H1'  | 1:15:A:C:H5'' | 8        | 0.27          |
| (1,913)  | 1:40:A:A:H8   | 1:39:A:C:H2'  | 1        | 0.27          |
| (1,913)  | 1:40:A:A:H8   | 1:39:A:C:H2'  | 9        | 0.27          |
| (1,882)  | 1:11:A:G:H1'  | 1:12:A:C:H4'  | 2        | 0.27          |
| (1,882)  | 1:11:A:G:H1'  | 1:12:A:C:H4'  | 10       | 0.27          |
| (1,878)  | 1:26:A:A:H2'  | 1:27:A:C:H4'  | 5        | 0.27          |
| (1,873)  | 1:20:A:A:H1'  | 1:21:A:C:H4'  | 1        | 0.27          |
| (1,868)  | 1:24:A:A:H8   | 1:23:A:C:H4'  | 4        | 0.27          |
| (1,868)  | 1:24:A:A:H8   | 1:23:A:C:H4'  | 9        | 0.27          |
| (1,852)  | 1:20:A:A:H2'  | 1:21:A:C:H6   | 6        | 0.27          |
| (1,830)  | 1:42:A:U:H2'  | 1:43:A:C:H6   | 9        | 0.27          |
| (1,825)  | 1:16:A:G:H5'  | 1:15:A:C:H1'  | 2        | 0.27          |
| (1,825)  | 1:16:A:G:H5'  | 1:15:A:C:H1'  | 4        | 0.27          |
| (1,606)  | 1:54:A:C:H5   | 1:53:A:U:H1'  | 4        | 0.27          |
| (1,541)  | 1:53:A:U:H4'  | 1:53:A:U:H5'  | 3        | 0.27          |
| (1,506)  | 1:28:A:U:H6   | 1:28:A:U:H3'  | 2        | 0.27          |
| (1,424)  | 1:49:A:G:H2'  | 1:50:A:A:H4'  | 5        | 0.27          |
| (1,396)  | 1:51:A:U:H3'  | 1:50:A:A:H1'  | 3        | 0.27          |
| (1,394)  | 1:9:A:G:H2'   | 1:8:A:A:H2    | 1        | 0.27          |
| (1,394)  | 1:9:A:G:H2'   | 1:8:A:A:H2    | 9        | 0.27          |
| (1,391)  | 1:27:A:C:H5   | 1:26:A:A:H2   | 5        | 0.27          |
| (1,381)  | 1:30:A:C:H4'  | 1:29:A:A:H1'  | 4        | 0.27          |
| (1,373)  | 1:23:A:C:H3'  | 1:24:A:A:H1'  | 1        | 0.27          |
| (1,373)  | 1:23:A:C:H3'  | 1:24:A:A:H1'  | 3        | 0.27          |
| (1,373)  | 1:23:A:C:H3'  | 1:24:A:A:H1'  | 5        | 0.27          |
| (1,352)  | 1:27:A:C:H5   | 1:26:A:A:H2'  | 5        | 0.27          |
| (1,352)  | 1:27:A:C:H5   | 1:26:A:A:H2'  | 6        | 0.27          |
| (1,352)  | 1:27:A:C:H5   | 1:26:A:A:H2'  | 7        | 0.27          |
| (1,352)  | 1:27:A:C:H5   | 1:26:A:A:H2'  | 10       | 0.27          |
| (1,332)  | 1:2:A:G:H3'   | 1:3:A:A:H8    | 10       | 0.27          |
| (1,321)  | 1:26:A:A:H3'  | 1:26:A:A:H2   | 5        | 0.27          |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 1        | 0.27          |
| (1,202)  | 1:4:A:A:H8    | 1:4:A:A:H2'   | 10       | 0.27          |
| (1,176)  | 1:25:A:A:H5'  | 1:25:A:A:H8   | 4        | 0.27          |
| (1,170)  | 1:3:A:A:H1'   | 1:4:A:A:H8    | 10       | 0.27          |
| (1,169)  | 1:3:A:A:H2'   | 1:3:A:A:H8    | 1        | 0.27          |
| (1,104)  | 1:21:A:C:H5   | 1:20:A:A:H4'  | 4        | 0.27          |
| (1,1330) | 1:38:A:C:H5   | 1:37:A:G:H3'  | 7        | 0.26          |
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 8        | 0.26          |
| (1,1297) | 1:8:A:A:H4'   | 1:9:A:G:H5''  | 2        | 0.26          |

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| Key      | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,1297) | 1:8:A:A:H4'  | 1:9:A:G:H5''  | 3        | 0.26          |
| (1,1297) | 1:8:A:A:H4'  | 1:9:A:G:H5''  | 9        | 0.26          |
| (1,1227) | 1:33:A:A:H8  | 1:32:A:G:H4'  | 3        | 0.26          |
| (1,1161) | 1:15:A:C:H3' | 1:16:A:G:H8   | 1        | 0.26          |
| (1,1161) | 1:15:A:C:H3' | 1:16:A:G:H8   | 9        | 0.26          |
| (1,1108) | 1:2:A:G:H8   | 1:2:A:G:H2'   | 2        | 0.26          |
| (1,989)  | 1:20:A:A:H2' | 1:21:A:C:H5   | 9        | 0.26          |
| (1,962)  | 1:44:A:A:H8  | 1:45:A:C:H5'  | 10       | 0.26          |
| (1,913)  | 1:40:A:A:H8  | 1:39:A:C:H2'  | 6        | 0.26          |
| (1,913)  | 1:40:A:A:H8  | 1:39:A:C:H2'  | 8        | 0.26          |
| (1,910)  | 1:44:A:A:H1' | 1:43:A:C:H2'  | 3        | 0.26          |
| (1,901)  | 1:22:A:U:H3' | 1:21:A:C:H2'  | 4        | 0.26          |
| (1,901)  | 1:22:A:U:H3' | 1:21:A:C:H2'  | 10       | 0.26          |
| (1,885)  | 1:37:A:G:H2' | 1:38:A:C:H4'  | 9        | 0.26          |
| (1,882)  | 1:11:A:G:H1' | 1:12:A:C:H4'  | 4        | 0.26          |
| (1,882)  | 1:11:A:G:H1' | 1:12:A:C:H4'  | 6        | 0.26          |
| (1,878)  | 1:26:A:A:H2' | 1:27:A:C:H4'  | 6        | 0.26          |
| (1,868)  | 1:24:A:A:H8  | 1:23:A:C:H4'  | 3        | 0.26          |
| (1,868)  | 1:24:A:A:H8  | 1:23:A:C:H4'  | 7        | 0.26          |
| (1,825)  | 1:16:A:G:H5' | 1:15:A:C:H1'  | 10       | 0.26          |
| (1,682)  | 1:55:A:C:H2' | 1:55:A:C:H6   | 4        | 0.26          |
| (1,678)  | 1:54:A:C:H4' | 1:54:A:C:H6   | 7        | 0.26          |
| (1,658)  | 1:27:A:C:H4' | 1:28:A:U:H5'' | 9        | 0.26          |
| (1,631)  | 1:29:A:A:H8  | 1:28:A:U:H3'  | 1        | 0.26          |
| (1,627)  | 1:47:A:C:H6  | 1:46:A:U:H2'  | 4        | 0.26          |
| (1,621)  | 1:54:A:C:H6  | 1:53:A:U:H2'  | 1        | 0.26          |
| (1,435)  | 1:30:A:C:H2' | 1:31:A:A:H5'' | 2        | 0.26          |
| (1,434)  | 1:51:A:U:H5  | 1:52:A:A:H8   | 9        | 0.26          |
| (1,394)  | 1:9:A:G:H2'  | 1:8:A:A:H2    | 4        | 0.26          |
| (1,394)  | 1:9:A:G:H2'  | 1:8:A:A:H2    | 5        | 0.26          |
| (1,391)  | 1:27:A:C:H5  | 1:26:A:A:H2   | 7        | 0.26          |
| (1,391)  | 1:27:A:C:H5  | 1:26:A:A:H2   | 10       | 0.26          |
| (1,332)  | 1:2:A:G:H3'  | 1:3:A:A:H8    | 8        | 0.26          |
| (1,236)  | 1:8:A:A:H5'' | 1:8:A:A:H1'   | 9        | 0.26          |
| (1,209)  | 1:24:A:A:H8  | 1:24:A:A:H2'  | 6        | 0.26          |
| (1,149)  | 1:50:A:A:H8  | 1:47:A:C:H5'  | 1        | 0.26          |
| (1,149)  | 1:50:A:A:H8  | 1:47:A:C:H5'' | 1        | 0.26          |
| (1,104)  | 1:21:A:C:H5  | 1:20:A:A:H4'  | 5        | 0.26          |
| (1,1330) | 1:38:A:C:H5  | 1:37:A:G:H3'  | 3        | 0.25          |
| (1,1317) | 1:59:A:U:H5  | 1:58:A:G:H3'  | 5        | 0.25          |
| (1,1297) | 1:8:A:A:H4'  | 1:9:A:G:H5''  | 5        | 0.25          |
| (1,1168) | 1:31:A:A:H1' | 1:32:A:G:H8   | 2        | 0.25          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1161) | 1:15:A:C:H3'  | 1:16:A:G:H8   | 2        | 0.25          |
| (1,1161) | 1:15:A:C:H3'  | 1:16:A:G:H8   | 5        | 0.25          |
| (1,1161) | 1:15:A:C:H3'  | 1:16:A:G:H8   | 8        | 0.25          |
| (1,1098) | 1:16:A:G:H8   | 1:16:A:G:H2'  | 4        | 0.25          |
| (1,1055) | 1:56:A:U:H4'  | 1:55:A:C:H3'  | 7        | 0.25          |
| (1,1050) | 1:31:A:A:H5'  | 1:30:A:C:H6   | 3        | 0.25          |
| (1,1048) | 1:44:A:A:H1'  | 1:54:A:C:H5   | 2        | 0.25          |
| (1,1013) | 1:24:A:A:H8   | 1:23:A:C:H1'  | 7        | 0.25          |
| (1,989)  | 1:20:A:A:H2'  | 1:21:A:C:H5   | 10       | 0.25          |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5   | 3        | 0.25          |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5   | 6        | 0.25          |
| (1,962)  | 1:44:A:A:H8   | 1:45:A:C:H5'  | 4        | 0.25          |
| (1,956)  | 1:14:A:U:H1'  | 1:15:A:C:H5'' | 9        | 0.25          |
| (1,908)  | 1:20:A:A:H8   | 1:19:A:C:H2'  | 6        | 0.25          |
| (1,895)  | 1:31:A:A:H8   | 1:30:A:C:H2'  | 1        | 0.25          |
| (1,895)  | 1:31:A:A:H8   | 1:30:A:C:H2'  | 9        | 0.25          |
| (1,882)  | 1:11:A:G:H1'  | 1:12:A:C:H4'  | 7        | 0.25          |
| (1,882)  | 1:11:A:G:H1'  | 1:12:A:C:H4'  | 8        | 0.25          |
| (1,882)  | 1:11:A:G:H1'  | 1:12:A:C:H4'  | 9        | 0.25          |
| (1,862)  | 1:53:A:U:H4'  | 1:54:A:C:H4'  | 3        | 0.25          |
| (1,860)  | 1:37:A:G:H4'  | 1:36:A:C:H4'  | 5        | 0.25          |
| (1,825)  | 1:16:A:G:H5'  | 1:15:A:C:H1'  | 5        | 0.25          |
| (1,825)  | 1:16:A:G:H5'  | 1:15:A:C:H1'  | 7        | 0.25          |
| (1,819)  | 1:43:A:C:H6   | 1:43:A:C:H1'  | 6        | 0.25          |
| (1,770)  | 1:21:A:C:H6   | 1:21:A:C:H5'' | 4        | 0.25          |
| (1,715)  | 1:36:A:C:H5'  | 1:36:A:C:H3'  | 7        | 0.25          |
| (1,659)  | 1:50:A:A:H2'  | 1:51:A:U:H4'  | 1        | 0.25          |
| (1,658)  | 1:27:A:C:H4'  | 1:28:A:U:H5'' | 2        | 0.25          |
| (1,587)  | 1:29:A:A:H4'  | 1:28:A:U:H6   | 9        | 0.25          |
| (1,541)  | 1:53:A:U:H4'  | 1:53:A:U:H5'  | 4        | 0.25          |
| (1,445)  | 1:53:A:U:H5'' | 1:53:A:U:H6   | 2        | 0.25          |
| (1,434)  | 1:51:A:U:H5   | 1:52:A:A:H8   | 2        | 0.25          |
| (1,391)  | 1:27:A:C:H5   | 1:26:A:A:H2   | 1        | 0.25          |
| (1,391)  | 1:27:A:C:H5   | 1:26:A:A:H2   | 9        | 0.25          |
| (1,381)  | 1:30:A:C:H4'  | 1:29:A:A:H1'  | 1        | 0.25          |
| (1,373)  | 1:23:A:C:H3'  | 1:24:A:A:H1'  | 6        | 0.25          |
| (1,352)  | 1:27:A:C:H5   | 1:26:A:A:H2'  | 3        | 0.25          |
| (1,236)  | 1:8:A:A:H5''  | 1:8:A:A:H1'   | 3        | 0.25          |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 7        | 0.25          |
| (1,194)  | 1:52:A:A:H5'  | 1:52:A:A:H4'  | 1        | 0.25          |
| (1,180)  | 1:25:A:A:H1'  | 1:26:A:A:H8   | 8        | 0.25          |
| (1,146)  | 1:24:A:A:H3'  | 1:23:A:C:H3'  | 9        | 0.25          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,109)  | 1:27:A:C:H3'  | 1:26:A:A:H3'  | 1        | 0.25          |
| (1,109)  | 1:27:A:C:H3'  | 1:26:A:A:H3'  | 2        | 0.25          |
| (1,109)  | 1:27:A:C:H4'  | 1:26:A:A:H3'  | 4        | 0.25          |
| (1,1308) | 1:18:A:C:H5   | 1:17:A:G:H5'  | 3        | 0.24          |
| (1,1269) | 1:18:A:C:H6   | 1:17:A:G:H3'  | 2        | 0.24          |
| (1,1266) | 1:50:A:A:H8   | 1:49:A:G:H2'  | 8        | 0.24          |
| (1,1225) | 1:47:A:C:H2'  | 1:49:A:G:H4'  | 2        | 0.24          |
| (1,1161) | 1:15:A:C:H3'  | 1:16:A:G:H8   | 3        | 0.24          |
| (1,1161) | 1:15:A:C:H3'  | 1:16:A:G:H8   | 4        | 0.24          |
| (1,1161) | 1:15:A:C:H3'  | 1:16:A:G:H8   | 7        | 0.24          |
| (1,1161) | 1:15:A:C:H3'  | 1:16:A:G:H8   | 10       | 0.24          |
| (1,1098) | 1:16:A:G:H8   | 1:16:A:G:H2'  | 5        | 0.24          |
| (1,1098) | 1:16:A:G:H8   | 1:16:A:G:H2'  | 6        | 0.24          |
| (1,1052) | 1:46:A:U:H2'  | 1:47:A:C:H3'  | 2        | 0.24          |
| (1,1027) | 1:37:A:G:H8   | 1:36:A:C:H1'  | 3        | 0.24          |
| (1,1013) | 1:24:A:A:H8   | 1:23:A:C:H1'  | 9        | 0.24          |
| (1,999)  | 1:14:A:U:H1'  | 1:15:A:C:H5   | 6        | 0.24          |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5   | 7        | 0.24          |
| (1,962)  | 1:44:A:A:H8   | 1:45:A:C:H5'  | 2        | 0.24          |
| (1,913)  | 1:40:A:A:H8   | 1:39:A:C:H2'  | 10       | 0.24          |
| (1,908)  | 1:20:A:A:H8   | 1:19:A:C:H2'  | 10       | 0.24          |
| (1,900)  | 1:28:A:U:H3'  | 1:27:A:C:H2'  | 5        | 0.24          |
| (1,895)  | 1:31:A:A:H8   | 1:30:A:C:H2'  | 6        | 0.24          |
| (1,882)  | 1:11:A:G:H1'  | 1:12:A:C:H4'  | 3        | 0.24          |
| (1,877)  | 1:22:A:U:H5'' | 1:21:A:C:H4'  | 3        | 0.24          |
| (1,862)  | 1:53:A:U:H4'  | 1:54:A:C:H4'  | 6        | 0.24          |
| (1,861)  | 1:53:A:U:H3'  | 1:54:A:C:H4'  | 9        | 0.24          |
| (1,859)  | 1:37:A:G:H8   | 1:36:A:C:H4'  | 3        | 0.24          |
| (1,848)  | 1:20:A:A:H1'  | 1:21:A:C:H6   | 1        | 0.24          |
| (1,830)  | 1:42:A:U:H2'  | 1:43:A:C:H6   | 3        | 0.24          |
| (1,825)  | 1:16:A:G:H5'  | 1:15:A:C:H1'  | 1        | 0.24          |
| (1,825)  | 1:16:A:G:H5'  | 1:15:A:C:H1'  | 6        | 0.24          |
| (1,823)  | 1:46:A:U:H4'  | 1:47:A:C:H6   | 4        | 0.24          |
| (1,819)  | 1:43:A:C:H6   | 1:43:A:C:H1'  | 2        | 0.24          |
| (1,819)  | 1:43:A:C:H6   | 1:43:A:C:H1'  | 8        | 0.24          |
| (1,815)  | 1:39:A:C:H5   | 1:39:A:C:H5'' | 3        | 0.24          |
| (1,770)  | 1:21:A:C:H6   | 1:21:A:C:H5'' | 6        | 0.24          |
| (1,682)  | 1:55:A:C:H2'  | 1:55:A:C:H6   | 1        | 0.24          |
| (1,678)  | 1:54:A:C:H4'  | 1:54:A:C:H6   | 4        | 0.24          |
| (1,668)  | 1:54:A:C:H6   | 1:53:A:U:H4'  | 4        | 0.24          |
| (1,665)  | 1:54:A:C:H6   | 1:53:A:U:H6   | 3        | 0.24          |
| (1,634)  | 1:29:A:A:H5'' | 1:28:A:U:H3'  | 5        | 0.24          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,506)  | 1:28:A:U:H6   | 1:28:A:U:H3'  | 10       | 0.24          |
| (1,434)  | 1:51:A:U:H5   | 1:52:A:A:H8   | 1        | 0.24          |
| (1,420)  | 1:51:A:U:H2'  | 1:50:A:A:H2   | 5        | 0.24          |
| (1,410)  | 1:2:A:G:H3'   | 1:3:A:A:H5'   | 1        | 0.24          |
| (1,410)  | 1:2:A:G:H3'   | 1:3:A:A:H5'   | 5        | 0.24          |
| (1,391)  | 1:27:A:C:H5   | 1:26:A:A:H2   | 6        | 0.24          |
