



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 07:33 AM UTC

PDB ID : 8R8P / pdb\_00008r8p  
BMRB ID : 34885  
Title : Solution structure of SMN-CX bound to the RNA helix formed upon SMN2 exon7 5'-splice site recognition  
Authors : Malard, F.; Campagne, S.  
Deposited on : 2023-11-29

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)  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

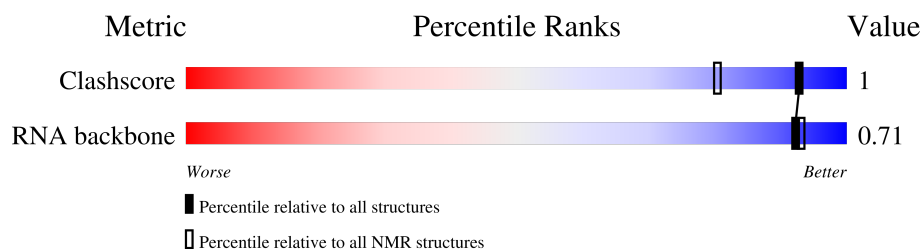
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*

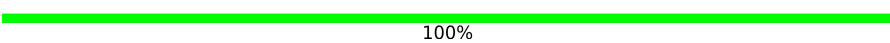
The overall completeness of chemical shifts assignment is 75%.

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     | 11     |  91% 9% |
| 2   | B     | 11     |  100%   |

## 2 Ensemble composition and analysis ⓘ

This entry contains 15 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 are 3 unique types of molecules in this entry. The entry contains 752 atoms, of which 258 are hydrogens and 0 are deuteriums.

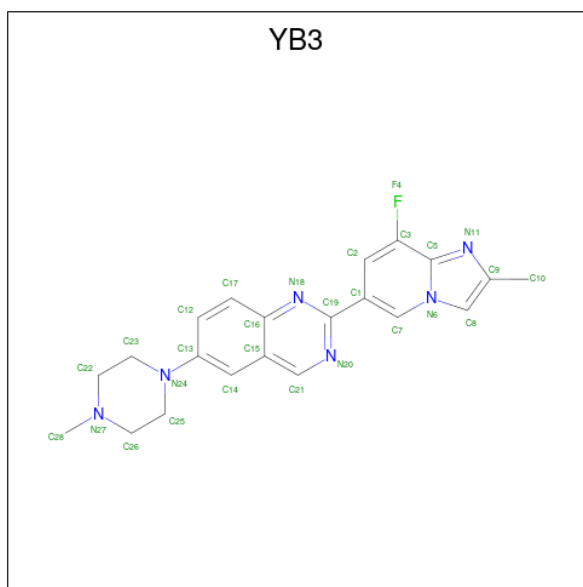
- Molecule 1 is a RNA chain called RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3').

| Mol | Chain | Residues | Atoms |     |     |    |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|-------|
| 1   | A     | 11       | Total | C   | H   | N  | O  | P  | 0     |
|     |       |          | 345   | 103 | 117 | 37 | 78 | 10 |       |

- Molecule 2 is a RNA chain called RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3').

| Mol | Chain | Residues | Atoms |     |     |    |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|-------|
| 2   | B     | 11       | Total | C   | H   | N  | O  | P  | 0     |
|     |       |          | 356   | 106 | 118 | 44 | 77 | 11 |       |

- Molecule 3 is 2-(8-fluoranyl-2-methyl-imidazo[1,2-a]pyridin-6-yl)-6-(4-methylpiperazin-1-yl)quinazoline (CCD ID: YB3) (formula: C<sub>21</sub>H<sub>21</sub>FN<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   |
|-----|-------|----------|-------|----|---|----|---|
| 3   | B     | 1        | Total | C  | F | H  | N |
|     |       |          | 51    | 21 | 1 | 23 | 6 |

## 4 Residue-property plots

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

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

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  91% 9%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

### 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 (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  91% 9%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

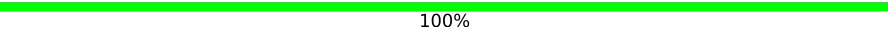
#### 4.2.2 Score per residue for model 2

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  82% 18%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.3 Score per residue for model 3

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  91% 9%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

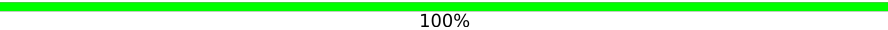
#### 4.2.4 Score per residue for model 4

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  91% 9%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

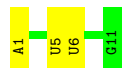
Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.5 Score per residue for model 5

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  73% 27%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.6 Score per residue for model 6

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  91% 9%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

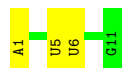
Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.7 Score per residue for model 7

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  73% 27%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

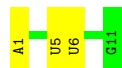
Chain B:  100%

There are no outlier residues in this chain.

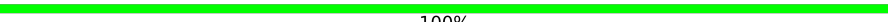
#### 4.2.8 Score per residue for model 8

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  73% 27%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

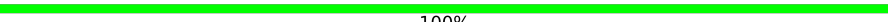
#### 4.2.9 Score per residue for model 9

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  91% 9%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

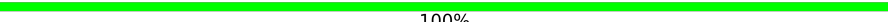
#### 4.2.10 Score per residue for model 10

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  82% 18%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

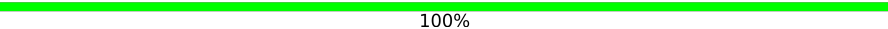
#### 4.2.11 Score per residue for model 11

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  91% 9%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.12 Score per residue for model 12

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  82% 18%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

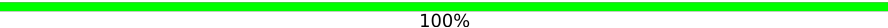
#### 4.2.13 Score per residue for model 13

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  82% 18%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.14 Score per residue for model 14

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  91% 9%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

#### 4.2.15 Score per residue for model 15

- Molecule 1: RNA (5'-R(\*AP\*UP\*AP\*CP\*(PSU)P\*(PSU)P\*AP\*CP\*CP\*UP\*G)-3')

Chain A:  91% 9%



- Molecule 2: RNA (5'-R(P\*GP\*GP\*AP\*GP\*UP\*AP\*AP\*GP\*UP\*CP\*U)-3')

Chain B:  100%

There are no outlier residues in this chain.

## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 15 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 |
|---------------|-----------------------|---------|
| Amber         | refinement            |         |
| CYANA         | structure calculation | 3.98    |

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                       | 341            |
| Number of shifts mapped to atoms             | 341            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 75%            |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

## 6 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: YB3, PSU

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 228   | 117      | 119      | 1±0     |
| All | All   | 7410  | 3870     | 3570     | 15      |

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 1.

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

| Atom-1      | Atom-2      | Clash(Å) | Distance(Å) | Models |       |
|-------------|-------------|----------|-------------|--------|-------|
|             |             |          |             | Worst  | Total |
| 1:A:1:A:OP2 | 1:A:1:A:OP1 | 0.42     | 2.38        | 10     | 15    |

### 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 ⓘ

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers | Suiteness |
|-----|-------|---------------|-------------------|-----------------|-----------|
| 1   | A     | 10/11 (91%)   | 0±0 (0±0%)        | 0±0 (0±0%)      | 0.68±0.00 |
| 2   | B     | 10/11 (91%)   | 0±0 (0±0%)        | 0±0 (0±0%)      | 0.73±0.00 |
| All | All   | 300/330 (91%) | 0 (0%)            | 0 (0%)          | 0.70      |

The overall RNA backbone suiteness is 0.71.

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are 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   | PSU  | A     | 5   | 1,2  | 18,21,22     | 0.75±0.02 | 0±0 (1±2%) |
| 1   | PSU  | A     | 6   | 1,2  | 18,21,22     | 0.75±0.03 | 0±0 (1±2%) |

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   | PSU  | A     | 5   | 1,2  | 21,30,33    | 0.78±0.02 | 0±0 (0±0%) |
| 1   | PSU  | A     | 6   | 1,2  | 21,30,33    | 0.78±0.02 | 0±0 (0±0%) |

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   | PSU  | A     | 6   | 1,2  | -       | 0±0,7,25,26 | 0±0,2,2,2 |
| 1   | PSU  | A     | 5   | 1,2  | -       | 0±0,7,25,26 | 0±0,2,2,2 |

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

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 6   | PSU  | C2-N1 | 2.12 | 1.39        | 1.36     | 10     | 5     |
| 1   | A     | 5   | PSU  | C2-N1 | 2.12 | 1.39        | 1.36     | 7      | 5     |

There are no bond-angle outliers.