| (1,291)  | 1:24:A:A:H8   | 1:24:A:A:H5'' | 2        | 0.24          |
| (1,257)  | 1:7:A:A:H3'   | 1:6:A:A:H2    | 2        | 0.24          |
| (1,257)  | 1:7:A:A:H3'   | 1:6:A:A:H2    | 7        | 0.24          |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 3        | 0.24          |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 4        | 0.24          |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 8        | 0.24          |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 9        | 0.24          |
| (1,209)  | 1:24:A:A:H8   | 1:24:A:A:H2'  | 7        | 0.24          |
| (1,203)  | 1:40:A:A:H8   | 1:40:A:A:H2'  | 6        | 0.24          |
| (1,194)  | 1:52:A:A:H5'  | 1:52:A:A:H4'  | 7        | 0.24          |
| (1,180)  | 1:25:A:A:H1'  | 1:26:A:A:H8   | 4        | 0.24          |
| (1,134)  | 1:50:A:A:H8   | 1:49:A:G:H5'  | 1        | 0.24          |
| (1,134)  | 1:50:A:A:H8   | 1:49:A:G:H5'' | 1        | 0.24          |
| (1,3)    | 1:41:A:G:H4'  | 1:40:A:A:H1'  | 6        | 0.24          |
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 3        | 0.23          |
| (1,1288) | 1:15:A:C:H5'  | 1:16:A:G:H5'' | 8        | 0.23          |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 4        | 0.23          |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 5        | 0.23          |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 6        | 0.23          |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 7        | 0.23          |
| (1,1268) | 1:42:A:U:H6   | 1:41:A:G:H3'  | 9        | 0.23          |
| (1,1227) | 1:33:A:A:H8   | 1:32:A:G:H4'  | 6        | 0.23          |
| (1,1227) | 1:33:A:A:H8   | 1:32:A:G:H4'  | 10       | 0.23          |
| (1,1218) | 1:31:A:A:H3'  | 1:32:A:G:H8   | 9        | 0.23          |
| (1,1211) | 1:50:A:A:H8   | 1:49:A:G:H1'  | 4        | 0.23          |
| (1,1168) | 1:31:A:A:H1'  | 1:32:A:G:H8   | 8        | 0.23          |
| (1,1161) | 1:15:A:C:H3'  | 1:16:A:G:H8   | 6        | 0.23          |
| (1,1098) | 1:16:A:G:H8   | 1:16:A:G:H2'  | 1        | 0.23          |
| (1,1055) | 1:56:A:U:H4'  | 1:55:A:C:H3'  | 6        | 0.23          |
| (1,1050) | 1:31:A:A:H5'  | 1:30:A:C:H6   | 2        | 0.23          |
| (1,1039) | 1:29:A:A:H3'  | 1:30:A:C:H5'  | 4        | 0.23          |
| (1,1013) | 1:24:A:A:H8   | 1:23:A:C:H1'  | 1        | 0.23          |
| (1,1013) | 1:24:A:A:H8   | 1:23:A:C:H1'  | 8        | 0.23          |
| (1,999)  | 1:14:A:U:H1'  | 1:15:A:C:H5   | 9        | 0.23          |
| (1,962)  | 1:44:A:A:H8   | 1:45:A:C:H5'  | 3        | 0.23          |
| (1,962)  | 1:44:A:A:H8   | 1:45:A:C:H5'  | 6        | 0.23          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,954)  | 1:37:A:G:H3'  | 1:38:A:C:H3'  | 9        | 0.23          |
| (1,927)  | 1:44:A:A:H8   | 1:43:A:C:H3'  | 7        | 0.23          |
| (1,913)  | 1:40:A:A:H8   | 1:39:A:C:H2'  | 7        | 0.23          |
| (1,910)  | 1:44:A:A:H1'  | 1:43:A:C:H2'  | 10       | 0.23          |
| (1,908)  | 1:20:A:A:H8   | 1:19:A:C:H2'  | 9        | 0.23          |
| (1,901)  | 1:22:A:U:H3'  | 1:21:A:C:H2'  | 5        | 0.23          |
| (1,895)  | 1:31:A:A:H8   | 1:30:A:C:H2'  | 10       | 0.23          |
| (1,883)  | 1:13:A:U:H5   | 1:12:A:C:H4'  | 3        | 0.23          |
| (1,883)  | 1:13:A:U:H5   | 1:12:A:C:H4'  | 7        | 0.23          |
| (1,883)  | 1:13:A:U:H5   | 1:12:A:C:H4'  | 10       | 0.23          |
| (1,871)  | 1:31:A:A:H8   | 1:30:A:C:H4'  | 7        | 0.23          |
| (1,868)  | 1:24:A:A:H8   | 1:23:A:C:H4'  | 8        | 0.23          |
| (1,848)  | 1:20:A:A:H1'  | 1:21:A:C:H6   | 3        | 0.23          |
| (1,825)  | 1:16:A:G:H5'  | 1:15:A:C:H1'  | 3        | 0.23          |
| (1,825)  | 1:16:A:G:H5'  | 1:15:A:C:H1'  | 9        | 0.23          |
| (1,770)  | 1:21:A:C:H6   | 1:21:A:C:H5'' | 1        | 0.23          |
| (1,770)  | 1:21:A:C:H6   | 1:21:A:C:H5'' | 3        | 0.23          |
| (1,770)  | 1:21:A:C:H6   | 1:21:A:C:H5'' | 7        | 0.23          |
| (1,682)  | 1:55:A:C:H2'  | 1:55:A:C:H6   | 6        | 0.23          |
| (1,682)  | 1:55:A:C:H2'  | 1:55:A:C:H6   | 9        | 0.23          |
| (1,678)  | 1:54:A:C:H4'  | 1:54:A:C:H6   | 6        | 0.23          |
| (1,632)  | 1:29:A:A:H4'  | 1:28:A:U:H3'  | 8        | 0.23          |
| (1,506)  | 1:28:A:U:H6   | 1:28:A:U:H3'  | 5        | 0.23          |
| (1,473)  | 1:14:A:U:H6   | 1:14:A:U:H3'  | 7        | 0.23          |
| (1,473)  | 1:14:A:U:H6   | 1:14:A:U:H3'  | 9        | 0.23          |
| (1,435)  | 1:30:A:C:H2'  | 1:31:A:A:H5'' | 5        | 0.23          |
| (1,425)  | 1:49:A:G:H4'  | 1:50:A:A:H4'  | 9        | 0.23          |
| (1,420)  | 1:51:A:U:H2'  | 1:50:A:A:H2   | 1        | 0.23          |
| (1,419)  | 1:19:A:C:H2'  | 1:20:A:A:H3'  | 9        | 0.23          |
| (1,396)  | 1:51:A:U:H3'  | 1:50:A:A:H1'  | 4        | 0.23          |
| (1,395)  | 1:28:A:U:H4'  | 1:29:A:A:H8   | 2        | 0.23          |
| (1,321)  | 1:26:A:A:H3'  | 1:26:A:A:H2   | 8        | 0.23          |
| (1,304)  | 1:29:A:A:H8   | 1:29:A:A:H5'' | 3        | 0.23          |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 2        | 0.23          |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 5        | 0.23          |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 6        | 0.23          |
| (1,213)  | 1:26:A:A:H8   | 1:26:A:A:H3'  | 3        | 0.23          |
| (1,209)  | 1:24:A:A:H8   | 1:24:A:A:H2'  | 1        | 0.23          |
| (1,202)  | 1:4:A:A:H8    | 1:4:A:A:H2'   | 5        | 0.23          |
| (1,107)  | 1:34:A:G:H2'  | 1:35:A:A:H2'  | 4        | 0.23          |
| (1,104)  | 1:21:A:C:H5   | 1:20:A:A:H4'  | 10       | 0.23          |
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 1        | 0.22          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 2        | 0.22          |
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 5        | 0.22          |
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 9        | 0.22          |
| (1,1308) | 1:18:A:C:H5   | 1:17:A:G:H5'  | 1        | 0.22          |
| (1,1288) | 1:15:A:C:H5'  | 1:16:A:G:H5'' | 7        | 0.22          |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 8        | 0.22          |
| (1,1224) | 1:31:A:A:H1'  | 1:32:A:G:H4'  | 8        | 0.22          |
| (1,1203) | 1:59:A:U:H3'  | 1:58:A:G:H1'  | 9        | 0.22          |
| (1,1168) | 1:31:A:A:H1'  | 1:32:A:G:H8   | 7        | 0.22          |
| (1,1098) | 1:16:A:G:H8   | 1:16:A:G:H2'  | 2        | 0.22          |
| (1,1098) | 1:16:A:G:H8   | 1:16:A:G:H2'  | 3        | 0.22          |
| (1,1098) | 1:16:A:G:H8   | 1:16:A:G:H2'  | 9        | 0.22          |
| (1,1098) | 1:16:A:G:H8   | 1:16:A:G:H2'  | 10       | 0.22          |
| (1,1055) | 1:56:A:U:H4'  | 1:55:A:C:H3'  | 3        | 0.22          |
| (1,1055) | 1:56:A:U:H4'  | 1:55:A:C:H3'  | 4        | 0.22          |
| (1,1052) | 1:46:A:U:H2'  | 1:47:A:C:H3'  | 8        | 0.22          |
| (1,1050) | 1:31:A:A:H5'  | 1:30:A:C:H6   | 9        | 0.22          |
| (1,1048) | 1:44:A:A:H1'  | 1:54:A:C:H5   | 9        | 0.22          |
| (1,1046) | 1:22:A:U:H6   | 1:21:A:C:H5   | 1        | 0.22          |
| (1,1046) | 1:22:A:U:H6   | 1:21:A:C:H5   | 9        | 0.22          |
| (1,962)  | 1:44:A:A:H8   | 1:45:A:C:H5'  | 5        | 0.22          |
| (1,962)  | 1:44:A:A:H8   | 1:45:A:C:H5'  | 8        | 0.22          |
| (1,954)  | 1:37:A:G:H3'  | 1:38:A:C:H3'  | 7        | 0.22          |
| (1,938)  | 1:28:A:U:H2'  | 1:27:A:C:H3'  | 8        | 0.22          |
| (1,901)  | 1:22:A:U:H3'  | 1:21:A:C:H2'  | 3        | 0.22          |
| (1,901)  | 1:22:A:U:H3'  | 1:21:A:C:H2'  | 6        | 0.22          |
| (1,893)  | 1:22:A:U:H6   | 1:21:A:C:H2'  | 10       | 0.22          |
| (1,883)  | 1:13:A:U:H5   | 1:12:A:C:H4'  | 5        | 0.22          |
| (1,883)  | 1:13:A:U:H5   | 1:12:A:C:H4'  | 9        | 0.22          |
| (1,878)  | 1:26:A:A:H2'  | 1:27:A:C:H4'  | 3        | 0.22          |
| (1,875)  | 1:28:A:U:H5   | 1:27:A:C:H4'  | 4        | 0.22          |
| (1,875)  | 1:28:A:U:H5   | 1:27:A:C:H4'  | 6        | 0.22          |
| (1,848)  | 1:20:A:A:H1'  | 1:21:A:C:H6   | 4        | 0.22          |
| (1,848)  | 1:20:A:A:H1'  | 1:21:A:C:H6   | 5        | 0.22          |
| (1,848)  | 1:20:A:A:H1'  | 1:21:A:C:H6   | 8        | 0.22          |
| (1,848)  | 1:20:A:A:H1'  | 1:21:A:C:H6   | 9        | 0.22          |
| (1,820)  | 1:50:A:A:H8   | 1:47:A:C:H6   | 1        | 0.22          |
| (1,770)  | 1:21:A:C:H6   | 1:21:A:C:H5'' | 2        | 0.22          |
| (1,770)  | 1:21:A:C:H6   | 1:21:A:C:H5'' | 5        | 0.22          |
| (1,770)  | 1:21:A:C:H6   | 1:21:A:C:H5'' | 10       | 0.22          |
| (1,682)  | 1:55:A:C:H2'  | 1:55:A:C:H6   | 7        | 0.22          |
| (1,665)  | 1:54:A:C:H6   | 1:53:A:U:H6   | 7        | 0.22          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,664)  | 1:58:A:G:H4'  | 1:59:A:U:H4'  | 1        | 0.22          |
| (1,634)  | 1:29:A:A:H5'' | 1:28:A:U:H3'  | 10       | 0.22          |
| (1,627)  | 1:47:A:C:H6   | 1:46:A:U:H2'  | 5        | 0.22          |
| (1,621)  | 1:54:A:C:H6   | 1:53:A:U:H2'  | 4        | 0.22          |
| (1,608)  | 1:45:A:C:H3'  | 1:46:A:U:H1'  | 3        | 0.22          |
| (1,581)  | 1:45:A:C:H4'  | 1:46:A:U:H6   | 10       | 0.22          |
| (1,473)  | 1:14:A:U:H6   | 1:14:A:U:H3'  | 8        | 0.22          |
| (1,383)  | 1:5:A:G:H1'   | 1:4:A:A:H1'   | 3        | 0.22          |
| (1,381)  | 1:30:A:C:H4'  | 1:29:A:A:H1'  | 9        | 0.22          |
| (1,304)  | 1:29:A:A:H8   | 1:29:A:A:H5'' | 10       | 0.22          |
| (1,231)  | 1:24:A:A:H5'' | 1:24:A:A:H1'  | 10       | 0.22          |
| (1,213)  | 1:26:A:A:H8   | 1:26:A:A:H3'  | 1        | 0.22          |
| (1,209)  | 1:24:A:A:H8   | 1:24:A:A:H2'  | 5        | 0.22          |
| (1,209)  | 1:24:A:A:H8   | 1:24:A:A:H2'  | 10       | 0.22          |
| (1,203)  | 1:40:A:A:H8   | 1:40:A:A:H2'  | 8        | 0.22          |
| (1,201)  | 1:20:A:A:H8   | 1:20:A:A:H2'  | 4        | 0.22          |
| (1,181)  | 1:8:A:A:H3'   | 1:8:A:A:H8    | 10       | 0.22          |
| (1,168)  | 1:50:A:A:H3'  | 1:50:A:A:H8   | 10       | 0.22          |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'  | 9        | 0.22          |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'' | 9        | 0.22          |
| (1,1288) | 1:15:A:C:H5'  | 1:16:A:G:H5'' | 3        | 0.21          |
| (1,1288) | 1:15:A:C:H5'  | 1:16:A:G:H5'' | 4        | 0.21          |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 3        | 0.21          |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 9        | 0.21          |
| (1,1264) | 1:38:A:C:H6   | 1:37:A:G:H2'  | 8        | 0.21          |
| (1,1227) | 1:33:A:A:H8   | 1:32:A:G:H4'  | 9        | 0.21          |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 3        | 0.21          |
| (1,1208) | 1:3:A:A:H8    | 1:2:A:G:H1'   | 4        | 0.21          |
| (1,1202) | 1:59:A:U:H5   | 1:58:A:G:H1'  | 4        | 0.21          |
| (1,1168) | 1:31:A:A:H1'  | 1:32:A:G:H8   | 6        | 0.21          |
| (1,1146) | 1:5:A:G:H8    | 1:5:A:G:H2'   | 8        | 0.21          |
| (1,1055) | 1:56:A:U:H4'  | 1:55:A:C:H3'  | 5        | 0.21          |
| (1,1052) | 1:46:A:U:H2'  | 1:47:A:C:H3'  | 3        | 0.21          |
| (1,1052) | 1:46:A:U:H2'  | 1:47:A:C:H3'  | 9        | 0.21          |
| (1,1051) | 1:31:A:A:H5'' | 1:30:A:C:H6   | 8        | 0.21          |
| (1,1050) | 1:31:A:A:H5'  | 1:30:A:C:H6   | 4        | 0.21          |
| (1,1046) | 1:22:A:U:H6   | 1:21:A:C:H5   | 6        | 0.21          |
| (1,999)  | 1:14:A:U:H1'  | 1:15:A:C:H5   | 1        | 0.21          |
| (1,999)  | 1:14:A:U:H1'  | 1:15:A:C:H5   | 7        | 0.21          |
| (1,989)  | 1:20:A:A:H2'  | 1:21:A:C:H5   | 3        | 0.21          |
| (1,928)  | 1:42:A:U:H3'  | 1:43:A:C:H3'  | 6        | 0.21          |
| (1,908)  | 1:20:A:A:H8   | 1:19:A:C:H2'  | 1        | 0.21          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,908) | 1:20:A:A:H8   | 1:19:A:C:H2'  | 2        | 0.21          |
| (1,908) | 1:20:A:A:H8   | 1:19:A:C:H2'  | 7        | 0.21          |
| (1,901) | 1:22:A:U:H3'  | 1:21:A:C:H2'  | 1        | 0.21          |
| (1,901) | 1:22:A:U:H3'  | 1:21:A:C:H2'  | 7        | 0.21          |
| (1,883) | 1:13:A:U:H5   | 1:12:A:C:H4'  | 1        | 0.21          |
| (1,878) | 1:26:A:A:H2'  | 1:27:A:C:H4'  | 1        | 0.21          |
| (1,875) | 1:28:A:U:H5   | 1:27:A:C:H4'  | 2        | 0.21          |
| (1,864) | 1:46:A:U:H1'  | 1:47:A:C:H4'  | 9        | 0.21          |
| (1,862) | 1:53:A:U:H4'  | 1:54:A:C:H4'  | 7        | 0.21          |
| (1,860) | 1:37:A:G:H4'  | 1:36:A:C:H4'  | 1        | 0.21          |
| (1,860) | 1:37:A:G:H4'  | 1:36:A:C:H4'  | 4        | 0.21          |
| (1,860) | 1:37:A:G:H4'  | 1:36:A:C:H4'  | 8        | 0.21          |
| (1,851) | 1:29:A:A:H4'  | 1:30:A:C:H6   | 7        | 0.21          |
| (1,848) | 1:20:A:A:H1'  | 1:21:A:C:H6   | 6        | 0.21          |
| (1,848) | 1:20:A:A:H1'  | 1:21:A:C:H6   | 7        | 0.21          |
| (1,848) | 1:20:A:A:H1'  | 1:21:A:C:H6   | 10       | 0.21          |
| (1,815) | 1:39:A:C:H5   | 1:39:A:C:H5'' | 1        | 0.21          |
| (1,770) | 1:21:A:C:H6   | 1:21:A:C:H5'' | 9        | 0.21          |
| (1,678) | 1:54:A:C:H4'  | 1:54:A:C:H6   | 5        | 0.21          |
| (1,675) | 1:52:A:A:H8   | 1:51:A:U:H2'  | 7        | 0.21          |
| (1,668) | 1:54:A:C:H6   | 1:53:A:U:H4'  | 5        | 0.21          |
| (1,668) | 1:54:A:C:H6   | 1:53:A:U:H4'  | 8        | 0.21          |
| (1,635) | 1:54:A:C:H6   | 1:53:A:U:H3'  | 1        | 0.21          |
| (1,634) | 1:29:A:A:H5'' | 1:28:A:U:H3'  | 4        | 0.21          |
| (1,541) | 1:53:A:U:H4'  | 1:53:A:U:H5'  | 6        | 0.21          |
| (1,503) | 1:14:A:U:H5   | 1:14:A:U:H2'  | 4        | 0.21          |
| (1,497) | 1:42:A:U:H6   | 1:42:A:U:H2'  | 10       | 0.21          |
| (1,473) | 1:14:A:U:H6   | 1:14:A:U:H3'  | 6        | 0.21          |
| (1,444) | 1:53:A:U:H4'  | 1:53:A:U:H6   | 1        | 0.21          |
| (1,443) | 1:46:A:U:H4'  | 1:46:A:U:H6   | 1        | 0.21          |
| (1,434) | 1:51:A:U:H5   | 1:52:A:A:H8   | 3        | 0.21          |
| (1,425) | 1:49:A:G:H4'  | 1:50:A:A:H4'  | 10       | 0.21          |
| (1,396) | 1:51:A:U:H3'  | 1:50:A:A:H1'  | 10       | 0.21          |
| (1,383) | 1:5:A:G:H1'   | 1:4:A:A:H1'   | 4        | 0.21          |
| (1,373) | 1:23:A:C:H3'  | 1:24:A:A:H1'  | 4        | 0.21          |
| (1,366) | 1:9:A:G:H8    | 1:8:A:A:H3'   | 1        | 0.21          |
| (1,366) | 1:9:A:G:H8    | 1:8:A:A:H3'   | 3        | 0.21          |
| (1,366) | 1:9:A:G:H8    | 1:8:A:A:H3'   | 9        | 0.21          |
| (1,366) | 1:9:A:G:H8    | 1:8:A:A:H3'   | 10       | 0.21          |
| (1,346) | 1:23:A:C:H1'  | 1:24:A:A:H4'  | 1        | 0.21          |
| (1,340) | 1:19:A:C:H4'  | 1:20:A:A:H8   | 8        | 0.21          |
| (1,257) | 1:7:A:A:H3'   | 1:6:A:A:H2    | 1        | 0.21          |

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| Key      | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,257)  | 1:7:A:A:H3'  | 1:6:A:A:H2    | 3        | 0.21          |
| (1,257)  | 1:7:A:A:H3'  | 1:6:A:A:H2    | 6        | 0.21          |
| (1,257)  | 1:7:A:A:H3'  | 1:6:A:A:H2    | 8        | 0.21          |
| (1,209)  | 1:24:A:A:H8  | 1:24:A:A:H2'  | 2        | 0.21          |
| (1,203)  | 1:40:A:A:H8  | 1:40:A:A:H2'  | 10       | 0.21          |
| (1,168)  | 1:50:A:A:H3' | 1:50:A:A:H8   | 3        | 0.21          |
| (1,168)  | 1:50:A:A:H3' | 1:50:A:A:H8   | 7        | 0.21          |
| (1,161)  | 1:24:A:A:H4' | 1:23:A:C:H1'  | 1        | 0.21          |
| (1,150)  | 1:46:A:U:H6  | 1:47:A:C:H5'  | 9        | 0.21          |
| (1,150)  | 1:46:A:U:H6  | 1:47:A:C:H5'' | 9        | 0.21          |
| (1,114)  | 1:45:A:C:H3' | 1:52:A:A:H5'  | 6        | 0.21          |
| (1,114)  | 1:45:A:C:H3' | 1:52:A:A:H5'' | 6        | 0.21          |
| (1,91)   | 1:21:A:C:H2' | 1:21:A:C:H5   | 3        | 0.21          |
| (1,1326) | 1:36:A:C:H2' | 1:37:A:G:H4'  | 3        | 0.2           |
| (1,1325) | 1:38:A:C:H5  | 1:37:A:G:H4'  | 7        | 0.2           |
| (1,1318) | 1:59:A:U:H3' | 1:58:A:G:H3'  | 1        | 0.2           |
| (1,1317) | 1:59:A:U:H5  | 1:58:A:G:H3'  | 1        | 0.2           |
| (1,1317) | 1:59:A:U:H5  | 1:58:A:G:H3'  | 7        | 0.2           |
| (1,1288) | 1:15:A:C:H5' | 1:16:A:G:H5'' | 5        | 0.2           |
| (1,1269) | 1:18:A:C:H6  | 1:17:A:G:H3'  | 1        | 0.2           |
| (1,1269) | 1:18:A:C:H6  | 1:17:A:G:H3'  | 3        | 0.2           |
| (1,1269) | 1:18:A:C:H6  | 1:17:A:G:H3'  | 7        | 0.2           |
| (1,1269) | 1:18:A:C:H6  | 1:17:A:G:H3'  | 10       | 0.2           |
| (1,1238) | 1:12:A:C:H5  | 1:11:A:G:H4'  | 7        | 0.2           |
| (1,1218) | 1:31:A:A:H3' | 1:32:A:G:H8   | 1        | 0.2           |
| (1,1218) | 1:31:A:A:H3' | 1:32:A:G:H8   | 6        | 0.2           |
| (1,1208) | 1:3:A:A:H8   | 1:2:A:G:H1'   | 10       | 0.2           |
| (1,1203) | 1:59:A:U:H3' | 1:58:A:G:H1'  | 6        | 0.2           |
| (1,1146) | 1:5:A:G:H8   | 1:5:A:G:H2'   | 6        | 0.2           |
| (1,1146) | 1:5:A:G:H8   | 1:5:A:G:H2'   | 9        | 0.2           |
| (1,1108) | 1:2:A:G:H8   | 1:2:A:G:H2'   | 3        | 0.2           |
| (1,1055) | 1:56:A:U:H4' | 1:55:A:C:H3'  | 1        | 0.2           |
| (1,1052) | 1:46:A:U:H2' | 1:47:A:C:H3'  | 6        | 0.2           |
| (1,1052) | 1:46:A:U:H2' | 1:47:A:C:H3'  | 7        | 0.2           |
| (1,1050) | 1:31:A:A:H5' | 1:30:A:C:H6   | 6        | 0.2           |
| (1,1046) | 1:22:A:U:H6  | 1:21:A:C:H5   | 10       | 0.2           |
| (1,1039) | 1:29:A:A:H3' | 1:30:A:C:H5'  | 2        | 0.2           |
| (1,1013) | 1:24:A:A:H8  | 1:23:A:C:H1'  | 3        | 0.2           |
| (1,999)  | 1:14:A:U:H1' | 1:15:A:C:H5   | 2        | 0.2           |
| (1,999)  | 1:14:A:U:H1' | 1:15:A:C:H5   | 8        | 0.2           |
| (1,997)  | 1:37:A:G:H2' | 1:38:A:C:H5   | 8        | 0.2           |
| (1,981)  | 1:53:A:U:H6  | 1:54:A:C:H5   | 9        | 0.2           |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,938) | 1:28:A:U:H2' | 1:27:A:C:H3'  | 3        | 0.2           |
| (1,932) | 1:28:A:U:H5  | 1:27:A:C:H3'  | 7        | 0.2           |
| (1,883) | 1:13:A:U:H5  | 1:12:A:C:H4'  | 4        | 0.2           |
| (1,868) | 1:24:A:A:H8  | 1:23:A:C:H4'  | 2        | 0.2           |
| (1,864) | 1:46:A:U:H1' | 1:47:A:C:H4'  | 7        | 0.2           |
| (1,859) | 1:37:A:G:H8  | 1:36:A:C:H4'  | 6        | 0.2           |
| (1,850) | 1:29:A:A:H1' | 1:30:A:C:H6   | 8        | 0.2           |
| (1,823) | 1:46:A:U:H4' | 1:47:A:C:H6   | 7        | 0.2           |
| (1,823) | 1:46:A:U:H4' | 1:47:A:C:H6   | 9        | 0.2           |
| (1,665) | 1:54:A:C:H6  | 1:53:A:U:H6   | 9        | 0.2           |
| (1,658) | 1:27:A:C:H4' | 1:28:A:U:H5'' | 3        | 0.2           |
| (1,617) | 1:47:A:C:H3' | 1:46:A:U:H3'  | 7        | 0.2           |
| (1,551) | 1:28:A:U:H3' | 1:28:A:U:H5'' | 7        | 0.2           |
| (1,503) | 1:14:A:U:H5  | 1:14:A:U:H2'  | 6        | 0.2           |
| (1,473) | 1:14:A:U:H6  | 1:14:A:U:H3'  | 1        | 0.2           |
| (1,473) | 1:14:A:U:H6  | 1:14:A:U:H3'  | 3        | 0.2           |
| (1,473) | 1:14:A:U:H6  | 1:14:A:U:H3'  | 4        | 0.2           |
| (1,444) | 1:53:A:U:H4' | 1:53:A:U:H6   | 10       | 0.2           |
| (1,425) | 1:49:A:G:H4' | 1:50:A:A:H4'  | 3        | 0.2           |
| (1,396) | 1:51:A:U:H3' | 1:50:A:A:H1'  | 6        | 0.2           |
| (1,381) | 1:30:A:C:H4' | 1:29:A:A:H1'  | 6        | 0.2           |
| (1,366) | 1:9:A:G:H8   | 1:8:A:A:H3'   | 4        | 0.2           |
| (1,366) | 1:9:A:G:H8   | 1:8:A:A:H3'   | 5        | 0.2           |
| (1,366) | 1:9:A:G:H8   | 1:8:A:A:H3'   | 6        | 0.2           |
| (1,339) | 1:28:A:U:H6  | 1:29:A:A:H8   | 7        | 0.2           |
| (1,338) | 1:30:A:C:H6  | 1:29:A:A:H8   | 2        | 0.2           |
| (1,329) | 1:31:A:A:H8  | 1:31:A:A:H5'' | 2        | 0.2           |
| (1,321) | 1:26:A:A:H3' | 1:26:A:A:H2   | 9        | 0.2           |
| (1,257) | 1:7:A:A:H3'  | 1:6:A:A:H2    | 5        | 0.2           |
| (1,213) | 1:26:A:A:H8  | 1:26:A:A:H3'  | 8        | 0.2           |
| (1,209) | 1:24:A:A:H8  | 1:24:A:A:H2'  | 9        | 0.2           |
| (1,203) | 1:40:A:A:H8  | 1:40:A:A:H2'  | 1        | 0.2           |
| (1,203) | 1:40:A:A:H8  | 1:40:A:A:H2'  | 2        | 0.2           |
| (1,202) | 1:4:A:A:H8   | 1:4:A:A:H2'   | 8        | 0.2           |
| (1,201) | 1:20:A:A:H8  | 1:20:A:A:H2'  | 1        | 0.2           |
| (1,181) | 1:8:A:A:H3'  | 1:8:A:A:H8    | 1        | 0.2           |
| (1,181) | 1:8:A:A:H3'  | 1:8:A:A:H8    | 4        | 0.2           |
| (1,181) | 1:8:A:A:H3'  | 1:8:A:A:H8    | 5        | 0.2           |
| (1,170) | 1:3:A:A:H1'  | 1:4:A:A:H8    | 6        | 0.2           |
| (1,169) | 1:3:A:A:H2'  | 1:3:A:A:H8    | 8        | 0.2           |
| (1,146) | 1:24:A:A:H3' | 1:23:A:C:H3'  | 3        | 0.2           |
| (1,146) | 1:24:A:A:H3' | 1:23:A:C:H3'  | 7        | 0.2           |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,139)  | 1:42:A:U:H3'  | 1:43:A:C:H6   | 8        | 0.2           |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'  | 7        | 0.2           |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'' | 7        | 0.2           |
| (1,104)  | 1:21:A:C:H5   | 1:20:A:A:H4'  | 1        | 0.2           |
| (1,91)   | 1:21:A:C:H2'  | 1:21:A:C:H5   | 6        | 0.2           |
| (1,91)   | 1:21:A:C:H2'  | 1:21:A:C:H5   | 9        | 0.2           |
| (1,1325) | 1:38:A:C:H5   | 1:37:A:G:H4'  | 4        | 0.19          |
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 10       | 0.19          |
| (1,1308) | 1:18:A:C:H5   | 1:17:A:G:H5'  | 2        | 0.19          |
| (1,1288) | 1:15:A:C:H5'  | 1:16:A:G:H5'' | 1        | 0.19          |
| (1,1288) | 1:15:A:C:H5'  | 1:16:A:G:H5'' | 9        | 0.19          |
| (1,1288) | 1:15:A:C:H5'  | 1:16:A:G:H5'' | 10       | 0.19          |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 10       | 0.19          |
| (1,1269) | 1:18:A:C:H6   | 1:17:A:G:H3'  | 5        | 0.19          |
| (1,1269) | 1:18:A:C:H6   | 1:17:A:G:H3'  | 8        | 0.19          |
| (1,1269) | 1:18:A:C:H6   | 1:17:A:G:H3'  | 9        | 0.19          |
| (1,1254) | 1:59:A:U:H6   | 1:58:A:G:H2'  | 2        | 0.19          |
| (1,1227) | 1:33:A:A:H8   | 1:32:A:G:H4'  | 7        | 0.19          |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 7        | 0.19          |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 8        | 0.19          |
| (1,1211) | 1:50:A:A:H8   | 1:49:A:G:H1'  | 9        | 0.19          |
| (1,1208) | 1:3:A:A:H8    | 1:2:A:G:H1'   | 9        | 0.19          |
| (1,1146) | 1:5:A:G:H8    | 1:5:A:G:H2'   | 1        | 0.19          |
| (1,1146) | 1:5:A:G:H8    | 1:5:A:G:H2'   | 2        | 0.19          |
| (1,1050) | 1:31:A:A:H5'  | 1:30:A:C:H6   | 10       | 0.19          |
| (1,1046) | 1:22:A:U:H6   | 1:21:A:C:H5   | 2        | 0.19          |
| (1,1046) | 1:22:A:U:H6   | 1:21:A:C:H5   | 3        | 0.19          |
| (1,1042) | 1:20:A:A:H3'  | 1:21:A:C:H5'' | 4        | 0.19          |
| (1,1042) | 1:20:A:A:H3'  | 1:21:A:C:H5'' | 9        | 0.19          |
| (1,1027) | 1:37:A:G:H8   | 1:36:A:C:H1'  | 8        | 0.19          |
| (1,999)  | 1:14:A:U:H1'  | 1:15:A:C:H5   | 5        | 0.19          |
| (1,989)  | 1:20:A:A:H2'  | 1:21:A:C:H5   | 2        | 0.19          |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5   | 2        | 0.19          |
| (1,962)  | 1:44:A:A:H8   | 1:45:A:C:H5'  | 1        | 0.19          |
| (1,962)  | 1:44:A:A:H8   | 1:45:A:C:H5'  | 9        | 0.19          |
| (1,921)  | 1:13:A:U:H3'  | 1:12:A:C:H2'  | 7        | 0.19          |
| (1,908)  | 1:20:A:A:H8   | 1:19:A:C:H2'  | 5        | 0.19          |
| (1,901)  | 1:22:A:U:H3'  | 1:21:A:C:H2'  | 8        | 0.19          |
| (1,898)  | 1:31:A:A:H1'  | 1:30:A:C:H2'  | 8        | 0.19          |
| (1,893)  | 1:22:A:U:H6   | 1:21:A:C:H2'  | 5        | 0.19          |
| (1,893)  | 1:22:A:U:H6   | 1:21:A:C:H2'  | 8        | 0.19          |
| (1,883)  | 1:13:A:U:H5   | 1:12:A:C:H4'  | 2        | 0.19          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,883) | 1:13:A:U:H5   | 1:12:A:C:H4'  | 6        | 0.19          |
| (1,878) | 1:26:A:A:H2'  | 1:27:A:C:H4'  | 8        | 0.19          |
| (1,875) | 1:28:A:U:H5   | 1:27:A:C:H4'  | 3        | 0.19          |
| (1,871) | 1:31:A:A:H8   | 1:30:A:C:H4'  | 3        | 0.19          |
| (1,868) | 1:24:A:A:H8   | 1:23:A:C:H4'  | 10       | 0.19          |
| (1,851) | 1:29:A:A:H4'  | 1:30:A:C:H6   | 3        | 0.19          |
| (1,830) | 1:42:A:U:H2'  | 1:43:A:C:H6   | 10       | 0.19          |
| (1,824) | 1:16:A:G:H1'  | 1:15:A:C:H1'  | 2        | 0.19          |
| (1,824) | 1:16:A:G:H1'  | 1:15:A:C:H1'  | 6        | 0.19          |
| (1,823) | 1:46:A:U:H4'  | 1:47:A:C:H6   | 10       | 0.19          |
| (1,815) | 1:39:A:C:H5   | 1:39:A:C:H5'' | 4        | 0.19          |
| (1,815) | 1:39:A:C:H5   | 1:39:A:C:H5'' | 6        | 0.19          |
| (1,815) | 1:39:A:C:H5   | 1:39:A:C:H5'' | 7        | 0.19          |
| (1,770) | 1:21:A:C:H6   | 1:21:A:C:H5'' | 8        | 0.19          |