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](#)

1 ligand 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        |
| 3   | YB3  | B     | 101 | -    | 32,32,32     | 1.72±0.02 | 6±0 (18±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 | Counts   | Bond angles |             |
|-----|------|-------|-----|------|----------|-------------|-------------|
|     |      |       |     |      |          | RMSZ        | #Z>2        |
| 3   | YB3  | B     | 101 | -    | 38,47,47 | 2.31±0.03   | 9±1 (23±2%) |

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     |
|-----|------|-------|-----|------|---------|-------------|-----------|
| 3   | YB3  | B     | 101 | -    | -       | 0±0,6,18,18 | 0±0,5,5,5 |

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

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
|     |       |     |      |         |      |             |          | Worst  | Total |
| 3   | B     | 101 | YB3  | C5-C3   | 6.05 | 1.37        | 1.42     | 11     | 15    |
| 3   | B     | 101 | YB3  | C19-N18 | 4.80 | 1.39        | 1.32     | 6      | 15    |
| 3   | B     | 101 | YB3  | C22-N27 | 2.68 | 1.52        | 1.46     | 12     | 15    |
| 3   | B     | 101 | YB3  | C2-C3   | 2.68 | 1.38        | 1.35     | 9      | 15    |
| 3   | B     | 101 | YB3  | C26-N27 | 2.67 | 1.52        | 1.46     | 9      | 15    |
| 3   | B     | 101 | YB3  | C28-N27 | 2.32 | 1.52        | 1.46     | 2      | 15    |

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

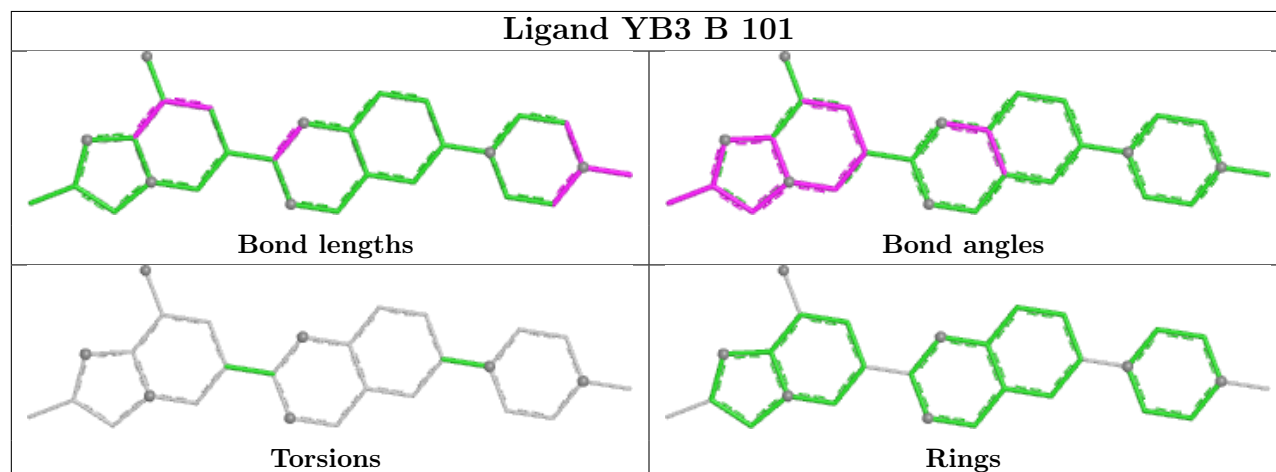
| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
|     |       |     |      |             |      |             |          | Worst  | Total |
| 3   | B     | 101 | YB3  | C8-N6-C5    | 6.62 | 104.40      | 106.87   | 3      | 15    |
| 3   | B     | 101 | YB3  | C7-C1-C2    | 5.90 | 123.88      | 117.65   | 9      | 15    |
| 3   | B     | 101 | YB3  | N6-C5-N11   | 5.54 | 114.90      | 111.05   | 3      | 15    |
| 3   | B     | 101 | YB3  | C10-C9-C8   | 5.47 | 122.72      | 129.00   | 10     | 15    |
| 3   | B     | 101 | YB3  | C8-N6-C7    | 4.46 | 125.75      | 130.04   | 13     | 15    |
| 3   | B     | 101 | YB3  | C10-C9-N11  | 3.99 | 125.01      | 119.58   | 1      | 15    |
| 3   | B     | 101 | YB3  | C15-C16-N18 | 2.45 | 118.88      | 122.25   | 5      | 15    |
| 3   | B     | 101 | YB3  | C1-C19-N20  | 2.41 | 115.10      | 117.12   | 5      | 6     |
| 3   | B     | 101 | YB3  | C23-C22-N27 | 2.32 | 114.58      | 110.86   | 4      | 11    |
| 3   | B     | 101 | YB3  | C1-C2-C3    | 2.24 | 117.88      | 120.57   | 12     | 11    |
| 3   | B     | 101 | YB3  | C14-C13-N24 | 2.08 | 119.76      | 122.11   | 13     | 1     |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 75% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping

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                  | 341 |
| Number of shifts mapped to atoms        | 341 |
| 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

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

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 282 atoms were assigned a chemical shift out of a possible 375. 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   | 220/220 (100%) | 120/120 (100%) | 100/100 (100%)  | 0/0 (—%)        |
| Base    | 62/155 (40%)   | 32/95 (34%)    | 30/35 (86%)     | 0/25 (0%)       |
| Overall | 282/375 (75%)  | 152/215 (71%)  | 130/135 (96%)   | 0/25 (0%)       |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 282 atoms were assigned a chemical shift out of a possible

375. 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   | 220/220 (100%) | 120/120 (100%)       | 100/100 (100%)        | 0/0 (—%)              |
| Base    | 62/155 (40%)   | 32/95 (34%)          | 30/35 (86%)           | 0/25 (0%)             |
| Overall | 282/375 (75%)  | 152/215 (71%)        | 130/135 (96%)         | 0/25 (0%)             |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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

There are no statistically unusual chemical shifts.

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

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

## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 419   |
| Intra-residue ( $ i-j =0$ )                              | 248   |
| Sequential ( $ i-j =1$ )                                 | 87    |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 0     |
| Long range ( $ i-j \geq 5$ )                             | 0     |
| Inter-chain                                              | 12    |
| Hydrogen bond restraints                                 | 72    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 165   |
| Number of unmapped restraints                            | 1     |
| Number of restraints per residue                         | 25.4  |
| Number of long range restraints per residue <sup>1</sup> | 0.0   |

<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)  | 17.0                                   | 0.2     |
| 0.2-0.5 (Medium) | 26.9                                   | 0.5     |
| >0.5 (Large)     | 18.3                                   | 8.45    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 37.1                                   | 9.92    |
| 10.0-20.0 (Medium) | 1.9                                    | 14.32   |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