| (1,678) | 1:54:A:C:H4'  | 1:54:A:C:H6   | 1        | 0.19          |
| (1,678) | 1:54:A:C:H4'  | 1:54:A:C:H6   | 3        | 0.19          |
| (1,668) | 1:54:A:C:H6   | 1:53:A:U:H4'  | 6        | 0.19          |
| (1,664) | 1:58:A:G:H4'  | 1:59:A:U:H4'  | 10       | 0.19          |
| (1,632) | 1:29:A:A:H4'  | 1:28:A:U:H3'  | 1        | 0.19          |
| (1,632) | 1:29:A:A:H4'  | 1:28:A:U:H3'  | 4        | 0.19          |
| (1,627) | 1:47:A:C:H6   | 1:46:A:U:H2'  | 1        | 0.19          |
| (1,608) | 1:45:A:C:H3'  | 1:46:A:U:H1'  | 6        | 0.19          |
| (1,593) | 1:50:A:A:H1'  | 1:51:A:U:H5   | 9        | 0.19          |
| (1,574) | 1:56:A:U:H5'' | 1:56:A:U:H4'  | 5        | 0.19          |
| (1,551) | 1:28:A:U:H3'  | 1:28:A:U:H5'' | 5        | 0.19          |
| (1,541) | 1:53:A:U:H4'  | 1:53:A:U:H5'  | 9        | 0.19          |
| (1,537) | 1:14:A:U:H4'  | 1:14:A:U:H5'  | 1        | 0.19          |
| (1,537) | 1:14:A:U:H4'  | 1:14:A:U:H5'  | 2        | 0.19          |
| (1,537) | 1:14:A:U:H4'  | 1:14:A:U:H5'  | 8        | 0.19          |
| (1,537) | 1:14:A:U:H4'  | 1:14:A:U:H5'  | 9        | 0.19          |
| (1,503) | 1:14:A:U:H5   | 1:14:A:U:H2'  | 10       | 0.19          |
| (1,478) | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 8        | 0.19          |
| (1,445) | 1:53:A:U:H5'' | 1:53:A:U:H6   | 3        | 0.19          |
| (1,435) | 1:30:A:C:H2'  | 1:31:A:A:H5'' | 4        | 0.19          |
| (1,435) | 1:30:A:C:H2'  | 1:31:A:A:H5'' | 9        | 0.19          |
| (1,425) | 1:49:A:G:H4'  | 1:50:A:A:H4'  | 6        | 0.19          |
| (1,424) | 1:49:A:G:H2'  | 1:50:A:A:H4'  | 1        | 0.19          |
| (1,419) | 1:19:A:C:H2'  | 1:20:A:A:H3'  | 5        | 0.19          |
| (1,419) | 1:19:A:C:H2'  | 1:20:A:A:H3'  | 7        | 0.19          |
| (1,418) | 1:19:A:C:H3'  | 1:20:A:A:H3'  | 1        | 0.19          |
| (1,394) | 1:9:A:G:H2'   | 1:8:A:A:H2    | 7        | 0.19          |
| (1,383) | 1:5:A:G:H1'   | 1:4:A:A:H1'   | 7        | 0.19          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,348)  | 1:46:A:U:H5'' | 1:52:A:A:H4'  | 5        | 0.19          |
| (1,346)  | 1:23:A:C:H1'  | 1:24:A:A:H4'  | 2        | 0.19          |
| (1,346)  | 1:23:A:C:H1'  | 1:24:A:A:H4'  | 5        | 0.19          |
| (1,346)  | 1:23:A:C:H1'  | 1:24:A:A:H4'  | 8        | 0.19          |
| (1,340)  | 1:19:A:C:H4'  | 1:20:A:A:H8   | 10       | 0.19          |
| (1,321)  | 1:26:A:A:H3'  | 1:26:A:A:H2   | 10       | 0.19          |
| (1,275)  | 1:40:A:A:H5'  | 1:40:A:A:H4'  | 2        | 0.19          |
| (1,275)  | 1:40:A:A:H5'  | 1:40:A:A:H4'  | 9        | 0.19          |
| (1,257)  | 1:7:A:A:H3'   | 1:6:A:A:H2    | 4        | 0.19          |
| (1,201)  | 1:20:A:A:H8   | 1:20:A:A:H2'  | 9        | 0.19          |
| (1,200)  | 1:8:A:A:H8    | 1:8:A:A:H2'   | 1        | 0.19          |
| (1,200)  | 1:8:A:A:H8    | 1:8:A:A:H2'   | 5        | 0.19          |
| (1,194)  | 1:52:A:A:H5'  | 1:52:A:A:H4'  | 6        | 0.19          |
| (1,181)  | 1:8:A:A:H3'   | 1:8:A:A:H8    | 8        | 0.19          |
| (1,180)  | 1:25:A:A:H1'  | 1:26:A:A:H8   | 10       | 0.19          |
| (1,163)  | 1:49:A:G:H2'  | 1:47:A:C:H3'  | 3        | 0.19          |
| (1,161)  | 1:24:A:A:H4'  | 1:23:A:C:H1'  | 2        | 0.19          |
| (1,161)  | 1:24:A:A:H4'  | 1:23:A:C:H1'  | 5        | 0.19          |
| (1,161)  | 1:24:A:A:H4'  | 1:23:A:C:H1'  | 8        | 0.19          |
| (1,91)   | 1:21:A:C:H2'  | 1:21:A:C:H5   | 1        | 0.19          |
| (1,91)   | 1:21:A:C:H2'  | 1:21:A:C:H5   | 2        | 0.19          |
| (1,91)   | 1:21:A:C:H2'  | 1:21:A:C:H5   | 4        | 0.19          |
| (1,91)   | 1:21:A:C:H2'  | 1:21:A:C:H5   | 10       | 0.19          |
| (1,3)    | 1:41:A:G:H4'  | 1:40:A:A:H1'  | 10       | 0.19          |
| (1,1330) | 1:38:A:C:H5   | 1:37:A:G:H3'  | 5        | 0.18          |
| (1,1330) | 1:38:A:C:H5   | 1:37:A:G:H3'  | 8        | 0.18          |
| (1,1325) | 1:38:A:C:H5   | 1:37:A:G:H4'  | 9        | 0.18          |
| (1,1306) | 1:40:A:A:H2'  | 1:41:A:G:H5'' | 2        | 0.18          |
| (1,1301) | 1:8:A:A:H2'   | 1:9:A:G:H5'   | 8        | 0.18          |
| (1,1288) | 1:15:A:C:H5'  | 1:16:A:G:H5'' | 2        | 0.18          |
| (1,1288) | 1:15:A:C:H5'  | 1:16:A:G:H5'' | 6        | 0.18          |
| (1,1269) | 1:18:A:C:H6   | 1:17:A:G:H3'  | 4        | 0.18          |
| (1,1269) | 1:18:A:C:H6   | 1:17:A:G:H3'  | 6        | 0.18          |
| (1,1238) | 1:12:A:C:H5   | 1:11:A:G:H4'  | 5        | 0.18          |
| (1,1238) | 1:12:A:C:H5   | 1:11:A:G:H4'  | 9        | 0.18          |
| (1,1224) | 1:31:A:A:H1'  | 1:32:A:G:H4'  | 2        | 0.18          |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 4        | 0.18          |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 6        | 0.18          |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 9        | 0.18          |
| (1,1208) | 1:3:A:A:H8    | 1:2:A:G:H1'   | 1        | 0.18          |
| (1,1208) | 1:3:A:A:H8    | 1:2:A:G:H1'   | 7        | 0.18          |
| (1,1178) | 1:38:A:C:H5   | 1:37:A:G:H8   | 6        | 0.18          |

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| Key      | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|----------|---------------|--------------|----------|---------------|
| (1,1146) | 1:5:A:G:H8    | 1:5:A:G:H2'  | 4        | 0.18          |
| (1,1146) | 1:5:A:G:H8    | 1:5:A:G:H2'  | 10       | 0.18          |
| (1,1106) | 1:49:A:G:H8   | 1:49:A:G:H3' | 10       | 0.18          |
| (1,1050) | 1:31:A:A:H5'  | 1:30:A:C:H6  | 5        | 0.18          |
| (1,1046) | 1:22:A:U:H6   | 1:21:A:C:H5  | 4        | 0.18          |
| (1,1046) | 1:22:A:U:H6   | 1:21:A:C:H5  | 7        | 0.18          |
| (1,999)  | 1:14:A:U:H1'  | 1:15:A:C:H5  | 3        | 0.18          |
| (1,999)  | 1:14:A:U:H1'  | 1:15:A:C:H5  | 4        | 0.18          |
| (1,999)  | 1:14:A:U:H1'  | 1:15:A:C:H5  | 10       | 0.18          |
| (1,981)  | 1:53:A:U:H6   | 1:54:A:C:H5  | 4        | 0.18          |
| (1,954)  | 1:37:A:G:H3'  | 1:38:A:C:H3' | 4        | 0.18          |
| (1,946)  | 1:40:A:A:H4'  | 1:39:A:C:H3' | 4        | 0.18          |
| (1,932)  | 1:28:A:U:H5   | 1:27:A:C:H3' | 5        | 0.18          |
| (1,908)  | 1:20:A:A:H8   | 1:19:A:C:H2' | 4        | 0.18          |
| (1,878)  | 1:26:A:A:H2'  | 1:27:A:C:H4' | 10       | 0.18          |
| (1,874)  | 1:22:A:U:H5   | 1:21:A:C:H4' | 2        | 0.18          |
| (1,871)  | 1:31:A:A:H8   | 1:30:A:C:H4' | 2        | 0.18          |
| (1,871)  | 1:31:A:A:H8   | 1:30:A:C:H4' | 9        | 0.18          |
| (1,868)  | 1:24:A:A:H8   | 1:23:A:C:H4' | 5        | 0.18          |
| (1,848)  | 1:20:A:A:H1'  | 1:21:A:C:H6  | 2        | 0.18          |
| (1,824)  | 1:16:A:G:H1'  | 1:15:A:C:H1' | 1        | 0.18          |
| (1,824)  | 1:16:A:G:H1'  | 1:15:A:C:H1' | 8        | 0.18          |
| (1,824)  | 1:16:A:G:H1'  | 1:15:A:C:H1' | 9        | 0.18          |
| (1,824)  | 1:16:A:G:H1'  | 1:15:A:C:H1' | 10       | 0.18          |
| (1,823)  | 1:46:A:U:H4'  | 1:47:A:C:H6  | 3        | 0.18          |
| (1,823)  | 1:46:A:U:H4'  | 1:47:A:C:H6  | 6        | 0.18          |
| (1,706)  | 1:15:A:C:H5'' | 1:15:A:C:H3' | 5        | 0.18          |
| (1,678)  | 1:54:A:C:H4'  | 1:54:A:C:H6  | 9        | 0.18          |
| (1,668)  | 1:54:A:C:H6   | 1:53:A:U:H4' | 1        | 0.18          |
| (1,668)  | 1:54:A:C:H6   | 1:53:A:U:H4' | 7        | 0.18          |
| (1,664)  | 1:58:A:G:H4'  | 1:59:A:U:H4' | 6        | 0.18          |
| (1,663)  | 1:58:A:G:H2'  | 1:59:A:U:H4' | 10       | 0.18          |
| (1,621)  | 1:54:A:C:H6   | 1:53:A:U:H2' | 9        | 0.18          |
| (1,620)  | 1:44:A:A:H8   | 1:42:A:U:H2' | 7        | 0.18          |
| (1,581)  | 1:45:A:C:H4'  | 1:46:A:U:H6  | 3        | 0.18          |
| (1,581)  | 1:45:A:C:H4'  | 1:46:A:U:H6  | 4        | 0.18          |
| (1,574)  | 1:56:A:U:H5'' | 1:56:A:U:H4' | 3        | 0.18          |
| (1,537)  | 1:14:A:U:H4'  | 1:14:A:U:H5' | 5        | 0.18          |
| (1,537)  | 1:14:A:U:H4'  | 1:14:A:U:H5' | 6        | 0.18          |
| (1,537)  | 1:14:A:U:H4'  | 1:14:A:U:H5' | 7        | 0.18          |
| (1,537)  | 1:14:A:U:H4'  | 1:14:A:U:H5' | 10       | 0.18          |
| (1,522)  | 1:59:A:U:H6   | 1:59:A:U:H3' | 10       | 0.18          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,503)  | 1:14:A:U:H5   | 1:14:A:U:H2'  | 1        | 0.18          |
| (1,503)  | 1:14:A:U:H5   | 1:14:A:U:H2'  | 3        | 0.18          |
| (1,503)  | 1:14:A:U:H5   | 1:14:A:U:H2'  | 8        | 0.18          |
| (1,503)  | 1:14:A:U:H5   | 1:14:A:U:H2'  | 9        | 0.18          |
| (1,500)  | 1:59:A:U:H6   | 1:59:A:U:H2'  | 10       | 0.18          |
| (1,478)  | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 1        | 0.18          |
| (1,478)  | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 9        | 0.18          |
| (1,473)  | 1:14:A:U:H6   | 1:14:A:U:H3'  | 2        | 0.18          |
| (1,436)  | 1:30:A:C:H2'  | 1:31:A:A:H5'  | 8        | 0.18          |
| (1,431)  | 1:28:A:U:H2'  | 1:29:A:A:H5'  | 10       | 0.18          |
| (1,424)  | 1:49:A:G:H2'  | 1:50:A:A:H4'  | 9        | 0.18          |
| (1,419)  | 1:19:A:C:H2'  | 1:20:A:A:H3'  | 2        | 0.18          |
| (1,396)  | 1:51:A:U:H3'  | 1:50:A:A:H1'  | 2        | 0.18          |
| (1,329)  | 1:31:A:A:H8   | 1:31:A:A:H5'' | 5        | 0.18          |
| (1,291)  | 1:24:A:A:H8   | 1:24:A:A:H5'' | 10       | 0.18          |
| (1,275)  | 1:40:A:A:H5'  | 1:40:A:A:H4'  | 3        | 0.18          |
| (1,213)  | 1:26:A:A:H8   | 1:26:A:A:H3'  | 10       | 0.18          |
| (1,200)  | 1:8:A:A:H8    | 1:8:A:A:H2'   | 3        | 0.18          |
| (1,200)  | 1:8:A:A:H8    | 1:8:A:A:H2'   | 4        | 0.18          |
| (1,200)  | 1:8:A:A:H8    | 1:8:A:A:H2'   | 8        | 0.18          |
| (1,200)  | 1:8:A:A:H8    | 1:8:A:A:H2'   | 9        | 0.18          |
| (1,197)  | 1:52:A:A:H8   | 1:52:A:A:H3'  | 3        | 0.18          |
| (1,168)  | 1:50:A:A:H3'  | 1:50:A:A:H8   | 4        | 0.18          |
| (1,150)  | 1:46:A:U:H6   | 1:47:A:C:H5'  | 7        | 0.18          |
| (1,150)  | 1:46:A:U:H6   | 1:47:A:C:H5'' | 7        | 0.18          |
| (1,107)  | 1:34:A:G:H2'  | 1:35:A:A:H2'  | 9        | 0.18          |
| (1,91)   | 1:21:A:C:H2'  | 1:21:A:C:H5   | 7        | 0.18          |
| (1,91)   | 1:21:A:C:H2'  | 1:21:A:C:H5   | 8        | 0.18          |
| (1,1325) | 1:38:A:C:H5   | 1:37:A:G:H4'  | 10       | 0.17          |
| (1,1309) | 1:33:A:A:H8   | 1:32:A:G:H2'  | 6        | 0.17          |
| (1,1309) | 1:33:A:A:H8   | 1:32:A:G:H2'  | 7        | 0.17          |
| (1,1227) | 1:33:A:A:H8   | 1:32:A:G:H4'  | 4        | 0.17          |
| (1,1227) | 1:33:A:A:H8   | 1:32:A:G:H4'  | 5        | 0.17          |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 1        | 0.17          |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 2        | 0.17          |
| (1,1218) | 1:31:A:A:H3'  | 1:32:A:G:H8   | 5        | 0.17          |
| (1,1208) | 1:3:A:A:H8    | 1:2:A:G:H1'   | 6        | 0.17          |
| (1,1206) | 1:8:A:A:H1'   | 1:9:A:G:H1'   | 7        | 0.17          |
| (1,1203) | 1:59:A:U:H3'  | 1:58:A:G:H1'  | 2        | 0.17          |
| (1,1178) | 1:38:A:C:H5   | 1:37:A:G:H8   | 3        | 0.17          |
| (1,1163) | 1:15:A:C:H5'  | 1:16:A:G:H8   | 6        | 0.17          |
| (1,1146) | 1:5:A:G:H8    | 1:5:A:G:H2'   | 3        | 0.17          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1106) | 1:49:A:G:H8   | 1:49:A:G:H3'  | 7        | 0.17          |
| (1,1055) | 1:56:A:U:H4'  | 1:55:A:C:H3'  | 2        | 0.17          |
| (1,1055) | 1:56:A:U:H4'  | 1:55:A:C:H3'  | 10       | 0.17          |
| (1,1050) | 1:31:A:A:H5'  | 1:30:A:C:H6   | 1        | 0.17          |
| (1,1046) | 1:22:A:U:H6   | 1:21:A:C:H5   | 8        | 0.17          |
| (1,1042) | 1:20:A:A:H3'  | 1:21:A:C:H5'' | 1        | 0.17          |
| (1,1042) | 1:20:A:A:H3'  | 1:21:A:C:H5'' | 8        | 0.17          |
| (1,1021) | 1:44:A:A:H2   | 1:45:A:C:H1'  | 1        | 0.17          |
| (1,1013) | 1:24:A:A:H8   | 1:23:A:C:H1'  | 4        | 0.17          |
| (1,913)  | 1:40:A:A:H8   | 1:39:A:C:H2'  | 3        | 0.17          |
| (1,893)  | 1:22:A:U:H6   | 1:21:A:C:H2'  | 2        | 0.17          |
| (1,893)  | 1:22:A:U:H6   | 1:21:A:C:H2'  | 7        | 0.17          |
| (1,886)  | 1:14:A:U:H4'  | 1:15:A:C:H2'  | 9        | 0.17          |
| (1,885)  | 1:37:A:G:H2'  | 1:38:A:C:H4'  | 10       | 0.17          |
| (1,883)  | 1:13:A:U:H5   | 1:12:A:C:H4'  | 8        | 0.17          |
| (1,874)  | 1:22:A:U:H5   | 1:21:A:C:H4'  | 6        | 0.17          |