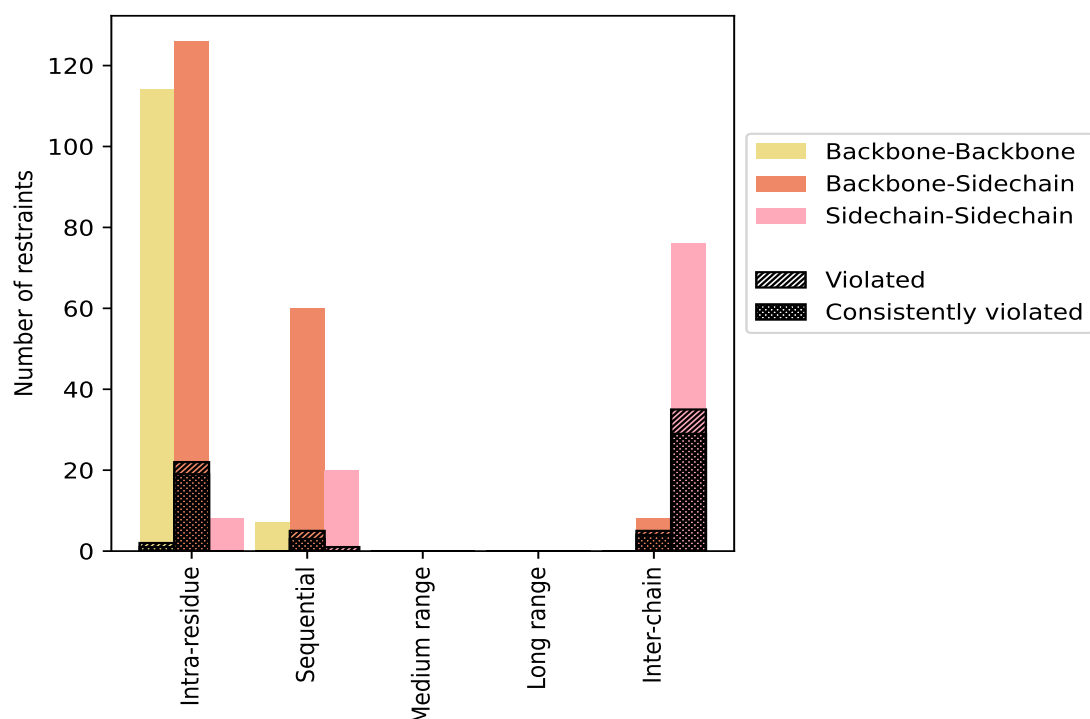
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count               | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                      |                      |
|------------------------------------------------------------|---------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|----------------------|
|                                                            |                     |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>       | % <sup>1</sup>       |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">248</a> | <a href="#">59.2</a>  | <a href="#">24</a>    | <a href="#">9.7</a>  | <a href="#">5.7</a>  | <a href="#">20</a>                 | <a href="#">8.1</a>  | <a href="#">4.8</a>  |
| Backbone-Backbone                                          | 114                 | 27.2                  | 2                     | 1.8                  | 0.5                  | 1                                  | 0.9                  | 0.2                  |
| Backbone-Sidechain                                         | 126                 | 30.1                  | 22                    | 17.5                 | 5.3                  | 19                                 | 15.1                 | 4.5                  |
| Sidechain-Sidechain                                        | 8                   | 1.9                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">87</a>  | <a href="#">20.8</a>  | <a href="#">6</a>     | <a href="#">6.9</a>  | <a href="#">1.4</a>  | <a href="#">3</a>                  | <a href="#">3.4</a>  | <a href="#">0.7</a>  |
| Backbone-Backbone                                          | 7                   | 1.7                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Backbone-Sidechain                                         | 60                  | 14.3                  | 5                     | 8.3                  | 1.2                  | 3                                  | 5.0                  | 0.7                  |
| Sidechain-Sidechain                                        | 20                  | 4.8                   | 1                     | 5.0                  | 0.2                  | 0                                  | 0.0                  | 0.0                  |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</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="#">Long range ( i-j ≥5)</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="#">Inter-chain</a>                                | <a href="#">12</a>  | <a href="#">2.9</a>   | <a href="#">5</a>     | <a href="#">41.7</a> | <a href="#">1.2</a>  | <a href="#">3</a>                  | <a href="#">25.0</a> | <a href="#">0.7</a>  |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Backbone-Sidechain                                         | 4                   | 1.0                   | 1                     | 25.0                 | 0.2                  | 0                                  | 0.0                  | 0.0                  |
| Sidechain-Sidechain                                        | 8                   | 1.9                   | 4                     | 50.0                 | 1.0                  | 3                                  | 37.5                 | 0.7                  |
| <a href="#">Hydrogen bond</a>                              | <a href="#">72</a>  | <a href="#">17.2</a>  | <a href="#">35</a>    | <a href="#">48.6</a> | <a href="#">8.4</a>  | <a href="#">30</a>                 | <a href="#">41.7</a> | <a href="#">7.2</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="#">419</a> | <a href="#">100.0</a> | <a href="#">70</a>    | <a href="#">16.7</a> | <a href="#">16.7</a> | <a href="#">56</a>                 | <a href="#">13.4</a> | <a href="#">13.4</a> |
| Backbone-Backbone                                          | 121                 | 28.9                  | 2                     | 1.7                  | 0.5                  | 1                                  | 0.8                  | 0.2                  |
| Backbone-Sidechain                                         | 194                 | 46.3                  | 32                    | 16.5                 | 7.6                  | 26                                 | 13.4                 | 6.2                  |
| Sidechain-Sidechain                                        | 104                 | 24.8                  | 36                    | 34.6                 | 8.6                  | 29                                 | 27.9                 | 6.9                  |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 21                   | 4               | 0               | 0               | 37              | 62    | 1.25     | 7.8     | 1.92                | 0.25       |
| 2        | 22                   | 3               | 0               | 0               | 36              | 61    | 1.27     | 7.71    | 1.93                | 0.27       |
| 3        | 22                   | 3               | 0               | 0               | 38              | 63    | 1.25     | 7.93    | 1.92                | 0.27       |
| 4        | 22                   | 4               | 0               | 0               | 37              | 63    | 1.24     | 8.15    | 1.93                | 0.26       |
| 5        | 23                   | 4               | 0               | 0               | 37              | 64    | 1.22     | 7.98    | 1.92                | 0.24       |
| 6        | 21                   | 3               | 0               | 0               | 38              | 62    | 1.27     | 7.95    | 1.94                | 0.26       |
| 7        | 22                   | 4               | 0               | 0               | 37              | 63    | 1.25     | 8.04    | 1.94                | 0.25       |
| 8        | 22                   | 3               | 0               | 0               | 36              | 61    | 1.28     | 7.72    | 1.93                | 0.28       |
| 9        | 22                   | 4               | 0               | 0               | 37              | 63    | 1.24     | 7.9     | 1.93                | 0.25       |
| 10       | 22                   | 3               | 0               | 0               | 38              | 63    | 1.24     | 7.87    | 1.92                | 0.27       |

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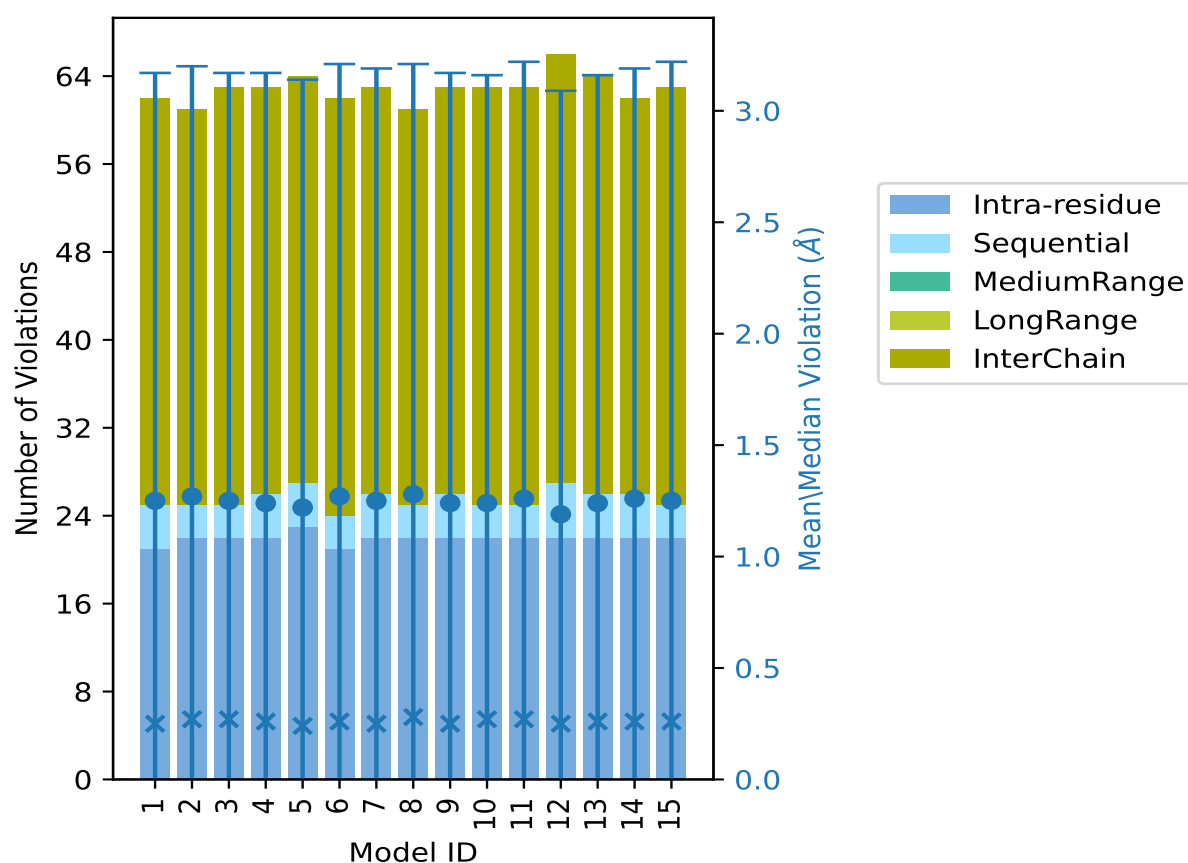
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 22                   | 3               | 0               | 0               | 38              | 63    | 1.26     | 8.41    | 1.96                | 0.27       |
| 12       | 22                   | 5               | 0               | 0               | 39              | 66    | 1.19     | 7.93    | 1.9                 | 0.25       |
| 13       | 22                   | 4               | 0               | 0               | 38              | 64    | 1.24     | 7.97    | 1.92                | 0.26       |
| 14       | 22                   | 4               | 0               | 0               | 36              | 62    | 1.26     | 7.83    | 1.93                | 0.26       |
| 15       | 22                   | 3               | 0               | 0               | 38              | 63    | 1.25     | 8.45    | 1.97                | 0.26       |