| (1,871)  | 1:31:A:A:H8   | 1:30:A:C:H4'  | 1        | 0.17          |
| (1,861)  | 1:53:A:U:H3'  | 1:54:A:C:H4'  | 3        | 0.17          |
| (1,850)  | 1:29:A:A:H1'  | 1:30:A:C:H6   | 9        | 0.17          |
| (1,824)  | 1:16:A:G:H1'  | 1:15:A:C:H1'  | 3        | 0.17          |
| (1,824)  | 1:16:A:G:H1'  | 1:15:A:C:H1'  | 4        | 0.17          |
| (1,824)  | 1:16:A:G:H1'  | 1:15:A:C:H1'  | 5        | 0.17          |
| (1,823)  | 1:46:A:U:H4'  | 1:47:A:C:H6   | 2        | 0.17          |
| (1,815)  | 1:39:A:C:H5   | 1:39:A:C:H5'' | 8        | 0.17          |
| (1,720)  | 1:47:A:C:H6   | 1:47:A:C:H2'  | 5        | 0.17          |
| (1,716)  | 1:47:A:C:H6   | 1:47:A:C:H3'  | 8        | 0.17          |
| (1,678)  | 1:54:A:C:H4'  | 1:54:A:C:H6   | 8        | 0.17          |
| (1,668)  | 1:54:A:C:H6   | 1:53:A:U:H4'  | 9        | 0.17          |
| (1,608)  | 1:45:A:C:H3'  | 1:46:A:U:H1'  | 1        | 0.17          |
| (1,608)  | 1:45:A:C:H3'  | 1:46:A:U:H1'  | 4        | 0.17          |
| (1,608)  | 1:45:A:C:H3'  | 1:46:A:U:H1'  | 5        | 0.17          |
| (1,608)  | 1:45:A:C:H3'  | 1:46:A:U:H1'  | 10       | 0.17          |
| (1,574)  | 1:56:A:U:H5'' | 1:56:A:U:H4'  | 4        | 0.17          |
| (1,537)  | 1:14:A:U:H4'  | 1:14:A:U:H5'  | 3        | 0.17          |
| (1,537)  | 1:14:A:U:H4'  | 1:14:A:U:H5'  | 4        | 0.17          |
| (1,503)  | 1:14:A:U:H5   | 1:14:A:U:H2'  | 2        | 0.17          |
| (1,503)  | 1:14:A:U:H5   | 1:14:A:U:H2'  | 5        | 0.17          |
| (1,478)  | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 6        | 0.17          |
| (1,478)  | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 7        | 0.17          |
| (1,473)  | 1:14:A:U:H6   | 1:14:A:U:H3'  | 5        | 0.17          |
| (1,444)  | 1:53:A:U:H4'  | 1:53:A:U:H6   | 5        | 0.17          |
| (1,412)  | 1:2:A:G:H2'   | 1:3:A:A:H5''  | 3        | 0.17          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,394)  | 1:9:A:G:H2'   | 1:8:A:A:H2    | 8        | 0.17          |
| (1,383)  | 1:5:A:G:H1'   | 1:4:A:A:H1'   | 6        | 0.17          |
| (1,366)  | 1:9:A:G:H8    | 1:8:A:A:H3'   | 2        | 0.17          |
| (1,348)  | 1:46:A:U:H5'' | 1:52:A:A:H4'  | 7        | 0.17          |
| (1,340)  | 1:19:A:C:H4'  | 1:20:A:A:H8   | 1        | 0.17          |
| (1,340)  | 1:19:A:C:H4'  | 1:20:A:A:H8   | 6        | 0.17          |
| (1,329)  | 1:31:A:A:H8   | 1:31:A:A:H5'' | 7        | 0.17          |
| (1,321)  | 1:26:A:A:H3'  | 1:26:A:A:H2   | 3        | 0.17          |
| (1,321)  | 1:26:A:A:H3'  | 1:26:A:A:H2   | 4        | 0.17          |
| (1,310)  | 1:31:A:A:H4'  | 1:31:A:A:H8   | 6        | 0.17          |
| (1,291)  | 1:24:A:A:H8   | 1:24:A:A:H5'' | 5        | 0.17          |
| (1,291)  | 1:24:A:A:H8   | 1:24:A:A:H5'' | 8        | 0.17          |
| (1,275)  | 1:40:A:A:H5'  | 1:40:A:A:H4'  | 6        | 0.17          |
| (1,275)  | 1:40:A:A:H5'  | 1:40:A:A:H4'  | 8        | 0.17          |
| (1,208)  | 1:6:A:A:H8    | 1:6:A:A:H2'   | 6        | 0.17          |
| (1,208)  | 1:6:A:A:H8    | 1:6:A:A:H2'   | 9        | 0.17          |
| (1,203)  | 1:40:A:A:H8   | 1:40:A:A:H2'  | 7        | 0.17          |
| (1,203)  | 1:40:A:A:H8   | 1:40:A:A:H2'  | 9        | 0.17          |
| (1,201)  | 1:20:A:A:H8   | 1:20:A:A:H2'  | 3        | 0.17          |
| (1,201)  | 1:20:A:A:H8   | 1:20:A:A:H2'  | 8        | 0.17          |
| (1,201)  | 1:20:A:A:H8   | 1:20:A:A:H2'  | 10       | 0.17          |
| (1,195)  | 1:52:A:A:H5'' | 1:52:A:A:H4'  | 2        | 0.17          |
| (1,194)  | 1:52:A:A:H5'  | 1:52:A:A:H4'  | 5        | 0.17          |
| (1,172)  | 1:29:A:A:H2'  | 1:29:A:A:H8   | 9        | 0.17          |
| (1,169)  | 1:3:A:A:H2'   | 1:3:A:A:H8    | 4        | 0.17          |
| (1,169)  | 1:3:A:A:H2'   | 1:3:A:A:H8    | 5        | 0.17          |
| (1,168)  | 1:50:A:A:H3'  | 1:50:A:A:H8   | 6        | 0.17          |
| (1,134)  | 1:50:A:A:H8   | 1:49:A:G:H5'  | 5        | 0.17          |
| (1,134)  | 1:50:A:A:H8   | 1:49:A:G:H5'' | 5        | 0.17          |
| (1,91)   | 1:21:A:C:H2'  | 1:21:A:C:H5   | 5        | 0.17          |
| (1,1325) | 1:38:A:C:H5   | 1:37:A:G:H4'  | 5        | 0.16          |
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 4        | 0.16          |
| (1,1311) | 1:12:A:C:H1'  | 1:11:A:G:H3'  | 6        | 0.16          |
| (1,1309) | 1:33:A:A:H8   | 1:32:A:G:H2'  | 3        | 0.16          |
| (1,1306) | 1:40:A:A:H2'  | 1:41:A:G:H5'' | 6        | 0.16          |
| (1,1295) | 1:31:A:A:H2'  | 1:32:A:G:H5'  | 8        | 0.16          |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 1        | 0.16          |
| (1,1270) | 1:12:A:C:H3'  | 1:11:A:G:H2'  | 4        | 0.16          |
| (1,1235) | 1:59:A:U:H5   | 1:58:A:G:H4'  | 3        | 0.16          |
| (1,1227) | 1:33:A:A:H8   | 1:32:A:G:H4'  | 2        | 0.16          |
| (1,1225) | 1:47:A:C:H2'  | 1:49:A:G:H4'  | 7        | 0.16          |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 10       | 0.16          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1197) | 1:56:A:U:H1'  | 1:57:A:G:H1'  | 3        | 0.16          |
| (1,1146) | 1:5:A:G:H8    | 1:5:A:G:H2'   | 5        | 0.16          |
| (1,1146) | 1:5:A:G:H8    | 1:5:A:G:H2'   | 7        | 0.16          |
| (1,1055) | 1:56:A:U:H4'  | 1:55:A:C:H3'  | 8        | 0.16          |
| (1,1055) | 1:56:A:U:H4'  | 1:55:A:C:H3'  | 9        | 0.16          |
| (1,1048) | 1:44:A:A:H1'  | 1:54:A:C:H5   | 5        | 0.16          |
| (1,1046) | 1:22:A:U:H6   | 1:21:A:C:H5   | 5        | 0.16          |
| (1,1027) | 1:37:A:G:H8   | 1:36:A:C:H1'  | 4        | 0.16          |
| (1,1027) | 1:37:A:G:H8   | 1:36:A:C:H1'  | 5        | 0.16          |
| (1,1013) | 1:24:A:A:H8   | 1:23:A:C:H1'  | 6        | 0.16          |
| (1,992)  | 1:28:A:U:H6   | 1:27:A:C:H5   | 6        | 0.16          |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5   | 4        | 0.16          |
| (1,962)  | 1:44:A:A:H8   | 1:45:A:C:H5'  | 7        | 0.16          |
| (1,960)  | 1:35:A:A:H2'  | 1:36:A:C:H5'' | 6        | 0.16          |
| (1,954)  | 1:37:A:G:H3'  | 1:38:A:C:H3'  | 1        | 0.16          |
| (1,954)  | 1:37:A:G:H3'  | 1:38:A:C:H3'  | 10       | 0.16          |
| (1,902)  | 1:22:A:U:H4'  | 1:21:A:C:H2'  | 9        | 0.16          |
| (1,900)  | 1:28:A:U:H3'  | 1:27:A:C:H2'  | 6        | 0.16          |
| (1,893)  | 1:22:A:U:H6   | 1:21:A:C:H2'  | 1        | 0.16          |
| (1,893)  | 1:22:A:U:H6   | 1:21:A:C:H2'  | 3        | 0.16          |
| (1,893)  | 1:22:A:U:H6   | 1:21:A:C:H2'  | 6        | 0.16          |
| (1,893)  | 1:22:A:U:H6   | 1:21:A:C:H2'  | 9        | 0.16          |
| (1,878)  | 1:26:A:A:H2'  | 1:27:A:C:H4'  | 2        | 0.16          |
| (1,875)  | 1:28:A:U:H5   | 1:27:A:C:H4'  | 9        | 0.16          |
| (1,874)  | 1:22:A:U:H5   | 1:21:A:C:H4'  | 3        | 0.16          |
| (1,874)  | 1:22:A:U:H5   | 1:21:A:C:H4'  | 4        | 0.16          |
| (1,871)  | 1:31:A:A:H8   | 1:30:A:C:H4'  | 5        | 0.16          |
| (1,862)  | 1:53:A:U:H4'  | 1:54:A:C:H4'  | 2        | 0.16          |
| (1,851)  | 1:29:A:A:H4'  | 1:30:A:C:H6   | 4        | 0.16          |
| (1,815)  | 1:39:A:C:H5   | 1:39:A:C:H5'' | 10       | 0.16          |
| (1,713)  | 1:36:A:C:H2'  | 1:36:A:C:H3'  | 7        | 0.16          |
| (1,706)  | 1:15:A:C:H5'' | 1:15:A:C:H3'  | 2        | 0.16          |
| (1,706)  | 1:15:A:C:H5'' | 1:15:A:C:H3'  | 3        | 0.16          |
| (1,706)  | 1:15:A:C:H5'' | 1:15:A:C:H3'  | 6        | 0.16          |
| (1,706)  | 1:15:A:C:H5'' | 1:15:A:C:H3'  | 7        | 0.16          |
| (1,706)  | 1:15:A:C:H5'' | 1:15:A:C:H3'  | 9        | 0.16          |
| (1,706)  | 1:15:A:C:H5'' | 1:15:A:C:H3'  | 10       | 0.16          |
| (1,668)  | 1:54:A:C:H6   | 1:53:A:U:H4'  | 3        | 0.16          |
| (1,668)  | 1:54:A:C:H6   | 1:53:A:U:H4'  | 10       | 0.16          |
| (1,665)  | 1:54:A:C:H6   | 1:53:A:U:H6   | 2        | 0.16          |
| (1,662)  | 1:27:A:C:H2'  | 1:28:A:U:H4'  | 7        | 0.16          |
| (1,628)  | 1:29:A:A:H8   | 1:28:A:U:H2'  | 4        | 0.16          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,607)  | 1:50:A:A:H2   | 1:51:A:U:H1'  | 8        | 0.16          |
| (1,603)  | 1:29:A:A:H8   | 1:28:A:U:H1'  | 8        | 0.16          |
| (1,581)  | 1:45:A:C:H4'  | 1:46:A:U:H6   | 8        | 0.16          |
| (1,574)  | 1:56:A:U:H5'' | 1:56:A:U:H4'  | 9        | 0.16          |
| (1,525)  | 1:59:A:U:H5'' | 1:59:A:U:H3'  | 7        | 0.16          |
| (1,503)  | 1:14:A:U:H5   | 1:14:A:U:H2'  | 7        | 0.16          |
| (1,497)  | 1:42:A:U:H6   | 1:42:A:U:H2'  | 3        | 0.16          |
| (1,482)  | 1:51:A:U:H5'' | 1:51:A:U:H3'  | 7        | 0.16          |
| (1,478)  | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 2        | 0.16          |
| (1,478)  | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 5        | 0.16          |
| (1,478)  | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 10       | 0.16          |
| (1,473)  | 1:14:A:U:H6   | 1:14:A:U:H3'  | 10       | 0.16          |
| (1,444)  | 1:53:A:U:H4'  | 1:53:A:U:H6   | 4        | 0.16          |
| (1,412)  | 1:2:A:G:H2'   | 1:3:A:A:H5''  | 5        | 0.16          |
| (1,396)  | 1:51:A:U:H3'  | 1:50:A:A:H1'  | 7        | 0.16          |
| (1,383)  | 1:5:A:G:H1'   | 1:4:A:A:H1'   | 8        | 0.16          |
| (1,383)  | 1:5:A:G:H1'   | 1:4:A:A:H1'   | 9        | 0.16          |
| (1,381)  | 1:30:A:C:H4'  | 1:29:A:A:H1'  | 10       | 0.16          |
| (1,307)  | 1:48:A:A:H3'  | 1:48:A:A:H5'  | 10       | 0.16          |
| (1,283)  | 1:20:A:A:H8   | 1:20:A:A:H5'' | 4        | 0.16          |
| (1,275)  | 1:40:A:A:H5'  | 1:40:A:A:H4'  | 10       | 0.16          |
| (1,257)  | 1:7:A:A:H3'   | 1:6:A:A:H2    | 10       | 0.16          |
| (1,203)  | 1:40:A:A:H8   | 1:40:A:A:H2'  | 5        | 0.16          |
| (1,201)  | 1:20:A:A:H8   | 1:20:A:A:H2'  | 6        | 0.16          |
| (1,181)  | 1:8:A:A:H3'   | 1:8:A:A:H8    | 3        | 0.16          |
| (1,181)  | 1:8:A:A:H3'   | 1:8:A:A:H8    | 9        | 0.16          |
| (1,176)  | 1:25:A:A:H5'  | 1:25:A:A:H8   | 8        | 0.16          |
| (1,128)  | 1:4:A:A:H3'   | 1:5:A:G:H1'   | 10       | 0.16          |
| (1,109)  | 1:27:A:C:H3'  | 1:26:A:A:H3'  | 10       | 0.16          |
| (1,1330) | 1:38:A:C:H5   | 1:37:A:G:H3'  | 4        | 0.15          |
| (1,1326) | 1:36:A:C:H2'  | 1:37:A:G:H4'  | 6        | 0.15          |
| (1,1317) | 1:59:A:U:H5   | 1:58:A:G:H3'  | 6        | 0.15          |
| (1,1316) | 1:59:A:U:H6   | 1:58:A:G:H3'  | 8        | 0.15          |
| (1,1306) | 1:40:A:A:H2'  | 1:41:A:G:H5'' | 9        | 0.15          |
| (1,1301) | 1:8:A:A:H2'   | 1:9:A:G:H5'   | 4        | 0.15          |
| (1,1301) | 1:8:A:A:H2'   | 1:9:A:G:H5'   | 5        | 0.15          |
| (1,1301) | 1:8:A:A:H2'   | 1:9:A:G:H5'   | 6        | 0.15          |
| (1,1301) | 1:8:A:A:H2'   | 1:9:A:G:H5'   | 9        | 0.15          |
| (1,1280) | 1:18:A:C:H5'' | 1:17:A:G:H2'  | 2        | 0.15          |
| (1,1270) | 1:12:A:C:H3'  | 1:11:A:G:H2'  | 2        | 0.15          |
| (1,1270) | 1:12:A:C:H3'  | 1:11:A:G:H2'  | 6        | 0.15          |
| (1,1254) | 1:59:A:U:H6   | 1:58:A:G:H2'  | 6        | 0.15          |

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| Key      | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,1254) | 1:59:A:U:H6  | 1:58:A:G:H2'  | 9        | 0.15          |
| (1,1224) | 1:31:A:A:H1' | 1:32:A:G:H4'  | 3        | 0.15          |
| (1,1224) | 1:31:A:A:H1' | 1:32:A:G:H4'  | 6        | 0.15          |
| (1,1216) | 1:33:A:A:H2  | 1:34:A:G:H1'  | 4        | 0.15          |
| (1,1212) | 1:29:A:A:H2  | 1:49:A:G:H1'  | 6        | 0.15          |
| (1,1211) | 1:50:A:A:H8  | 1:49:A:G:H1'  | 6        | 0.15          |
| (1,1203) | 1:59:A:U:H3' | 1:58:A:G:H1'  | 8        | 0.15          |
| (1,1178) | 1:38:A:C:H5  | 1:37:A:G:H8   | 8        | 0.15          |
| (1,1163) | 1:15:A:C:H5' | 1:16:A:G:H8   | 1        | 0.15          |
| (1,1163) | 1:15:A:C:H5' | 1:16:A:G:H8   | 2        | 0.15          |
| (1,1163) | 1:15:A:C:H5' | 1:16:A:G:H8   | 3        | 0.15          |
| (1,1163) | 1:15:A:C:H5' | 1:16:A:G:H8   | 10       | 0.15          |
| (1,1106) | 1:49:A:G:H8  | 1:49:A:G:H3'  | 9        | 0.15          |
| (1,1042) | 1:20:A:A:H3' | 1:21:A:C:H5'' | 6        | 0.15          |
| (1,1042) | 1:20:A:A:H3' | 1:21:A:C:H5'' | 7        | 0.15          |
| (1,1029) | 1:26:A:A:H2' | 1:27:A:C:H5'' | 4        | 0.15          |
| (1,1021) | 1:44:A:A:H2  | 1:45:A:C:H1'  | 5        | 0.15          |
| (1,992)  | 1:28:A:U:H6  | 1:27:A:C:H5   | 9        | 0.15          |