<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

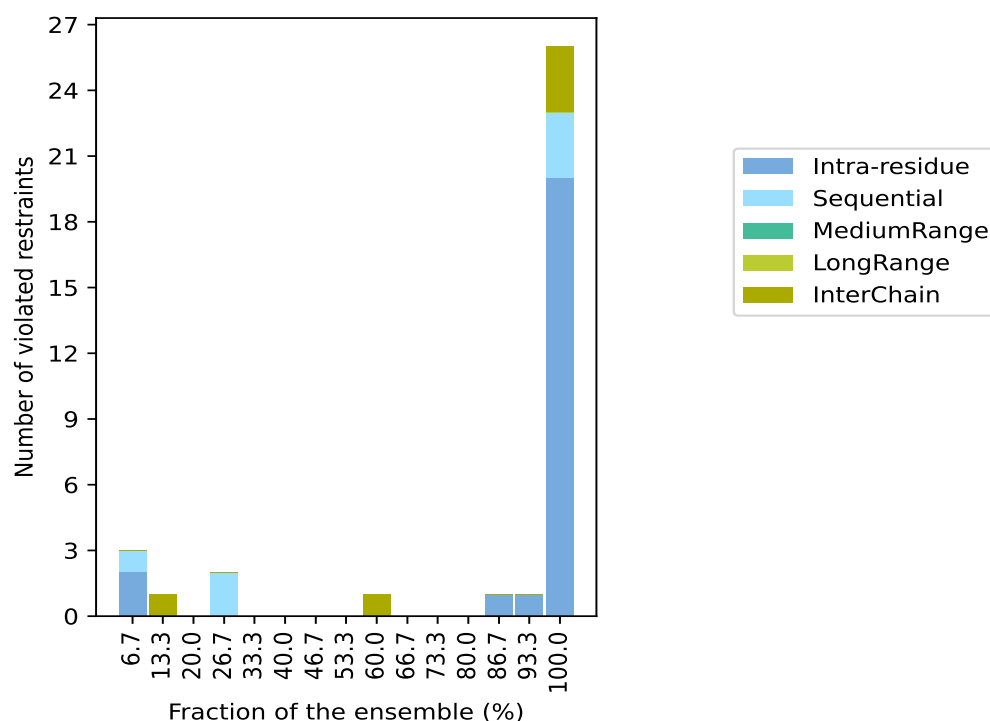
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 312(IR:224, SQ:81, MR:0, LR:0, IC:7) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 2                             | 1               | 0               | 0               | 0               | 3     | 1                        | 6.7   |
| 0                             | 0               | 0               | 0               | 1               | 1     | 2                        | 13.3  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 3                        | 20.0  |
| 0                             | 2               | 0               | 0               | 0               | 2     | 4                        | 26.7  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 5                        | 33.3  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 6                        | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 7                        | 46.7  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 8                        | 53.3  |
| 0                             | 0               | 0               | 0               | 1               | 1     | 9                        | 60.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 10                       | 66.7  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 73.3  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 80.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 13                       | 86.7  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 14                       | 93.3  |
| 20                            | 3               | 0               | 0               | 3               | 26    | 15                       | 100.0 |

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

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

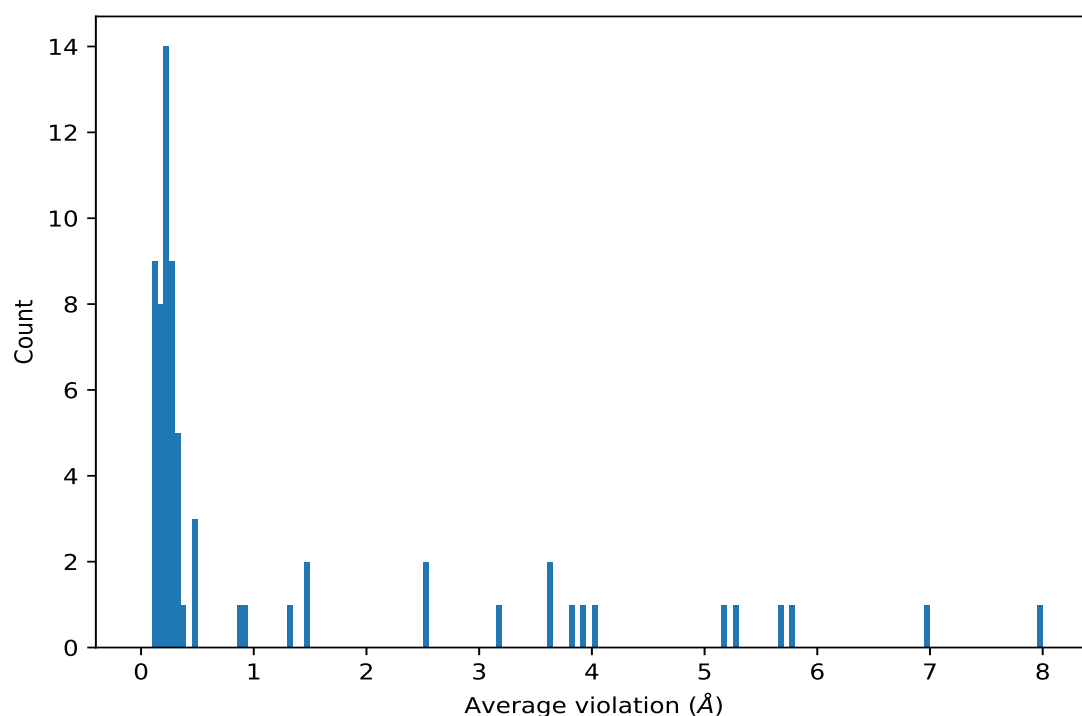
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1        | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|------------------|---------------------|----------|---------------------|------------|
| (5,1)   | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 15                  | 7.98     | 0.21                | 7.93       |
| (4,1)   | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 15                  | 6.95     | 0.1                 | 6.95       |
| (6,13)  | 1:5:A:PSU:H3' | 2:18:B:A:N1      | 15                  | 5.75     | 0.02                | 5.75       |
| (6,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1      | 15                  | 5.68     | 0.02                | 5.69       |
| (1,13)  | 1:5:A:PSU:H3' | 2:18:B:A:N1      | 15                  | 5.25     | 0.02                | 5.25       |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1      | 15                  | 5.18     | 0.02                | 5.19       |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'      | 15                  | 4.03     | 0.01                | 4.03       |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4'     | 15                  | 3.91     | 0.01                | 3.91       |
| (2,249) | 2:16:B:U:H5   | 2:16:B:U:H4'     | 15                  | 3.82     | 0.01                | 3.82       |
| (2,322) | 2:21:B:C:H5   | 2:21:B:C:H4'     | 15                  | 3.65     | 0.01                | 3.65       |
| (2,324) | 2:21:B:C:H5   | 2:21:B:C:H4'     | 15                  | 3.65     | 0.01                | 3.65       |
| (2,25)  | 1:2:A:U:H4'   | 1:2:A:U:H5       | 15                  | 3.19     | 0.01                | 3.19       |
| (2,67)  | 1:4:A:C:H4'   | 1:4:A:C:H5       | 15                  | 2.54     | 0.01                | 2.54       |
| (2,67)  | 1:4:A:C:H4'   | 1:4:A:C:H5       | 15                  | 2.54     | 0.01                | 2.54       |
| (2,24)  | 1:2:A:U:H4'   | 1:2:A:U:H5       | 15                  | 1.49     | 0.01                | 1.49       |
| (2,248) | 2:16:B:U:H5   | 2:16:B:U:H3'     | 15                  | 1.47     | 0.02                | 1.48       |

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| Key     | Atom-1       | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|--------------|-----------------|---------------------|----------|---------------------|------------|
| (2,66)  | 1:4:A:C:H3'  | 1:4:A:C:H5      | 15                  | 1.34     | 0.03                | 1.34       |
| (4,2)   | 1:9:A:C:H6   | 3:101:B:YB3:H12 | 15                  | 0.91     | 0.06                | 0.92       |
| (2,132) | 1:8:A:C:H1'  | 1:9:A:C:H5      | 15                  | 0.89     | 0.07                | 0.89       |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1'     | 15                  | 0.49     | 0.01                | 0.5        |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1'     | 15                  | 0.49     | 0.01                | 0.49       |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5      | 15                  | 0.47     | 0.02                | 0.47       |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5     | 15                  | 0.38     | 0.05                | 0.38       |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1     | 15                  | 0.33     | 0.02                | 0.33       |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4     | 15                  | 0.32     | 0.04                | 0.3        |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1'    | 15                  | 0.31     | 0.0                 | 0.31       |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2    | 15                  | 0.29     | 0.04                | 0.28       |
| (2,58)  | 1:4:A:C:H1'  | 1:4:A:C:H5      | 15                  | 0.28     | 0.0                 | 0.28       |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6     | 15                  | 0.28     | 0.05                | 0.27       |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5      | 15                  | 0.27     | 0.01                | 0.27       |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4     | 15                  | 0.27     | 0.03                | 0.27       |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1     | 15                  | 0.25     | 0.01                | 0.25       |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1      | 15                  | 0.25     | 0.01                | 0.25       |
| (6,26)  | 1:8:A:C:N4   | 2:15:B:G:O6     | 15                  | 0.25     | 0.03                | 0.26       |
| (6,4)   | 1:1:A:A:N6   | 2:22:B:U:O4     | 15                  | 0.25     | 0.03                | 0.26       |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6      | 15                  | 0.24     | 0.02                | 0.24       |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1     | 15                  | 0.23     | 0.02                | 0.23       |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1     | 15                  | 0.23     | 0.02                | 0.23       |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1     | 15                  | 0.23     | 0.02                | 0.23       |
| (2,40)  | 1:3:A:A:H2'  | 1:3:A:A:H3'     | 15                  | 0.22     | 0.0                 | 0.22       |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4     | 15                  | 0.22     | 0.04                | 0.21       |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2    | 15                  | 0.22     | 0.02                | 0.23       |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6     | 15                  | 0.22     | 0.03                | 0.23       |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5      | 15                  | 0.22     | 0.01                | 0.22       |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'     | 15                  | 0.22     | 0.01                | 0.22       |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6     | 15                  | 0.21     | 0.06                | 0.21       |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6     | 15                  | 0.21     | 0.02                | 0.2        |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1     | 15                  | 0.21     | 0.01                | 0.2        |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2    | 15                  | 0.2      | 0.04                | 0.18       |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1      | 15                  | 0.19     | 0.02                | 0.19       |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1      | 15                  | 0.19     | 0.01                | 0.18       |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4     | 15                  | 0.18     | 0.03                | 0.19       |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6     | 15                  | 0.18     | 0.01                | 0.19       |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1     | 15                  | 0.17     | 0.01                | 0.17       |
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4     | 15                  | 0.16     | 0.03                | 0.16       |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1      | 15                  | 0.16     | 0.01                | 0.16       |
| (6,5)   | 2:20:B:U:H3  | 1:3:A:A:N1      | 15                  | 0.14     | 0.01                | 0.14       |
| (2,164) | 1:11:A:G:H2' | 1:11:A:G:H8     | 14                  | 0.17     | 0.06                | 0.14       |