| (1,965)  | 1:20:A:A:H2' | 1:21:A:C:H5'  | 6        | 0.15          |
| (1,965)  | 1:20:A:A:H2' | 1:21:A:C:H5'  | 7        | 0.15          |
| (1,951)  | 1:37:A:G:H1' | 1:38:A:C:H3'  | 2        | 0.15          |
| (1,938)  | 1:28:A:U:H2' | 1:27:A:C:H3'  | 10       | 0.15          |
| (1,934)  | 1:28:A:U:H3' | 1:27:A:C:H3'  | 8        | 0.15          |
| (1,929)  | 1:31:A:A:H8  | 1:30:A:C:H3'  | 10       | 0.15          |
| (1,921)  | 1:13:A:U:H3' | 1:12:A:C:H2'  | 5        | 0.15          |
| (1,913)  | 1:40:A:A:H8  | 1:39:A:C:H2'  | 4        | 0.15          |
| (1,908)  | 1:20:A:A:H8  | 1:19:A:C:H2'  | 3        | 0.15          |
| (1,905)  | 1:56:A:U:H6  | 1:55:A:C:H2'  | 10       | 0.15          |
| (1,902)  | 1:22:A:U:H4' | 1:21:A:C:H2'  | 2        | 0.15          |
| (1,902)  | 1:22:A:U:H4' | 1:21:A:C:H2'  | 3        | 0.15          |
| (1,900)  | 1:28:A:U:H3' | 1:27:A:C:H2'  | 7        | 0.15          |
| (1,895)  | 1:31:A:A:H8  | 1:30:A:C:H2'  | 4        | 0.15          |
| (1,893)  | 1:22:A:U:H6  | 1:21:A:C:H2'  | 4        | 0.15          |
| (1,885)  | 1:37:A:G:H2' | 1:38:A:C:H4'  | 2        | 0.15          |
| (1,874)  | 1:22:A:U:H5  | 1:21:A:C:H4'  | 1        | 0.15          |
| (1,874)  | 1:22:A:U:H5  | 1:21:A:C:H4'  | 5        | 0.15          |
| (1,871)  | 1:31:A:A:H8  | 1:30:A:C:H4'  | 4        | 0.15          |
| (1,860)  | 1:37:A:G:H4' | 1:36:A:C:H4'  | 7        | 0.15          |
| (1,830)  | 1:42:A:U:H2' | 1:43:A:C:H6   | 2        | 0.15          |
| (1,824)  | 1:16:A:G:H1' | 1:15:A:C:H1'  | 7        | 0.15          |
| (1,724)  | 1:43:A:C:H6  | 1:43:A:C:H2'  | 10       | 0.15          |
| (1,713)  | 1:36:A:C:H2' | 1:36:A:C:H3'  | 2        | 0.15          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,706)  | 1:15:A:C:H5'' | 1:15:A:C:H3'  | 4        | 0.15          |
| (1,706)  | 1:15:A:C:H5'' | 1:15:A:C:H3'  | 8        | 0.15          |
| (1,678)  | 1:54:A:C:H4'  | 1:54:A:C:H6   | 10       | 0.15          |
| (1,664)  | 1:58:A:G:H4'  | 1:59:A:U:H4'  | 7        | 0.15          |
| (1,659)  | 1:50:A:A:H2'  | 1:51:A:U:H4'  | 5        | 0.15          |
| (1,632)  | 1:29:A:A:H4'  | 1:28:A:U:H3'  | 6        | 0.15          |
| (1,608)  | 1:45:A:C:H3'  | 1:46:A:U:H1'  | 2        | 0.15          |
| (1,581)  | 1:45:A:C:H4'  | 1:46:A:U:H6   | 6        | 0.15          |
| (1,574)  | 1:56:A:U:H5'' | 1:56:A:U:H4'  | 1        | 0.15          |
| (1,574)  | 1:56:A:U:H5'' | 1:56:A:U:H4'  | 10       | 0.15          |
| (1,443)  | 1:46:A:U:H4'  | 1:46:A:U:H6   | 5        | 0.15          |
| (1,437)  | 1:30:A:C:H4'  | 1:31:A:A:H5'' | 8        | 0.15          |
| (1,435)  | 1:30:A:C:H2'  | 1:31:A:A:H5'' | 10       | 0.15          |
| (1,426)  | 1:45:A:C:H1'  | 1:44:A:A:H2'  | 10       | 0.15          |
| (1,412)  | 1:2:A:G:H2'   | 1:3:A:A:H5''  | 1        | 0.15          |
| (1,409)  | 1:2:A:G:H2'   | 1:3:A:A:H5'   | 6        | 0.15          |
| (1,383)  | 1:5:A:G:H1'   | 1:4:A:A:H1'   | 5        | 0.15          |
| (1,378)  | 1:5:A:G:H1'   | 1:6:A:A:H1'   | 3        | 0.15          |
| (1,346)  | 1:23:A:C:H1'  | 1:24:A:A:H4'  | 10       | 0.15          |
| (1,338)  | 1:30:A:C:H6   | 1:29:A:A:H8   | 6        | 0.15          |
| (1,335)  | 1:23:A:C:H5   | 1:24:A:A:H8   | 7        | 0.15          |
| (1,321)  | 1:26:A:A:H3'  | 1:26:A:A:H2   | 2        | 0.15          |
| (1,321)  | 1:26:A:A:H3'  | 1:26:A:A:H2   | 6        | 0.15          |
| (1,310)  | 1:31:A:A:H4'  | 1:31:A:A:H8   | 3        | 0.15          |
| (1,310)  | 1:31:A:A:H4'  | 1:31:A:A:H8   | 9        | 0.15          |
| (1,307)  | 1:48:A:A:H3'  | 1:48:A:A:H5'  | 9        | 0.15          |
| (1,291)  | 1:24:A:A:H8   | 1:24:A:A:H5'' | 4        | 0.15          |
| (1,213)  | 1:26:A:A:H8   | 1:26:A:A:H3'  | 4        | 0.15          |
| (1,202)  | 1:4:A:A:H8    | 1:4:A:A:H2'   | 3        | 0.15          |
| (1,200)  | 1:8:A:A:H8    | 1:8:A:A:H2'   | 10       | 0.15          |
| (1,169)  | 1:3:A:A:H2'   | 1:3:A:A:H8    | 2        | 0.15          |
| (1,168)  | 1:50:A:A:H3'  | 1:50:A:A:H8   | 2        | 0.15          |
| (1,163)  | 1:49:A:G:H2'  | 1:47:A:C:H3'  | 5        | 0.15          |
| (1,161)  | 1:24:A:A:H4'  | 1:23:A:C:H1'  | 10       | 0.15          |
| (1,146)  | 1:24:A:A:H3'  | 1:23:A:C:H3'  | 8        | 0.15          |
| (1,139)  | 1:42:A:U:H3'  | 1:43:A:C:H6   | 2        | 0.15          |
| (1,104)  | 1:21:A:C:H5   | 1:20:A:A:H4'  | 6        | 0.15          |
| (1,1330) | 1:38:A:C:H5   | 1:37:A:G:H3'  | 2        | 0.14          |
| (1,1330) | 1:38:A:C:H5   | 1:37:A:G:H3'  | 6        | 0.14          |
| (1,1325) | 1:38:A:C:H5   | 1:37:A:G:H4'  | 1        | 0.14          |
| (1,1317) | 1:59:A:U:H5   | 1:58:A:G:H3'  | 2        | 0.14          |
| (1,1316) | 1:59:A:U:H6   | 1:58:A:G:H3'  | 5        | 0.14          |

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| Key      | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,1306) | 1:40:A:A:H2' | 1:41:A:G:H5'' | 1        | 0.14          |
| (1,1306) | 1:40:A:A:H2' | 1:41:A:G:H5'' | 5        | 0.14          |
| (1,1306) | 1:40:A:A:H2' | 1:41:A:G:H5'' | 8        | 0.14          |
| (1,1306) | 1:40:A:A:H2' | 1:41:A:G:H5'' | 10       | 0.14          |
| (1,1270) | 1:12:A:C:H3' | 1:11:A:G:H2'  | 9        | 0.14          |
| (1,1268) | 1:42:A:U:H6  | 1:41:A:G:H3'  | 3        | 0.14          |
| (1,1259) | 1:59:A:U:H5  | 1:58:A:G:H2'  | 3        | 0.14          |
| (1,1238) | 1:12:A:C:H5  | 1:11:A:G:H4'  | 4        | 0.14          |
| (1,1238) | 1:12:A:C:H5  | 1:11:A:G:H4'  | 8        | 0.14          |
| (1,1235) | 1:59:A:U:H5  | 1:58:A:G:H4'  | 9        | 0.14          |
| (1,1227) | 1:33:A:A:H8  | 1:32:A:G:H4'  | 1        | 0.14          |
| (1,1220) | 1:3:A:A:H8   | 1:2:A:G:H4'   | 3        | 0.14          |
| (1,1216) | 1:33:A:A:H2  | 1:34:A:G:H1'  | 1        | 0.14          |
| (1,1211) | 1:50:A:A:H8  | 1:49:A:G:H1'  | 2        | 0.14          |
| (1,1211) | 1:50:A:A:H8  | 1:49:A:G:H1'  | 3        | 0.14          |
| (1,1208) | 1:3:A:A:H8   | 1:2:A:G:H1'   | 2        | 0.14          |
| (1,1208) | 1:3:A:A:H8   | 1:2:A:G:H1'   | 5        | 0.14          |
| (1,1203) | 1:59:A:U:H3' | 1:58:A:G:H1'  | 3        | 0.14          |
| (1,1163) | 1:15:A:C:H5' | 1:16:A:G:H8   | 4        | 0.14          |
| (1,1163) | 1:15:A:C:H5' | 1:16:A:G:H8   | 7        | 0.14          |
| (1,1163) | 1:15:A:C:H5' | 1:16:A:G:H8   | 8        | 0.14          |
| (1,1163) | 1:15:A:C:H5' | 1:16:A:G:H8   | 9        | 0.14          |
| (1,1048) | 1:44:A:A:H1' | 1:54:A:C:H5   | 7        | 0.14          |
| (1,1039) | 1:29:A:A:H3' | 1:30:A:C:H5'  | 7        | 0.14          |
| (1,1027) | 1:37:A:G:H8  | 1:36:A:C:H1'  | 2        | 0.14          |
| (1,1025) | 1:46:A:U:H3' | 1:47:A:C:H1'  | 8        | 0.14          |
| (1,1021) | 1:44:A:A:H2  | 1:45:A:C:H1'  | 9        | 0.14          |
| (1,1008) | 1:42:A:U:H3' | 1:43:A:C:H1'  | 5        | 0.14          |
| (1,1006) | 1:44:A:A:H2  | 1:55:A:C:H1'  | 9        | 0.14          |
| (1,997)  | 1:37:A:G:H2' | 1:38:A:C:H5   | 3        | 0.14          |
| (1,965)  | 1:20:A:A:H2' | 1:21:A:C:H5'  | 4        | 0.14          |
| (1,965)  | 1:20:A:A:H2' | 1:21:A:C:H5'  | 8        | 0.14          |
| (1,954)  | 1:37:A:G:H3' | 1:38:A:C:H3'  | 5        | 0.14          |
| (1,940)  | 1:22:A:U:H6  | 1:21:A:C:H3'  | 10       | 0.14          |
| (1,939)  | 1:28:A:U:H6  | 1:27:A:C:H3'  | 1        | 0.14          |
| (1,939)  | 1:28:A:U:H6  | 1:27:A:C:H3'  | 8        | 0.14          |
| (1,927)  | 1:44:A:A:H8  | 1:43:A:C:H3'  | 1        | 0.14          |
| (1,899)  | 1:31:A:A:H3' | 1:30:A:C:H2'  | 3        | 0.14          |
| (1,898)  | 1:31:A:A:H1' | 1:30:A:C:H2'  | 6        | 0.14          |
| (1,895)  | 1:31:A:A:H8  | 1:30:A:C:H2'  | 5        | 0.14          |
| (1,860)  | 1:37:A:G:H4' | 1:36:A:C:H4'  | 2        | 0.14          |
| (1,823)  | 1:46:A:U:H4' | 1:47:A:C:H6   | 1        | 0.14          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,823) | 1:46:A:U:H4'  | 1:47:A:C:H6   | 5        | 0.14          |
| (1,820) | 1:50:A:A:H8   | 1:47:A:C:H6   | 5        | 0.14          |
| (1,763) | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 2        | 0.14          |
| (1,763) | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 3        | 0.14          |
| (1,763) | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 4        | 0.14          |
| (1,763) | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 5        | 0.14          |
| (1,763) | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 6        | 0.14          |
| (1,763) | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 7        | 0.14          |
| (1,763) | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 9        | 0.14          |
| (1,763) | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 10       | 0.14          |
| (1,713) | 1:36:A:C:H2'  | 1:36:A:C:H3'  | 10       | 0.14          |
| (1,706) | 1:15:A:C:H5'' | 1:15:A:C:H3'  | 1        | 0.14          |
| (1,670) | 1:52:A:A:H2'  | 1:53:A:U:H5'  | 7        | 0.14          |
| (1,664) | 1:58:A:G:H4'  | 1:59:A:U:H4'  | 2        | 0.14          |
| (1,664) | 1:58:A:G:H4'  | 1:59:A:U:H4'  | 4        | 0.14          |
| (1,664) | 1:58:A:G:H4'  | 1:59:A:U:H4'  | 9        | 0.14          |
| (1,662) | 1:27:A:C:H2'  | 1:28:A:U:H4'  | 5        | 0.14          |
| (1,649) | 1:45:A:C:H4'  | 1:46:A:U:H5'' | 9        | 0.14          |
| (1,629) | 1:57:A:G:H8   | 1:56:A:U:H2'  | 8        | 0.14          |
| (1,628) | 1:29:A:A:H8   | 1:28:A:U:H2'  | 2        | 0.14          |
| (1,593) | 1:50:A:A:H1'  | 1:51:A:U:H5   | 3        | 0.14          |
| (1,593) | 1:50:A:A:H1'  | 1:51:A:U:H5   | 4        | 0.14          |
| (1,581) | 1:45:A:C:H4'  | 1:46:A:U:H6   | 9        | 0.14          |
| (1,574) | 1:56:A:U:H5'' | 1:56:A:U:H4'  | 8        | 0.14          |
| (1,524) | 1:59:A:U:H2'  | 1:59:A:U:H3'  | 8        | 0.14          |
| (1,506) | 1:28:A:U:H6   | 1:28:A:U:H3'  | 9        | 0.14          |
| (1,482) | 1:51:A:U:H5'' | 1:51:A:U:H3'  | 10       | 0.14          |
| (1,481) | 1:51:A:U:H2'  | 1:51:A:U:H3'  | 1        | 0.14          |
| (1,478) | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 3        | 0.14          |
| (1,426) | 1:45:A:C:H1'  | 1:44:A:A:H2'  | 8        | 0.14          |
| (1,410) | 1:2:A:G:H3'   | 1:3:A:A:H5'   | 9        | 0.14          |
| (1,383) | 1:5:A:G:H1'   | 1:4:A:A:H1'   | 2        | 0.14          |
| (1,366) | 1:9:A:G:H8    | 1:8:A:A:H3'   | 7        | 0.14          |
| (1,346) | 1:23:A:C:H1'  | 1:24:A:A:H4'  | 3        | 0.14          |
| (1,340) | 1:19:A:C:H4'  | 1:20:A:A:H8   | 4        | 0.14          |
| (1,296) | 1:3:A:A:H3'   | 1:3:A:A:H5'   | 9        | 0.14          |
| (1,283) | 1:20:A:A:H8   | 1:20:A:A:H5'' | 10       | 0.14          |
| (1,280) | 1:52:A:A:H5'' | 1:52:A:A:H3'  | 1        | 0.14          |
| (1,280) | 1:52:A:A:H5'' | 1:52:A:A:H3'  | 6        | 0.14          |
| (1,275) | 1:40:A:A:H5'  | 1:40:A:A:H4'  | 1        | 0.14          |
| (1,275) | 1:40:A:A:H5'  | 1:40:A:A:H4'  | 4        | 0.14          |
| (1,257) | 1:7:A:A:H3'   | 1:6:A:A:H2    | 9        | 0.14          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,208)  | 1:6:A:A:H8    | 1:6:A:A:H2'   | 3        | 0.14          |
| (1,201)  | 1:20:A:A:H8   | 1:20:A:A:H2'  | 7        | 0.14          |
| (1,200)  | 1:8:A:A:H8    | 1:8:A:A:H2'   | 7        | 0.14          |
| (1,196)  | 1:52:A:A:H8   | 1:52:A:A:H2'  | 3        | 0.14          |
| (1,195)  | 1:52:A:A:H5'' | 1:52:A:A:H4'  | 3        | 0.14          |
| (1,163)  | 1:49:A:G:H2'  | 1:47:A:C:H3'  | 1        | 0.14          |
| (1,161)  | 1:24:A:A:H4'  | 1:23:A:C:H1'  | 3        | 0.14          |
| (1,150)  | 1:46:A:U:H6   | 1:47:A:C:H5'  | 4        | 0.14          |
| (1,150)  | 1:46:A:U:H6   | 1:47:A:C:H5'' | 4        | 0.14          |
| (1,150)  | 1:46:A:U:H6   | 1:47:A:C:H5'  | 10       | 0.14          |
| (1,150)  | 1:46:A:U:H6   | 1:47:A:C:H5'' | 10       | 0.14          |
| (1,146)  | 1:24:A:A:H3'  | 1:23:A:C:H3'  | 1        | 0.14          |
| (1,104)  | 1:21:A:C:H5   | 1:20:A:A:H4'  | 8        | 0.14          |
| (1,1330) | 1:38:A:C:H5   | 1:37:A:G:H3'  | 1        | 0.13          |
| (1,1329) | 1:38:A:C:H6   | 1:37:A:G:H3'  | 9        | 0.13          |
| (1,1328) | 1:12:A:C:H6   | 1:11:A:G:H5'' | 1        | 0.13          |
| (1,1328) | 1:12:A:C:H6   | 1:11:A:G:H5'' | 2        | 0.13          |
| (1,1325) | 1:38:A:C:H5   | 1:37:A:G:H4'  | 2        | 0.13          |
| (1,1318) | 1:59:A:U:H3'  | 1:58:A:G:H3'  | 7        | 0.13          |
| (1,1317) | 1:59:A:U:H5   | 1:58:A:G:H3'  | 9        | 0.13          |
| (1,1314) | 1:12:A:C:H4'  | 1:11:A:G:H3'  | 8        | 0.13          |
| (1,1309) | 1:33:A:A:H8   | 1:32:A:G:H2'  | 2        | 0.13          |
| (1,1309) | 1:33:A:A:H8   | 1:32:A:G:H2'  | 4        | 0.13          |
| (1,1309) | 1:33:A:A:H8   | 1:32:A:G:H2'  | 10       | 0.13          |
| (1,1301) | 1:8:A:A:H2'   | 1:9:A:G:H5'   | 3        | 0.13          |
| (1,1301) | 1:8:A:A:H2'   | 1:9:A:G:H5'   | 10       | 0.13          |
| (1,1270) | 1:12:A:C:H3'  | 1:11:A:G:H2'  | 7        | 0.13          |
| (1,1259) | 1:59:A:U:H5   | 1:58:A:G:H2'  | 9        | 0.13          |
| (1,1254) | 1:59:A:U:H6   | 1:58:A:G:H2'  | 3        | 0.13          |
| (1,1238) | 1:12:A:C:H5   | 1:11:A:G:H4'  | 10       | 0.13          |
| (1,1224) | 1:31:A:A:H1'  | 1:32:A:G:H4'  | 10       | 0.13          |
| (1,1221) | 1:6:A:A:H5''  | 1:5:A:G:H4'   | 5        | 0.13          |
| (1,1212) | 1:29:A:A:H2   | 1:49:A:G:H1'  | 2        | 0.13          |
| (1,1197) | 1:56:A:U:H1'  | 1:57:A:G:H1'  | 2        | 0.13          |
| (1,1197) | 1:56:A:U:H1'  | 1:57:A:G:H1'  | 7        | 0.13          |
| (1,1180) | 1:36:A:C:H6   | 1:37:A:G:H8   | 6        | 0.13          |
| (1,1179) | 1:38:A:C:H6   | 1:37:A:G:H8   | 7        | 0.13          |
| (1,1179) | 1:38:A:C:H6   | 1:37:A:G:H8   | 8        | 0.13          |
| (1,1050) | 1:31:A:A:H5'  | 1:30:A:C:H6   | 7        | 0.13          |
| (1,1048) | 1:44:A:A:H1'  | 1:54:A:C:H5   | 3        | 0.13          |
| (1,1042) | 1:20:A:A:H3'  | 1:21:A:C:H5'' | 5        | 0.13          |
| (1,1039) | 1:29:A:A:H3'  | 1:30:A:C:H5'  | 5        | 0.13          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1027) | 1:37:A:G:H8   | 1:36:A:C:H1'  | 1        | 0.13          |
| (1,1006) | 1:44:A:A:H2   | 1:55:A:C:H1'  | 6        | 0.13          |
| (1,1006) | 1:44:A:A:H2   | 1:55:A:C:H1'  | 8        | 0.13          |
| (1,981)  | 1:53:A:U:H6   | 1:54:A:C:H5   | 6        | 0.13          |
| (1,965)  | 1:20:A:A:H2'  | 1:21:A:C:H5'  | 9        | 0.13          |
| (1,951)  | 1:37:A:G:H1'  | 1:38:A:C:H3'  | 10       | 0.13          |
| (1,940)  | 1:22:A:U:H6   | 1:21:A:C:H3'  | 9        | 0.13          |
| (1,939)  | 1:28:A:U:H6   | 1:27:A:C:H3'  | 6        | 0.13          |
| (1,938)  | 1:28:A:U:H2'  | 1:27:A:C:H3'  | 1        | 0.13          |
| (1,928)  | 1:42:A:U:H3'  | 1:43:A:C:H3'  | 3        | 0.13          |
| (1,928)  | 1:42:A:U:H3'  | 1:43:A:C:H3'  | 9        | 0.13          |
| (1,921)  | 1:13:A:U:H3'  | 1:12:A:C:H2'  | 6        | 0.13          |
| (1,921)  | 1:13:A:U:H3'  | 1:12:A:C:H2'  | 9        | 0.13          |
| (1,905)  | 1:56:A:U:H6   | 1:55:A:C:H2'  | 5        | 0.13          |
| (1,901)  | 1:22:A:U:H3'  | 1:21:A:C:H2'  | 9        | 0.13          |
| (1,899)  | 1:31:A:A:H3'  | 1:30:A:C:H2'  | 2        | 0.13          |
| (1,895)  | 1:31:A:A:H8   | 1:30:A:C:H2'  | 3        | 0.13          |
| (1,885)  | 1:37:A:G:H2'  | 1:38:A:C:H4'  | 5        | 0.13          |
| (1,878)  | 1:26:A:A:H2'  | 1:27:A:C:H4'  | 9        | 0.13          |
| (1,872)  | 1:26:A:A:H2   | 1:27:A:C:H4'  | 6        | 0.13          |
| (1,871)  | 1:31:A:A:H8   | 1:30:A:C:H4'  | 6        | 0.13          |
| (1,829)  | 1:13:A:U:H1'  | 1:15:A:C:H6   | 1        | 0.13          |
| (1,763)  | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 1        | 0.13          |
| (1,763)  | 1:15:A:C:H4'  | 1:15:A:C:H5'  | 8        | 0.13          |
| (1,733)  | 1:43:A:C:H6   | 1:43:A:C:H3'  | 4        | 0.13          |
| (1,681)  | 1:54:A:C:H2'  | 1:55:A:C:H6   | 5        | 0.13          |
| (1,664)  | 1:58:A:G:H4'  | 1:59:A:U:H4'  | 3        | 0.13          |
| (1,632)  | 1:29:A:A:H4'  | 1:28:A:U:H3'  | 5        | 0.13          |
| (1,593)  | 1:50:A:A:H1'  | 1:51:A:U:H5   | 6        | 0.13          |
| (1,593)  | 1:50:A:A:H1'  | 1:51:A:U:H5   | 10       | 0.13          |
| (1,574)  | 1:56:A:U:H5'' | 1:56:A:U:H4'  | 7        | 0.13          |
| (1,551)  | 1:28:A:U:H3'  | 1:28:A:U:H5'' | 4        | 0.13          |
| (1,524)  | 1:59:A:U:H2'  | 1:59:A:U:H3'  | 2        | 0.13          |
| (1,524)  | 1:59:A:U:H2'  | 1:59:A:U:H3'  | 5        | 0.13          |
| (1,481)  | 1:51:A:U:H2'  | 1:51:A:U:H3'  | 5        | 0.13          |
| (1,478)  | 1:14:A:U:H5'' | 1:14:A:U:H3'  | 4        | 0.13          |
| (1,455)  | 1:59:A:U:H3'  | 1:59:A:U:H5   | 4        | 0.13          |
| (1,446)  | 1:59:A:U:H5   | 1:59:A:U:H6   | 4        | 0.13          |
| (1,435)  | 1:30:A:C:H2'  | 1:31:A:A:H5'' | 1        | 0.13          |
| (1,426)  | 1:45:A:C:H1'  | 1:44:A:A:H2'  | 3        | 0.13          |
| (1,426)  | 1:45:A:C:H1'  | 1:44:A:A:H2'  | 4        | 0.13          |
| (1,426)  | 1:45:A:C:H1'  | 1:44:A:A:H2'  | 5        | 0.13          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,426)  | 1:45:A:C:H1'  | 1:44:A:A:H2'  | 6        | 0.13          |
| (1,425)  | 1:49:A:G:H4'  | 1:50:A:A:H4'  | 8        | 0.13          |
| (1,424)  | 1:49:A:G:H2'  | 1:50:A:A:H4'  | 4        | 0.13          |
| (1,419)  | 1:19:A:C:H2'  | 1:20:A:A:H3'  | 3        | 0.13          |
| (1,418)  | 1:19:A:C:H3'  | 1:20:A:A:H3'  | 4        | 0.13          |
| (1,412)  | 1:2:A:G:H2'   | 1:3:A:A:H5''  | 4        | 0.13          |
| (1,383)  | 1:5:A:G:H1'   | 1:4:A:A:H1'   | 1        | 0.13          |
| (1,378)  | 1:5:A:G:H1'   | 1:6:A:A:H1'   | 4        | 0.13          |
| (1,371)  | 1:45:A:C:H5   | 1:44:A:A:H1'  | 7        | 0.13          |
| (1,348)  | 1:46:A:U:H5'' | 1:52:A:A:H4'  | 10       | 0.13          |
| (1,299)  | 1:3:A:A:H8    | 1:3:A:A:H5''  | 5        | 0.13          |
| (1,291)  | 1:24:A:A:H8   | 1:24:A:A:H5'' | 6        | 0.13          |
| (1,275)  | 1:40:A:A:H5'  | 1:40:A:A:H4'  | 5        | 0.13          |
| (1,203)  | 1:40:A:A:H8   | 1:40:A:A:H2'  | 3        | 0.13          |
| (1,201)  | 1:20:A:A:H8   | 1:20:A:A:H2'  | 5        | 0.13          |
| (1,195)  | 1:52:A:A:H5'' | 1:52:A:A:H4'  | 9        | 0.13          |
| (1,181)  | 1:8:A:A:H3'   | 1:8:A:A:H8    | 6        | 0.13          |
| (1,128)  | 1:4:A:A:H3'   | 1:5:A:G:H1'   | 2        | 0.13          |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'  | 3        | 0.13          |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'' | 3        | 0.13          |
| (1,105)  | 1:27:A:C:H5   | 1:26:A:A:H4'  | 7        | 0.13          |
| (1,3)    | 1:41:A:G:H4'  | 1:40:A:A:H1'  | 3        | 0.13          |
| (1,1328) | 1:12:A:C:H6   | 1:11:A:G:H5'' | 3        | 0.12          |
| (1,1317) | 1:59:A:U:H5   | 1:58:A:G:H3'  | 3        | 0.12          |
| (1,1314) | 1:12:A:C:H4'  | 1:11:A:G:H3'  | 7        | 0.12          |
| (1,1309) | 1:33:A:A:H8   | 1:32:A:G:H2'  | 9        | 0.12          |
| (1,1301) | 1:8:A:A:H2'   | 1:9:A:G:H5'   | 1        | 0.12          |
| (1,1301) | 1:8:A:A:H2'   | 1:9:A:G:H5'   | 7        | 0.12          |
| (1,1270) | 1:12:A:C:H3'  | 1:11:A:G:H2'  | 10       | 0.12          |
| (1,1264) | 1:38:A:C:H6   | 1:37:A:G:H2'  | 3        | 0.12          |
| (1,1254) | 1:59:A:U:H6   | 1:58:A:G:H2'  | 5        | 0.12          |
| (1,1249) | 1:50:A:A:H5'' | 1:49:A:G:H3'  | 1        | 0.12          |
| (1,1238) | 1:12:A:C:H5   | 1:11:A:G:H4'  | 3        | 0.12          |
| (1,1235) | 1:59:A:U:H5   | 1:58:A:G:H4'  | 2        | 0.12          |
| (1,1216) | 1:33:A:A:H2   | 1:34:A:G:H1'  | 6        | 0.12          |
| (1,1197) | 1:56:A:U:H1'  | 1:57:A:G:H1'  | 4        | 0.12          |
| (1,1191) | 1:59:A:U:H6   | 1:58:A:G:H8   | 4        | 0.12          |
| (1,1163) | 1:15:A:C:H5'  | 1:16:A:G:H8   | 5        | 0.12          |
| (1,1106) | 1:49:A:G:H8   | 1:49:A:G:H3'  | 2        | 0.12          |
| (1,1053) | 1:46:A:U:H4'  | 1:45:A:C:H3'  | 2        | 0.12          |
| (1,1035) | 1:31:A:A:H8   | 1:30:A:C:H6   | 9        | 0.12          |
| (1,1032) | 1:29:A:A:H3'  | 1:30:A:C:H6   | 8        | 0.12          |

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| Key      | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|----------|--------------|---------------|----------|---------------|
| (1,1026) | 1:50:A:A:H4' | 1:47:A:C:H1'  | 8        | 0.12          |
| (1,1016) | 1:22:A:U:H1' | 1:23:A:C:H1'  | 1        | 0.12          |
| (1,1008) | 1:42:A:U:H3' | 1:43:A:C:H1'  | 4        | 0.12          |
| (1,1007) | 1:44:A:A:H8  | 1:43:A:C:H1'  | 4        | 0.12          |
| (1,1006) | 1:44:A:A:H2  | 1:55:A:C:H1'  | 2        | 0.12          |
| (1,992)  | 1:28:A:U:H6  | 1:27:A:C:H5   | 2        | 0.12          |
| (1,961)  | 1:35:A:A:H2' | 1:36:A:C:H5'  | 1        | 0.12          |
| (1,954)  | 1:37:A:G:H3' | 1:38:A:C:H3'  | 2        | 0.12          |
| (1,946)  | 1:40:A:A:H4' | 1:39:A:C:H3'  | 5        | 0.12          |
| (1,946)  | 1:40:A:A:H4' | 1:39:A:C:H3'  | 9        | 0.12          |
| (1,940)  | 1:22:A:U:H6  | 1:21:A:C:H3'  | 7        | 0.12          |
| (1,928)  | 1:42:A:U:H3' | 1:43:A:C:H3'  | 10       | 0.12          |
| (1,912)  | 1:13:A:U:H6  | 1:12:A:C:H2'  | 4        | 0.12          |
| (1,905)  | 1:56:A:U:H6  | 1:55:A:C:H2'  | 8        | 0.12          |
| (1,902)  | 1:22:A:U:H4' | 1:21:A:C:H2'  | 1        | 0.12          |
| (1,900)  | 1:28:A:U:H3' | 1:27:A:C:H2'  | 1        | 0.12          |
| (1,886)  | 1:14:A:U:H4' | 1:15:A:C:H2'  | 1        | 0.12          |
| (1,885)  | 1:37:A:G:H2' | 1:38:A:C:H4'  | 7        | 0.12          |
| (1,874)  | 1:22:A:U:H5  | 1:21:A:C:H4'  | 9        | 0.12          |
| (1,872)  | 1:26:A:A:H2  | 1:27:A:C:H4'  | 8        | 0.12          |
| (1,865)  | 1:46:A:U:H3' | 1:47:A:C:H4'  | 8        | 0.12          |
| (1,860)  | 1:37:A:G:H4' | 1:36:A:C:H4'  | 10       | 0.12          |
| (1,851)  | 1:29:A:A:H4' | 1:30:A:C:H6   | 10       | 0.12          |
| (1,832)  | 1:56:A:U:H6  | 1:55:A:C:H6   | 5        | 0.12          |
| (1,829)  | 1:13:A:U:H1' | 1:15:A:C:H6   | 8        | 0.12          |
| (1,829)  | 1:13:A:U:H1' | 1:15:A:C:H6   | 10       | 0.12          |
| (1,815)  | 1:39:A:C:H5  | 1:39:A:C:H5'' | 9        | 0.12          |
| (1,793)  | 1:27:A:C:H6  | 1:27:A:C:H5   | 3        | 0.12          |
| (1,793)  | 1:27:A:C:H6  | 1:27:A:C:H5   | 4        | 0.12          |
| (1,793)  | 1:27:A:C:H6  | 1:27:A:C:H5   | 5        | 0.12          |
| (1,793)  | 1:27:A:C:H6  | 1:27:A:C:H5   | 6        | 0.12          |
| (1,793)  | 1:27:A:C:H6  | 1:27:A:C:H5   | 8        | 0.12          |
| (1,793)  | 1:27:A:C:H6  | 1:27:A:C:H5   | 9        | 0.12          |
| (1,748)  | 1:12:A:C:H2' | 1:12:A:C:H3'  | 2        | 0.12          |
| (1,681)  | 1:54:A:C:H2' | 1:55:A:C:H6   | 4        | 0.12          |
| (1,665)  | 1:54:A:C:H6  | 1:53:A:U:H6   | 6        | 0.12          |
| (1,649)  | 1:45:A:C:H4' | 1:46:A:U:H5'' | 1        | 0.12          |
| (1,637)  | 1:23:A:C:H3' | 1:22:A:U:H3'  | 10       | 0.12          |
| (1,629)  | 1:57:A:G:H8  | 1:56:A:U:H2'  | 2        | 0.12          |
| (1,629)  | 1:57:A:G:H8  | 1:56:A:U:H2'  | 10       | 0.12          |
| (1,620)  | 1:44:A:A:H8  | 1:42:A:U:H2'  | 3        | 0.12          |
| (1,620)  | 1:44:A:A:H8  | 1:42:A:U:H2'  | 9        | 0.12          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,608)  | 1:45:A:C:H3'  | 1:46:A:U:H1'  | 8        | 0.12          |
| (1,593)  | 1:50:A:A:H1'  | 1:51:A:U:H5   | 7        | 0.12          |
| (1,581)  | 1:45:A:C:H4'  | 1:46:A:U:H6   | 1        | 0.12          |
| (1,581)  | 1:45:A:C:H4'  | 1:46:A:U:H6   | 7        | 0.12          |
| (1,574)  | 1:56:A:U:H5'' | 1:56:A:U:H4'  | 2        | 0.12          |
| (1,541)  | 1:53:A:U:H4'  | 1:53:A:U:H5'  | 2        | 0.12          |
| (1,528)  | 1:56:A:U:H2'  | 1:56:A:U:H3'  | 2        | 0.12          |
| (1,524)  | 1:59:A:U:H2'  | 1:59:A:U:H3'  | 3        | 0.12          |
| (1,524)  | 1:59:A:U:H2'  | 1:59:A:U:H3'  | 4        | 0.12          |
| (1,524)  | 1:59:A:U:H2'  | 1:59:A:U:H3'  | 7        | 0.12          |
| (1,500)  | 1:59:A:U:H6   | 1:59:A:U:H2'  | 7        | 0.12          |
| (1,497)  | 1:42:A:U:H6   | 1:42:A:U:H2'  | 9        | 0.12          |
| (1,435)  | 1:30:A:C:H2'  | 1:31:A:A:H5'' | 6        | 0.12          |
| (1,431)  | 1:28:A:U:H2'  | 1:29:A:A:H5'  | 4        | 0.12          |
| (1,378)  | 1:5:A:G:H1'   | 1:6:A:A:H1'   | 5        | 0.12          |
| (1,378)  | 1:5:A:G:H1'   | 1:6:A:A:H1'   | 6        | 0.12          |
| (1,348)  | 1:46:A:U:H5'' | 1:52:A:A:H4'  | 4        | 0.12          |
| (1,346)  | 1:23:A:C:H1'  | 1:24:A:A:H4'  | 7        | 0.12          |
| (1,335)  | 1:23:A:C:H5   | 1:24:A:A:H8   | 9        | 0.12          |
| (1,321)  | 1:26:A:A:H3'  | 1:26:A:A:H2   | 1        | 0.12          |
| (1,304)  | 1:29:A:A:H8   | 1:29:A:A:H5'' | 6        | 0.12          |
| (1,283)  | 1:20:A:A:H8   | 1:20:A:A:H5'' | 1        | 0.12          |
| (1,208)  | 1:6:A:A:H8    | 1:6:A:A:H2'   | 5        | 0.12          |
| (1,208)  | 1:6:A:A:H8    | 1:6:A:A:H2'   | 10       | 0.12          |