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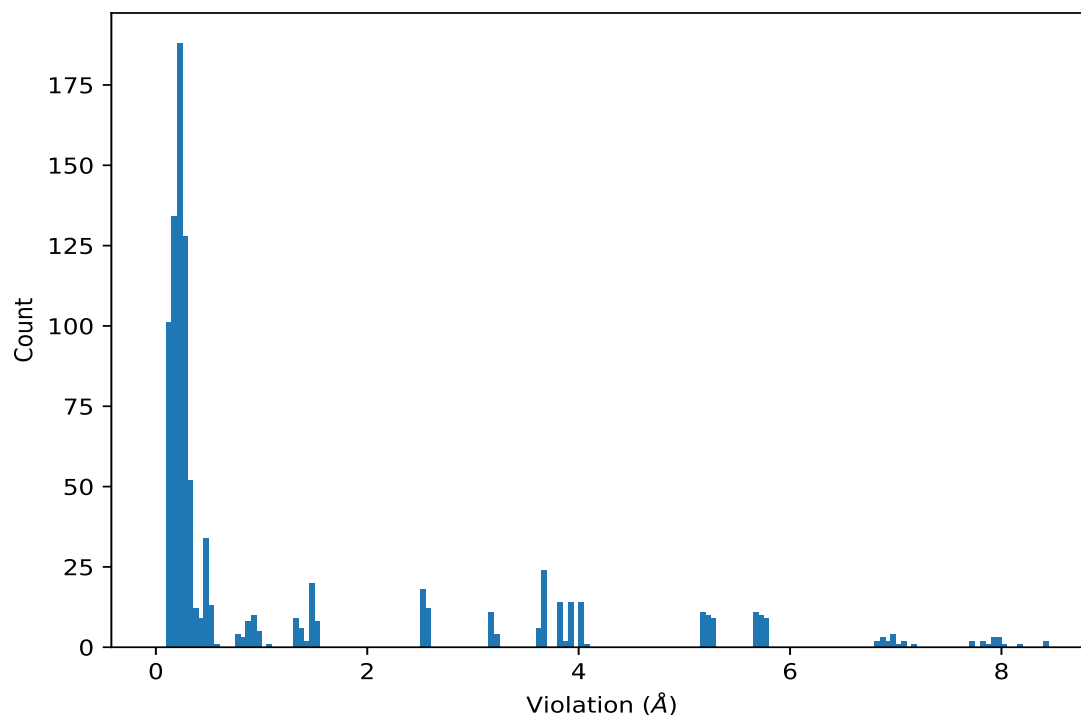
| Key     | Atom-1        | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|------------------|---------------------|----------|---------------------|------------|
| (6,27)  | 1:8:A:C:N3    | 2:15:B:G:H1      | 14                  | 0.14     | 0.02                | 0.14       |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 14                  | 0.12     | 0.02                | 0.12       |
| (6,19)  | 2:17:B:A:H61  | 1:6:A:PSU:O2     | 13                  | 0.13     | 0.02                | 0.13       |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 13                  | 0.11     | 0.01                | 0.11       |
| (6,30)  | 1:9:A:C:N4    | 2:13:B:G:O6      | 12                  | 0.13     | 0.02                | 0.13       |
| (5,2)   | 1:9:A:C:H5    | 3:101:B:YB3:H28A | 9                   | 0.34     | 0.23                | 0.17       |
| (5,2)   | 1:8:A:C:H6    | 3:101:B:YB3:H28A | 9                   | 0.34     | 0.23                | 0.17       |
| (2,53)  | 1:3:A:A:H8    | 1:2:A:U:H4'      | 4                   | 0.11     | 0.01                | 0.11       |
| (2,137) | 1:8:A:C:H3'   | 1:9:A:C:H6       | 4                   | 0.11     | 0.0                 | 0.11       |
| (2,97)  | 1:6:A:PSU:H2' | 2:17:B:A:H2      | 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) |
|--------|---------------|------------------|----------|---------------|
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 15       | 8.45          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 11       | 8.41          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 4        | 8.15          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 7        | 8.04          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 5        | 7.98          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 13       | 7.97          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 6        | 7.95          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 3        | 7.93          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 12       | 7.93          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 9        | 7.9           |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 10       | 7.87          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 14       | 7.83          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 1        | 7.8           |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 8        | 7.72          |
| (5,1)  | 2:14:B:A:H8   | 3:101:B:YB3:H25B | 2        | 7.71          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 15       | 7.19          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 5        | 7.07          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 7        | 7.07          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 11       | 7.03          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 13       | 6.98          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 6        | 6.97          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 14       | 6.96          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 12       | 6.95          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 9        | 6.94          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 10       | 6.94          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 4        | 6.89          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 1        | 6.85          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 3        | 6.85          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 8        | 6.81          |
| (4,1)  | 2:13:B:G:H8   | 3:101:B:YB3:H25B | 2        | 6.8           |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1      | 9        | 5.78          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1      | 12       | 5.77          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1      | 15       | 5.77          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1      | 11       | 5.76          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1      | 6        | 5.75          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1      | 7        | 5.75          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1      | 8        | 5.75          |

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| Key    | Atom-1        | Atom-2      | Model ID | Violation (Å) |
|--------|---------------|-------------|----------|---------------|
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 13       | 5.75          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 14       | 5.75          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 3        | 5.74          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 3        | 5.74          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 1        | 5.73          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 2        | 5.73          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 2        | 5.72          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 4        | 5.72          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 10       | 5.72          |
| (6,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 5        | 5.71          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 11       | 5.7           |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 12       | 5.7           |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 5        | 5.69          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 7        | 5.69          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 8        | 5.69          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 15       | 5.69          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 13       | 5.68          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 6        | 5.67          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 1        | 5.66          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 4        | 5.66          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 10       | 5.66          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 14       | 5.66          |
| (6,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 9        | 5.65          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 9        | 5.28          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 12       | 5.27          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 15       | 5.27          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 11       | 5.26          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 6        | 5.25          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 7        | 5.25          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 8        | 5.25          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 13       | 5.25          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 14       | 5.25          |
| (1,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 3        | 5.24          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 3        | 5.24          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 1        | 5.23          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 2        | 5.23          |
| (1,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 2        | 5.22          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 4        | 5.22          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 10       | 5.22          |
| (1,13) | 1:5:A:PSU:H3' | 2:18:B:A:N1 | 5        | 5.21          |
| (1,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 11       | 5.2           |
| (1,17) | 1:6:A:PSU:H3' | 2:17:B:A:N1 | 12       | 5.2           |

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| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 5        | 5.19          |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 7        | 5.19          |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 8        | 5.19          |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 15       | 5.19          |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 13       | 5.18          |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 6        | 5.17          |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 1        | 5.16          |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 4        | 5.16          |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 10       | 5.16          |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 14       | 5.16          |
| (1,17)  | 1:6:A:PSU:H3' | 2:17:B:A:N1  | 9        | 5.15          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 11       | 4.05          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 6        | 4.04          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 8        | 4.04          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 9        | 4.04          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 15       | 4.04          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 1        | 4.03          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 3        | 4.03          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 4        | 4.03          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 10       | 4.03          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 2        | 4.02          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 5        | 4.02          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 7        | 4.02          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 13       | 4.02          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 12       | 4.01          |
| (2,150) | 1:9:A:C:H5    | 1:9:A:C:H4'  | 14       | 4.01          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 2        | 3.94          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 3        | 3.92          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 6        | 3.92          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 9        | 3.92          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 13       | 3.92          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 1        | 3.91          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 7        | 3.91          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 8        | 3.91          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 10       | 3.91          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 11       | 3.91          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 14       | 3.91          |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 5        | 3.9           |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 12       | 3.9           |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 15       | 3.9           |
| (2,245) | 2:16:B:U:H5   | 2:16:B:U:H4' | 4        | 3.89          |
| (2,249) | 2:16:B:U:H5   | 2:16:B:U:H4' | 2        | 3.85          |

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| Key     | Atom-1      | Atom-2       | Model ID | Violation (Å) |
|---------|-------------|--------------|----------|---------------|
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 3        | 3.83          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 6        | 3.83          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 9        | 3.83          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 13       | 3.83          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 1        | 3.82          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 7        | 3.82          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 8        | 3.82          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 10       | 3.82          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 11       | 3.82          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 14       | 3.82          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 5        | 3.81          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 12       | 3.81          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 15       | 3.81          |
| (2,249) | 2:16:B:U:H5 | 2:16:B:U:H4' | 4        | 3.8           |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 4        | 3.67          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 7        | 3.67          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 4        | 3.67          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 7        | 3.67          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 6        | 3.66          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 10       | 3.66          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 12       | 3.66          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 6        | 3.66          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 10       | 3.66          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 12       | 3.66          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 1        | 3.65          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 2        | 3.65          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 3        | 3.65          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 8        | 3.65          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 9        | 3.65          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 11       | 3.65          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 13       | 3.65          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 1        | 3.65          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 2        | 3.65          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 3        | 3.65          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 8        | 3.65          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 9        | 3.65          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 11       | 3.65          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 13       | 3.65          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 5        | 3.64          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 5        | 3.64          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 14       | 3.63          |
| (2,324) | 2:21:B:C:H5 | 2:21:B:C:H4' | 15       | 3.63          |

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| Key     | Atom-1      | Atom-2       | Model ID | Violation (Å) |
|---------|-------------|--------------|----------|---------------|
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 14       | 3.63          |
| (2,322) | 2:21:B:C:H5 | 2:21:B:C:H4' | 15       | 3.63          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 12       | 3.21          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 13       | 3.2           |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 14       | 3.2           |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 15       | 3.2           |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 2        | 3.19          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 3        | 3.19          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 4        | 3.19          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 6        | 3.19          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 9        | 3.19          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 10       | 3.19          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 11       | 3.19          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 1        | 3.18          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 5        | 3.18          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 8        | 3.18          |
| (2,25)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 7        | 3.17          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 12       | 2.56          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 12       | 2.56          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 15       | 2.56          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 15       | 2.56          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 9        | 2.55          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 9        | 2.55          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 11       | 2.55          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 11       | 2.55          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 13       | 2.55          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 13       | 2.55          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 14       | 2.55          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 14       | 2.55          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 1        | 2.54          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 1        | 2.54          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 4        | 2.54          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 4        | 2.54          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 8        | 2.54          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 8        | 2.54          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 10       | 2.54          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 10       | 2.54          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 2        | 2.53          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 2        | 2.53          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 3        | 2.53          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 3        | 2.53          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 5        | 2.53          |

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| Key     | Atom-1      | Atom-2       | Model ID | Violation (Å) |
|---------|-------------|--------------|----------|---------------|
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 5        | 2.53          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 6        | 2.53          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 6        | 2.53          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 7        | 2.52          |
| (2,67)  | 1:4:A:C:H4' | 1:4:A:C:H5   | 7        | 2.52          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 12       | 1.51          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 2        | 1.5           |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 10       | 1.5           |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 11       | 1.5           |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 13       | 1.5           |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 13       | 1.5           |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 14       | 1.5           |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 15       | 1.5           |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 3        | 1.49          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 2        | 1.49          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 3        | 1.49          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 4        | 1.49          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 6        | 1.49          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 9        | 1.49          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 10       | 1.49          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 11       | 1.49          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 1        | 1.48          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 7        | 1.48          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 15       | 1.48          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 1        | 1.48          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 5        | 1.48          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 8        | 1.48          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 6        | 1.47          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 14       | 1.47          |
| (2,24)  | 1:2:A:U:H4' | 1:2:A:U:H5   | 7        | 1.47          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 8        | 1.46          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 9        | 1.46          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 12       | 1.46          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 4        | 1.44          |
| (2,248) | 2:16:B:U:H5 | 2:16:B:U:H3' | 5        | 1.43          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5   | 12       | 1.39          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5   | 14       | 1.38          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5   | 11       | 1.37          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5   | 15       | 1.37          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5   | 13       | 1.36          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5   | 8        | 1.35          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5   | 1        | 1.34          |

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| Key     | Atom-1      | Atom-2           | Model ID | Violation (Å) |
|---------|-------------|------------------|----------|---------------|
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5       | 2        | 1.34          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5       | 5        | 1.34          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5       | 9        | 1.34          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5       | 6        | 1.33          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5       | 10       | 1.33          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5       | 4        | 1.32          |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5       | 3        | 1.3           |
| (2,66)  | 1:4:A:C:H3' | 1:4:A:C:H5       | 7        | 1.3           |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 3        | 1.06          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 13       | 0.99          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 12       | 0.98          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 10       | 0.97          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 14       | 0.97          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 6        | 0.95          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 1        | 0.94          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 7        | 0.94          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 13       | 0.94          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 6        | 0.93          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 2        | 0.93          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 8        | 0.92          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 9        | 0.91          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 5        | 0.91          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 9        | 0.91          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 14       | 0.9           |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 1        | 0.89          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 2        | 0.88          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 5        | 0.88          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 11       | 0.88          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 7        | 0.88          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 10       | 0.87          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 12       | 0.87          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 4        | 0.85          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 8        | 0.84          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 15       | 0.82          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 15       | 0.81          |
| (4,2)   | 1:9:A:C:H6  | 3:101:B:YB3:H12  | 3        | 0.79          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 4        | 0.79          |
| (2,132) | 1:8:A:C:H1' | 1:9:A:C:H5       | 11       | 0.76          |
| (5,2)   | 1:9:A:C:H5  | 3:101:B:YB3:H28A | 11       | 0.75          |
| (5,2)   | 1:9:A:C:H5  | 3:101:B:YB3:H28A | 6        | 0.56          |
| (5,2)   | 1:9:A:C:H5  | 3:101:B:YB3:H28A | 8        | 0.53          |
| (5,2)   | 1:9:A:C:H5  | 3:101:B:YB3:H28A | 13       | 0.53          |

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| Key     | Atom-1       | Atom-2      | Model ID | Violation (Å) |
|---------|--------------|-------------|----------|---------------|
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 3        | 0.52          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 8        | 0.5           |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 11       | 0.5           |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 1        | 0.5           |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 5        | 0.5           |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 7        | 0.5           |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 8        | 0.5           |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 9        | 0.5           |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 12       | 0.5           |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 14       | 0.5           |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5  | 10       | 0.5           |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 1        | 0.49          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 2        | 0.49          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 5        | 0.49          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 6        | 0.49          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 9        | 0.49          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 13       | 0.49          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 14       | 0.49          |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 10       | 0.49          |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 13       | 0.49          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5  | 6        | 0.49          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5  | 7        | 0.49          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5  | 9        | 0.49          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5  | 11       | 0.49          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5 | 12       | 0.48          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 3        | 0.48          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 4        | 0.48          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 7        | 0.48          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 10       | 0.48          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 12       | 0.48          |
| (2,147) | 1:9:A:C:H5   | 1:9:A:C:H1' | 15       | 0.48          |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 2        | 0.48          |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 6        | 0.48          |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 11       | 0.48          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5  | 3        | 0.48          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5 | 7        | 0.47          |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 4        | 0.47          |
| (2,128) | 1:8:A:C:H5   | 1:8:A:C:H1' | 15       | 0.47          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5  | 1        | 0.47          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5  | 5        | 0.47          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5  | 13       | 0.47          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5  | 2        | 0.46          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5   | 12       | 0.46          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5   | 15       | 0.46          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5   | 8        | 0.45          |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 4        | 0.44          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5   | 4        | 0.44          |
| (2,19)  | 1:2:A:U:H2'  | 1:2:A:U:H5   | 14       | 0.44          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 14       | 0.43          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 10       | 0.42          |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 7        | 0.41          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6  | 4        | 0.4           |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 5        | 0.4           |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 15       | 0.4           |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 4        | 0.39          |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 13       | 0.39          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 13       | 0.39          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 11       | 0.38          |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 12       | 0.38          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 3        | 0.38          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 11       | 0.38          |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 10       | 0.37          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 2        | 0.37          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 6        | 0.36          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 9        | 0.36          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 1        | 0.35          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 9        | 0.34          |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 1        | 0.34          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 8        | 0.34          |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 8        | 0.33          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 7        | 0.33          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 8        | 0.33          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 12       | 0.33          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 13       | 0.33          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 15       | 0.33          |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 13       | 0.33          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 3        | 0.32          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 4        | 0.32          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 10       | 0.32          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 15       | 0.32          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 4        | 0.32          |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 14       | 0.31          |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 15       | 0.31          |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 6        | 0.31          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 14       | 0.31          |
| (6,26)  | 1:8:A:C:N4   | 2:15:B:G:O6  | 3        | 0.31          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 3        | 0.31          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 13       | 0.31          |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 5        | 0.31          |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 2        | 0.31          |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 8        | 0.31          |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 11       | 0.31          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 7        | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 1        | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 2        | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 3        | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 4        | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 5        | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 6        | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 7        | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 8        | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 9        | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 11       | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 13       | 0.31          |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 14       | 0.31          |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 1        | 0.3           |
| (6,32)  | 1:9:A:C:N3   | 2:13:B:G:N1  | 5        | 0.3           |
| (6,26)  | 1:8:A:C:N4   | 2:15:B:G:O6  | 8        | 0.3           |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 3        | 0.3           |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 14       | 0.3           |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2 | 4        | 0.3           |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 3        | 0.3           |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 5        | 0.3           |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 6        | 0.3           |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 14       | 0.3           |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 13       | 0.3           |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 10       | 0.3           |
| (2,309) | 2:20:B:U:H5  | 2:20:B:U:H1' | 12       | 0.3           |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 11       | 0.29          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 7        | 0.29          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 8        | 0.29          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 11       | 0.29          |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 6        | 0.29          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 12       | 0.29          |
| (2,58)  | 1:4:A:C:H1'  | 1:4:A:C:H5   | 2        | 0.29          |
| (2,58)  | 1:4:A:C:H1'  | 1:4:A:C:H5   | 7        | 0.29          |