| (1,202)  | 1:4:A:A:H8    | 1:4:A:A:H2'   | 4        | 0.12          |
| (1,202)  | 1:4:A:A:H8    | 1:4:A:A:H2'   | 7        | 0.12          |
| (1,202)  | 1:4:A:A:H8    | 1:4:A:A:H2'   | 9        | 0.12          |
| (1,200)  | 1:8:A:A:H8    | 1:8:A:A:H2'   | 6        | 0.12          |
| (1,195)  | 1:52:A:A:H5'' | 1:52:A:A:H4'  | 4        | 0.12          |
| (1,169)  | 1:3:A:A:H2'   | 1:3:A:A:H8    | 10       | 0.12          |
| (1,161)  | 1:24:A:A:H4'  | 1:23:A:C:H1'  | 7        | 0.12          |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'  | 2        | 0.12          |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'' | 2        | 0.12          |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'  | 10       | 0.12          |
| (1,114)  | 1:45:A:C:H3'  | 1:52:A:A:H5'' | 10       | 0.12          |
| (1,105)  | 1:27:A:C:H5   | 1:26:A:A:H4'  | 5        | 0.12          |
| (1,1330) | 1:38:A:C:H5   | 1:37:A:G:H3'  | 10       | 0.11          |
| (1,1328) | 1:12:A:C:H6   | 1:11:A:G:H5'' | 4        | 0.11          |
| (1,1328) | 1:12:A:C:H6   | 1:11:A:G:H5'' | 6        | 0.11          |
| (1,1316) | 1:59:A:U:H6   | 1:58:A:G:H3'  | 1        | 0.11          |
| (1,1316) | 1:59:A:U:H6   | 1:58:A:G:H3'  | 7        | 0.11          |
| (1,1306) | 1:40:A:A:H2'  | 1:41:A:G:H5'' | 3        | 0.11          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,1306) | 1:40:A:A:H2'  | 1:41:A:G:H5'' | 4        | 0.11          |
| (1,1306) | 1:40:A:A:H2'  | 1:41:A:G:H5'' | 7        | 0.11          |
| (1,1254) | 1:59:A:U:H6   | 1:58:A:G:H2'  | 7        | 0.11          |
| (1,1254) | 1:59:A:U:H6   | 1:58:A:G:H2'  | 8        | 0.11          |
| (1,1238) | 1:12:A:C:H5   | 1:11:A:G:H4'  | 1        | 0.11          |
| (1,1234) | 1:15:A:C:H5'' | 1:16:A:G:H4'  | 5        | 0.11          |
| (1,1224) | 1:31:A:A:H1'  | 1:32:A:G:H4'  | 9        | 0.11          |
| (1,1212) | 1:29:A:A:H2   | 1:49:A:G:H1'  | 9        | 0.11          |
| (1,1212) | 1:29:A:A:H2   | 1:49:A:G:H1'  | 10       | 0.11          |
| (1,1207) | 1:8:A:A:H3'   | 1:9:A:G:H1'   | 9        | 0.11          |
| (1,1160) | 1:15:A:C:H1'  | 1:16:A:G:H8   | 5        | 0.11          |
| (1,1060) | 1:1:A:GTP:H1' | 1:2:A:G:H8    | 3        | 0.11          |
| (1,1053) | 1:46:A:U:H4'  | 1:45:A:C:H3'  | 8        | 0.11          |
| (1,1026) | 1:50:A:A:H4'  | 1:47:A:C:H1'  | 2        | 0.11          |
| (1,997)  | 1:37:A:G:H2'  | 1:38:A:C:H5   | 7        | 0.11          |
| (1,984)  | 1:20:A:A:H1'  | 1:21:A:C:H5   | 1        | 0.11          |
| (1,981)  | 1:53:A:U:H6   | 1:54:A:C:H5   | 3        | 0.11          |
| (1,980)  | 1:46:A:U:H3'  | 1:47:A:C:H5   | 8        | 0.11          |
| (1,951)  | 1:37:A:G:H1'  | 1:38:A:C:H3'  | 7        | 0.11          |
| (1,948)  | 1:13:A:U:H1'  | 1:12:A:C:H3'  | 9        | 0.11          |
| (1,946)  | 1:40:A:A:H4'  | 1:39:A:C:H3'  | 3        | 0.11          |
| (1,928)  | 1:42:A:U:H3'  | 1:43:A:C:H3'  | 4        | 0.11          |
| (1,927)  | 1:44:A:A:H8   | 1:43:A:C:H3'  | 4        | 0.11          |
| (1,921)  | 1:13:A:U:H3'  | 1:12:A:C:H2'  | 1        | 0.11          |
| (1,914)  | 1:13:A:U:H5   | 1:12:A:C:H2'  | 2        | 0.11          |
| (1,912)  | 1:13:A:U:H6   | 1:12:A:C:H2'  | 1        | 0.11          |
| (1,912)  | 1:13:A:U:H6   | 1:12:A:C:H2'  | 10       | 0.11          |
| (1,900)  | 1:28:A:U:H3'  | 1:27:A:C:H2'  | 3        | 0.11          |
| (1,899)  | 1:31:A:A:H3'  | 1:30:A:C:H2'  | 7        | 0.11          |
| (1,895)  | 1:31:A:A:H8   | 1:30:A:C:H2'  | 7        | 0.11          |
| (1,886)  | 1:14:A:U:H4'  | 1:15:A:C:H2'  | 8        | 0.11          |
| (1,885)  | 1:37:A:G:H2'  | 1:38:A:C:H4'  | 4        | 0.11          |
| (1,872)  | 1:26:A:A:H2   | 1:27:A:C:H4'  | 3        | 0.11          |
| (1,872)  | 1:26:A:A:H2   | 1:27:A:C:H4'  | 10       | 0.11          |
| (1,829)  | 1:13:A:U:H1'  | 1:15:A:C:H6   | 4        | 0.11          |
| (1,815)  | 1:39:A:C:H5   | 1:39:A:C:H5'' | 2        | 0.11          |
| (1,793)  | 1:27:A:C:H6   | 1:27:A:C:H5   | 1        | 0.11          |
| (1,793)  | 1:27:A:C:H6   | 1:27:A:C:H5   | 2        | 0.11          |
| (1,793)  | 1:27:A:C:H6   | 1:27:A:C:H5   | 7        | 0.11          |
| (1,793)  | 1:27:A:C:H6   | 1:27:A:C:H5   | 10       | 0.11          |
| (1,748)  | 1:12:A:C:H2'  | 1:12:A:C:H3'  | 7        | 0.11          |
| (1,748)  | 1:12:A:C:H2'  | 1:12:A:C:H3'  | 8        | 0.11          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,742) | 1:39:A:C:H6   | 1:39:A:C:H3'  | 9        | 0.11          |
| (1,714) | 1:36:A:C:H5'' | 1:36:A:C:H3'  | 9        | 0.11          |
| (1,713) | 1:36:A:C:H2'  | 1:36:A:C:H3'  | 9        | 0.11          |
| (1,632) | 1:29:A:A:H4'  | 1:28:A:U:H3'  | 10       | 0.11          |
| (1,628) | 1:29:A:A:H8   | 1:28:A:U:H2'  | 7        | 0.11          |
| (1,617) | 1:47:A:C:H3'  | 1:46:A:U:H3'  | 9        | 0.11          |
| (1,587) | 1:29:A:A:H4'  | 1:28:A:U:H6   | 3        | 0.11          |
| (1,574) | 1:56:A:U:H5'' | 1:56:A:U:H4'  | 6        | 0.11          |
| (1,528) | 1:56:A:U:H2'  | 1:56:A:U:H3'  | 4        | 0.11          |
| (1,528) | 1:56:A:U:H2'  | 1:56:A:U:H3'  | 7        | 0.11          |
| (1,524) | 1:59:A:U:H2'  | 1:59:A:U:H3'  | 1        | 0.11          |
| (1,524) | 1:59:A:U:H2'  | 1:59:A:U:H3'  | 6        | 0.11          |
| (1,510) | 1:53:A:U:H6   | 1:53:A:U:H3'  | 9        | 0.11          |
| (1,497) | 1:42:A:U:H6   | 1:42:A:U:H2'  | 8        | 0.11          |
| (1,482) | 1:51:A:U:H5'' | 1:51:A:U:H3'  | 6        | 0.11          |
| (1,446) | 1:59:A:U:H5   | 1:59:A:U:H6   | 5        | 0.11          |
| (1,446) | 1:59:A:U:H5   | 1:59:A:U:H6   | 8        | 0.11          |
| (1,446) | 1:59:A:U:H5   | 1:59:A:U:H6   | 10       | 0.11          |
| (1,425) | 1:49:A:G:H4'  | 1:50:A:A:H4'  | 4        | 0.11          |
| (1,424) | 1:49:A:G:H2'  | 1:50:A:A:H4'  | 6        | 0.11          |
| (1,418) | 1:19:A:C:H3'  | 1:20:A:A:H3'  | 8        | 0.11          |
| (1,418) | 1:19:A:C:H3'  | 1:20:A:A:H3'  | 10       | 0.11          |
| (1,414) | 1:53:A:U:H4'  | 1:35:A:A:H2   | 9        | 0.11          |
| (1,412) | 1:2:A:G:H2'   | 1:3:A:A:H5''  | 2        | 0.11          |
| (1,410) | 1:2:A:G:H3'   | 1:3:A:A:H5'   | 10       | 0.11          |
| (1,409) | 1:2:A:G:H2'   | 1:3:A:A:H5'   | 7        | 0.11          |
| (1,367) | 1:9:A:G:H1'   | 1:8:A:A:H3'   | 9        | 0.11          |
| (1,348) | 1:46:A:U:H5'' | 1:52:A:A:H4'  | 2        | 0.11          |
| (1,346) | 1:23:A:C:H1'  | 1:24:A:A:H4'  | 9        | 0.11          |
| (1,329) | 1:31:A:A:H8   | 1:31:A:A:H5'' | 3        | 0.11          |
| (1,310) | 1:31:A:A:H4'  | 1:31:A:A:H8   | 4        | 0.11          |
| (1,310) | 1:31:A:A:H4'  | 1:31:A:A:H8   | 7        | 0.11          |
| (1,304) | 1:29:A:A:H8   | 1:29:A:A:H5'' | 4        | 0.11          |
| (1,304) | 1:29:A:A:H8   | 1:29:A:A:H5'' | 5        | 0.11          |
| (1,296) | 1:3:A:A:H3'   | 1:3:A:A:H5'   | 6        | 0.11          |
| (1,265) | 1:48:A:A:H2'  | 1:48:A:A:H3'  | 9        | 0.11          |
| (1,208) | 1:6:A:A:H8    | 1:6:A:A:H2'   | 1        | 0.11          |
| (1,208) | 1:6:A:A:H8    | 1:6:A:A:H2'   | 2        | 0.11          |
| (1,208) | 1:6:A:A:H8    | 1:6:A:A:H2'   | 4        | 0.11          |
| (1,202) | 1:4:A:A:H8    | 1:4:A:A:H2'   | 1        | 0.11          |
| (1,172) | 1:29:A:A:H2'  | 1:29:A:A:H8   | 8        | 0.11          |
| (1,161) | 1:24:A:A:H4'  | 1:23:A:C:H1'  | 9        | 0.11          |

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| Key      | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|----------|---------------|---------------|----------|---------------|
| (1,138)  | 1:47:A:C:H2'  | 1:49:A:G:H5'  | 1        | 0.11          |
| (1,138)  | 1:47:A:C:H2'  | 1:49:A:G:H5'' | 1        | 0.11          |
| (1,129)  | 1:4:A:A:H3'   | 1:5:A:G:H4'   | 10       | 0.11          |
| (1,128)  | 1:4:A:A:H3'   | 1:5:A:G:H1'   | 5        | 0.11          |
| (1,107)  | 1:34:A:G:H2'  | 1:35:A:A:H2'  | 10       | 0.11          |
| (1,86)   | 1:47:A:C:H6   | 1:47:A:C:H5'  | 5        | 0.11          |
| (1,86)   | 1:47:A:C:H6   | 1:47:A:C:H5'' | 5        | 0.11          |
| (1,1318) | 1:59:A:U:H3'  | 1:58:A:G:H3'  | 5        | 0.1           |
| (1,1265) | 1:38:A:C:H1'  | 1:37:A:G:H2'  | 6        | 0.1           |
| (1,1238) | 1:12:A:C:H5   | 1:11:A:G:H4'  | 2        | 0.1           |
| (1,1220) | 1:3:A:A:H8    | 1:2:A:G:H4'   | 1        | 0.1           |
| (1,1175) | 1:47:A:C:H2'  | 1:49:A:G:H8   | 3        | 0.1           |
| (1,1160) | 1:15:A:C:H1'  | 1:16:A:G:H8   | 1        | 0.1           |
| (1,1160) | 1:15:A:C:H1'  | 1:16:A:G:H8   | 6        | 0.1           |
| (1,1160) | 1:15:A:C:H1'  | 1:16:A:G:H8   | 9        | 0.1           |
| (1,1060) | 1:1:A:GTP:H1' | 1:2:A:G:H8    | 2        | 0.1           |
| (1,1006) | 1:44:A:A:H2   | 1:55:A:C:H1'  | 10       | 0.1           |
| (1,968)  | 1:22:A:U:H4'  | 1:23:A:C:H5'' | 5        | 0.1           |
| (1,965)  | 1:20:A:A:H2'  | 1:21:A:C:H5'  | 3        | 0.1           |
| (1,965)  | 1:20:A:A:H2'  | 1:21:A:C:H5'  | 5        | 0.1           |
| (1,960)  | 1:35:A:A:H2'  | 1:36:A:C:H5'' | 3        | 0.1           |
| (1,951)  | 1:37:A:G:H1'  | 1:38:A:C:H3'  | 8        | 0.1           |
| (1,929)  | 1:31:A:A:H8   | 1:30:A:C:H3'  | 5        | 0.1           |
| (1,928)  | 1:42:A:U:H3'  | 1:43:A:C:H3'  | 2        | 0.1           |
| (1,912)  | 1:13:A:U:H6   | 1:12:A:C:H2'  | 3        | 0.1           |
| (1,912)  | 1:13:A:U:H6   | 1:12:A:C:H2'  | 5        | 0.1           |
| (1,905)  | 1:56:A:U:H6   | 1:55:A:C:H2'  | 7        | 0.1           |
| (1,899)  | 1:31:A:A:H3'  | 1:30:A:C:H2'  | 5        | 0.1           |
| (1,899)  | 1:31:A:A:H3'  | 1:30:A:C:H2'  | 10       | 0.1           |
| (1,886)  | 1:14:A:U:H4'  | 1:15:A:C:H2'  | 2        | 0.1           |
| (1,885)  | 1:37:A:G:H2'  | 1:38:A:C:H4'  | 1        | 0.1           |
| (1,874)  | 1:22:A:U:H5   | 1:21:A:C:H4'  | 8        | 0.1           |
| (1,874)  | 1:22:A:U:H5   | 1:21:A:C:H4'  | 10       | 0.1           |
| (1,872)  | 1:26:A:A:H2   | 1:27:A:C:H4'  | 1        | 0.1           |
| (1,829)  | 1:13:A:U:H1'  | 1:15:A:C:H6   | 9        | 0.1           |
| (1,748)  | 1:12:A:C:H2'  | 1:12:A:C:H3'  | 1        | 0.1           |
| (1,748)  | 1:12:A:C:H2'  | 1:12:A:C:H3'  | 3        | 0.1           |
| (1,748)  | 1:12:A:C:H2'  | 1:12:A:C:H3'  | 6        | 0.1           |
| (1,748)  | 1:12:A:C:H2'  | 1:12:A:C:H3'  | 9        | 0.1           |
| (1,719)  | 1:27:A:C:H6   | 1:27:A:C:H2'  | 6        | 0.1           |
| (1,713)  | 1:36:A:C:H2'  | 1:36:A:C:H3'  | 1        | 0.1           |
| (1,681)  | 1:54:A:C:H2'  | 1:55:A:C:H6   | 1        | 0.1           |

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| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,681) | 1:54:A:C:H2' | 1:55:A:C:H6   | 8        | 0.1           |
| (1,629) | 1:57:A:G:H8  | 1:56:A:U:H2'  | 1        | 0.1           |
| (1,629) | 1:57:A:G:H8  | 1:56:A:U:H2'  | 7        | 0.1           |
| (1,629) | 1:57:A:G:H8  | 1:56:A:U:H2'  | 9        | 0.1           |
| (1,617) | 1:47:A:C:H3' | 1:46:A:U:H3'  | 2        | 0.1           |
| (1,581) | 1:45:A:C:H4' | 1:46:A:U:H6   | 2        | 0.1           |
| (1,528) | 1:56:A:U:H2' | 1:56:A:U:H3'  | 3        | 0.1           |
| (1,528) | 1:56:A:U:H2' | 1:56:A:U:H3'  | 6        | 0.1           |
| (1,524) | 1:59:A:U:H2' | 1:59:A:U:H3'  | 9        | 0.1           |
| (1,481) | 1:51:A:U:H2' | 1:51:A:U:H3'  | 2        | 0.1           |
| (1,481) | 1:51:A:U:H2' | 1:51:A:U:H3'  | 6        | 0.1           |
| (1,456) | 1:56:A:U:H6  | 1:56:A:U:H5   | 5        | 0.1           |
| (1,456) | 1:56:A:U:H6  | 1:56:A:U:H5   | 8        | 0.1           |
| (1,456) | 1:56:A:U:H6  | 1:56:A:U:H5   | 10       | 0.1           |
| (1,446) | 1:59:A:U:H5  | 1:59:A:U:H6   | 1        | 0.1           |
| (1,446) | 1:59:A:U:H5  | 1:59:A:U:H6   | 7        | 0.1           |
| (1,414) | 1:53:A:U:H4' | 1:35:A:A:H2   | 7        | 0.1           |
| (1,378) | 1:5:A:G:H1'  | 1:6:A:A:H1'   | 2        | 0.1           |
| (1,329) | 1:31:A:A:H8  | 1:31:A:A:H5'' | 4        | 0.1           |
| (1,310) | 1:31:A:A:H4' | 1:31:A:A:H8   | 1        | 0.1           |
| (1,299) | 1:3:A:A:H8   | 1:3:A:A:H5''  | 10       | 0.1           |
| (1,221) | 1:29:A:A:H8  | 1:29:A:A:H3'  | 10       | 0.1           |
| (1,201) | 1:20:A:A:H8  | 1:20:A:A:H2'  | 2        | 0.1           |
| (1,150) | 1:46:A:U:H6  | 1:47:A:C:H5'  | 3        | 0.1           |
| (1,150) | 1:46:A:U:H6  | 1:47:A:C:H5'' | 3        | 0.1           |
| (1,128) | 1:4:A:A:H3'  | 1:5:A:G:H1'   | 1        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found