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| Key    | Atom-1      | Atom-2       | Model ID | Violation (Å) |
|--------|-------------|--------------|----------|---------------|
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 8        | 0.29          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 9        | 0.29          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 13       | 0.29          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 14       | 0.29          |
| (6,32) | 1:9:A:C:N3  | 2:13:B:G:N1  | 2        | 0.28          |
| (6,31) | 1:9:A:C:N3  | 2:13:B:G:H1  | 11       | 0.28          |
| (6,26) | 1:8:A:C:N4  | 2:15:B:G:O6  | 10       | 0.28          |
| (6,25) | 1:8:A:C:H41 | 2:15:B:G:O6  | 3        | 0.28          |
| (6,25) | 1:8:A:C:H41 | 2:15:B:G:O6  | 8        | 0.28          |
| (6,24) | 1:7:A:A:N6  | 2:16:B:U:O4  | 1        | 0.28          |
| (6,24) | 1:7:A:A:N6  | 2:16:B:U:O4  | 10       | 0.28          |
| (6,16) | 2:18:B:A:N6 | 1:5:A:PSU:O2 | 7        | 0.28          |
| (6,16) | 2:18:B:A:N6 | 1:5:A:PSU:O2 | 11       | 0.28          |
| (6,12) | 1:4:A:C:N3  | 2:19:B:G:N1  | 8        | 0.28          |
| (6,8)  | 1:3:A:A:N6  | 2:20:B:U:O4  | 4        | 0.28          |
| (6,8)  | 1:3:A:A:N6  | 2:20:B:U:O4  | 15       | 0.28          |
| (6,4)  | 1:1:A:A:N6  | 2:22:B:U:O4  | 2        | 0.28          |
| (6,4)  | 1:1:A:A:N6  | 2:22:B:U:O4  | 5        | 0.28          |
| (6,4)  | 1:1:A:A:N6  | 2:22:B:U:O4  | 7        | 0.28          |
| (6,4)  | 1:1:A:A:N6  | 2:22:B:U:O4  | 9        | 0.28          |
| (6,4)  | 1:1:A:A:N6  | 2:22:B:U:O4  | 10       | 0.28          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 1        | 0.28          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 3        | 0.28          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 4        | 0.28          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 5        | 0.28          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 6        | 0.28          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 10       | 0.28          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 11       | 0.28          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 12       | 0.28          |
| (2,58) | 1:4:A:C:H1' | 1:4:A:C:H5   | 15       | 0.28          |
| (2,17) | 1:2:A:U:H1' | 1:2:A:U:H5   | 2        | 0.28          |
| (2,17) | 1:2:A:U:H1' | 1:2:A:U:H5   | 4        | 0.28          |
| (2,17) | 1:2:A:U:H1' | 1:2:A:U:H5   | 8        | 0.28          |
| (2,17) | 1:2:A:U:H1' | 1:2:A:U:H5   | 14       | 0.28          |
| (6,36) | 1:10:A:U:N3 | 2:12:B:G:O6  | 2        | 0.27          |
| (6,36) | 1:10:A:U:N3 | 2:12:B:G:O6  | 3        | 0.27          |
| (6,36) | 1:10:A:U:N3 | 2:12:B:G:O6  | 6        | 0.27          |
| (6,36) | 1:10:A:U:N3 | 2:12:B:G:O6  | 10       | 0.27          |
| (6,28) | 1:8:A:C:N3  | 2:15:B:G:N1  | 3        | 0.27          |
| (6,26) | 1:8:A:C:N4  | 2:15:B:G:O6  | 2        | 0.27          |
| (6,26) | 1:8:A:C:N4  | 2:15:B:G:O6  | 6        | 0.27          |
| (6,26) | 1:8:A:C:N4  | 2:15:B:G:O6  | 9        | 0.27          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (6,26)  | 1:8:A:C:N4   | 2:15:B:G:O6  | 14       | 0.27          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 9        | 0.27          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 9        | 0.27          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 11       | 0.27          |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 2        | 0.27          |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 10       | 0.27          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 3        | 0.27          |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 9        | 0.27          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 10       | 0.27          |
| (6,4)   | 1:1:A:A:N6   | 2:22:B:U:O4  | 6        | 0.27          |
| (2,297) | 2:19:B:G:H1' | 2:20:B:U:H5  | 1        | 0.27          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 1        | 0.27          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 3        | 0.27          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 5        | 0.27          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 10       | 0.27          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 12       | 0.27          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 15       | 0.27          |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 5        | 0.26          |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 10       | 0.26          |
| (6,26)  | 1:8:A:C:N4   | 2:15:B:G:O6  | 13       | 0.26          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 15       | 0.26          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 3        | 0.26          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 4        | 0.26          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 8        | 0.26          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 13       | 0.26          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 15       | 0.26          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 11       | 0.26          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 12       | 0.26          |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 8        | 0.26          |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 12       | 0.26          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 4        | 0.26          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 6        | 0.26          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 12       | 0.26          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 13       | 0.26          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 15       | 0.26          |
| (6,8)   | 1:3:A:A:N6   | 2:20:B:U:O4  | 1        | 0.26          |
| (6,4)   | 1:1:A:A:N6   | 2:22:B:U:O4  | 3        | 0.26          |
| (6,4)   | 1:1:A:A:N6   | 2:22:B:U:O4  | 15       | 0.26          |
| (2,164) | 1:11:A:G:H2' | 1:11:A:G:H8  | 2        | 0.26          |
| (2,164) | 1:11:A:G:H2' | 1:11:A:G:H8  | 4        | 0.26          |
| (2,164) | 1:11:A:G:H2' | 1:11:A:G:H8  | 6        | 0.26          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 5        | 0.26          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 14       | 0.26          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 6        | 0.26          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 7        | 0.26          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 9        | 0.26          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 11       | 0.26          |
| (2,17)  | 1:2:A:U:H1'  | 1:2:A:U:H5   | 13       | 0.26          |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 12       | 0.25          |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 13       | 0.25          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6  | 8        | 0.25          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 1        | 0.25          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 9        | 0.25          |
| (6,26)  | 1:8:A:C:N4   | 2:15:B:G:O6  | 7        | 0.25          |
| (6,26)  | 1:8:A:C:N4   | 2:15:B:G:O6  | 12       | 0.25          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 9        | 0.25          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 2        | 0.25          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 5        | 0.25          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 6        | 0.25          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 14       | 0.25          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 2        | 0.25          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 6        | 0.25          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 7        | 0.25          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 10       | 0.25          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 12       | 0.25          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 14       | 0.25          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 7        | 0.25          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 9        | 0.25          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 14       | 0.25          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 15       | 0.25          |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 9        | 0.25          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 7        | 0.25          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 10       | 0.25          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 14       | 0.25          |
| (2,164) | 1:11:A:G:H2' | 1:11:A:G:H8  | 3        | 0.25          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 1        | 0.25          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 8        | 0.25          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 12       | 0.25          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6  | 14       | 0.24          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 7        | 0.24          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 8        | 0.24          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 13       | 0.24          |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 2        | 0.24          |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 9        | 0.24          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 12       | 0.24          |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 13       | 0.24          |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 14       | 0.24          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 2        | 0.24          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 6        | 0.24          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 10       | 0.24          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 14       | 0.24          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 1        | 0.24          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 3        | 0.24          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 4        | 0.24          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 5        | 0.24          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 10       | 0.24          |
| (6,16)  | 2:18:B:A:N6  | 1:5:A:PSU:O2 | 15       | 0.24          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2 | 1        | 0.24          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 9        | 0.24          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 1        | 0.24          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 2        | 0.24          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 5        | 0.24          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 9        | 0.24          |
| (6,12)  | 1:4:A:C:N3   | 2:19:B:G:N1  | 11       | 0.24          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 6        | 0.24          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 8        | 0.24          |
| (6,4)   | 1:1:A:A:N6   | 2:22:B:U:O4  | 11       | 0.24          |
| (6,4)   | 1:1:A:A:N6   | 2:22:B:U:O4  | 12       | 0.24          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 2        | 0.24          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 6        | 0.24          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 7        | 0.24          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 15       | 0.24          |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'  | 5        | 0.24          |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5   | 5        | 0.24          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6  | 1        | 0.23          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6  | 15       | 0.23          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 3        | 0.23          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 12       | 0.23          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 15       | 0.23          |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 6        | 0.23          |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 7        | 0.23          |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 8        | 0.23          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 13       | 0.23          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 4        | 0.23          |
| (6,24)  | 1:7:A:A:N6   | 2:16:B:U:O4  | 12       | 0.23          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4  | 3        | 0.23          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 1        | 0.23          |
| (6,22)  | 2:16:B:U:N3  | 1:7:A:A:N1   | 5        | 0.23          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 10       | 0.23          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 12       | 0.23          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 13       | 0.23          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 1        | 0.23          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 3        | 0.23          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 8        | 0.23          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2 | 13       | 0.23          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 15       | 0.23          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 12       | 0.23          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 15       | 0.23          |
| (6,4)   | 1:1:A:A:N6   | 2:22:B:U:O4  | 13       | 0.23          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 4        | 0.23          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 9        | 0.23          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 10       | 0.23          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 11       | 0.23          |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'  | 2        | 0.23          |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'  | 3        | 0.23          |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5   | 2        | 0.23          |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5   | 3        | 0.23          |
| (2,40)  | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 1        | 0.23          |
| (2,40)  | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 3        | 0.23          |
| (2,40)  | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 7        | 0.23          |
| (2,40)  | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 8        | 0.23          |
| (2,40)  | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 12       | 0.23          |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 9        | 0.22          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6  | 2        | 0.22          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6  | 6        | 0.22          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 4        | 0.22          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 6        | 0.22          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 10       | 0.22          |
| (6,26)  | 1:8:A:C:N4   | 2:15:B:G:O6  | 4        | 0.22          |
| (6,26)  | 1:8:A:C:N4   | 2:15:B:G:O6  | 5        | 0.22          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4  | 13       | 0.22          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 2        | 0.22          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 15       | 0.22          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 11       | 0.22          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 6        | 0.22          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 3        | 0.22          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 11       | 0.22          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 8        | 0.22          |

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| Key    | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|--------|--------------|--------------|----------|---------------|
| (6,4)  | 1:1:A:A:N6   | 2:22:B:U:O4  | 1        | 0.22          |
| (6,4)  | 1:1:A:A:N6   | 2:22:B:U:O4  | 14       | 0.22          |
| (2,68) | 1:4:A:C:H5   | 1:4:A:C:H2'  | 1        | 0.22          |
| (2,68) | 1:4:A:C:H5   | 1:4:A:C:H2'  | 4        | 0.22          |
| (2,68) | 1:4:A:C:H5   | 1:4:A:C:H2'  | 7        | 0.22          |
| (2,68) | 1:4:A:C:H5   | 1:4:A:C:H2'  | 11       | 0.22          |
| (2,68) | 1:4:A:C:H5   | 1:4:A:C:H2'  | 15       | 0.22          |
| (2,63) | 1:4:A:C:H2'  | 1:4:A:C:H5   | 1        | 0.22          |
| (2,63) | 1:4:A:C:H2'  | 1:4:A:C:H5   | 4        | 0.22          |
| (2,63) | 1:4:A:C:H2'  | 1:4:A:C:H5   | 7        | 0.22          |
| (2,63) | 1:4:A:C:H2'  | 1:4:A:C:H5   | 11       | 0.22          |
| (2,63) | 1:4:A:C:H2'  | 1:4:A:C:H5   | 15       | 0.22          |
| (2,40) | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 2        | 0.22          |
| (2,40) | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 4        | 0.22          |
| (2,40) | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 5        | 0.22          |
| (2,40) | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 6        | 0.22          |
| (2,40) | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 9        | 0.22          |
| (2,40) | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 10       | 0.22          |
| (2,40) | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 11       | 0.22          |
| (2,40) | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 13       | 0.22          |
| (2,40) | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 14       | 0.22          |
| (2,40) | 1:3:A:A:H2'  | 1:3:A:A:H3'  | 15       | 0.22          |
| (6,35) | 1:10:A:U:H3  | 2:12:B:G:O6  | 3        | 0.21          |
| (6,35) | 1:10:A:U:H3  | 2:12:B:G:O6  | 11       | 0.21          |
| (6,31) | 1:9:A:C:N3   | 2:13:B:G:H1  | 5        | 0.21          |
| (6,31) | 1:9:A:C:N3   | 2:13:B:G:H1  | 14       | 0.21          |
| (6,28) | 1:8:A:C:N3   | 2:15:B:G:N1  | 1        | 0.21          |
| (6,28) | 1:8:A:C:N3   | 2:15:B:G:N1  | 4        | 0.21          |
| (6,28) | 1:8:A:C:N3   | 2:15:B:G:N1  | 5        | 0.21          |
| (6,26) | 1:8:A:C:N4   | 2:15:B:G:O6  | 1        | 0.21          |
| (6,26) | 1:8:A:C:N4   | 2:15:B:G:O6  | 11       | 0.21          |
| (6,25) | 1:8:A:C:H41  | 2:15:B:G:O6  | 7        | 0.21          |
| (6,23) | 1:7:A:A:H61  | 2:16:B:U:O4  | 8        | 0.21          |
| (6,23) | 1:7:A:A:H61  | 2:16:B:U:O4  | 11       | 0.21          |
| (6,20) | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 6        | 0.21          |
| (6,20) | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 14       | 0.21          |
| (6,18) | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 4        | 0.21          |
| (6,18) | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 5        | 0.21          |
| (6,18) | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 6        | 0.21          |
| (6,18) | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 13       | 0.21          |
| (6,15) | 2:18:B:A:H61 | 1:5:A:PSU:O2 | 3        | 0.21          |
| (6,15) | 2:18:B:A:H61 | 1:5:A:PSU:O2 | 5        | 0.21          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2 | 14       | 0.21          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 4        | 0.21          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 12       | 0.21          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 13       | 0.21          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 14       | 0.21          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 1        | 0.21          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 10       | 0.21          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 2        | 0.21          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 3        | 0.21          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 8        | 0.21          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 14       | 0.21          |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1   | 4        | 0.21          |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1   | 13       | 0.21          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 9        | 0.21          |
| (2,171) | 1:11:A:G:H5' | 1:11:A:G:H8  | 5        | 0.21          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 13       | 0.21          |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'  | 6        | 0.21          |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'  | 8        | 0.21          |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'  | 9        | 0.21          |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'  | 10       | 0.21          |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'  | 13       | 0.21          |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5   | 6        | 0.21          |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5   | 8        | 0.21          |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5   | 9        | 0.21          |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5   | 10       | 0.21          |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5   | 13       | 0.21          |
| (6,36)  | 1:10:A:U:N3  | 2:12:B:G:O6  | 7        | 0.2           |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 11       | 0.2           |
| (6,26)  | 1:8:A:C:N4   | 2:15:B:G:O6  | 15       | 0.2           |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 12       | 0.2           |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4  | 1        | 0.2           |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4  | 7        | 0.2           |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 9        | 0.2           |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 1        | 0.2           |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 5        | 0.2           |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 7        | 0.2           |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 8        | 0.2           |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 2        | 0.2           |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 4        | 0.2           |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 9        | 0.2           |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 13       | 0.2           |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 5        | 0.2           |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 6        | 0.2           |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 2        | 0.2           |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 13       | 0.2           |
| (6,4)   | 1:1:A:A:N6   | 2:22:B:U:O4  | 4        | 0.2           |
| (6,4)   | 1:1:A:A:N6   | 2:22:B:U:O4  | 8        | 0.2           |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1   | 6        | 0.2           |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1   | 9        | 0.2           |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1   | 12       | 0.2           |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1   | 14       | 0.2           |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 8        | 0.2           |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'  | 12       | 0.2           |
| (2,68)  | 1:4:A:C:H5   | 1:4:A:C:H2'  | 14       | 0.2           |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5   | 12       | 0.2           |
| (2,63)  | 1:4:A:C:H2'  | 1:4:A:C:H5   | 14       | 0.2           |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6  | 10       | 0.19          |
| (6,31)  | 1:9:A:C:N3   | 2:13:B:G:H1  | 2        | 0.19          |
| (6,28)  | 1:8:A:C:N3   | 2:15:B:G:N1  | 15       | 0.19          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 1        | 0.19          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 4        | 0.19          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4  | 9        | 0.19          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4  | 10       | 0.19          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 8        | 0.19          |
| (6,18)  | 1:6:A:PSU:N3 | 2:17:B:A:N1  | 2        | 0.19          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2 | 6        | 0.19          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 2        | 0.19          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 3        | 0.19          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 10       | 0.19          |
| (6,14)  | 1:5:A:PSU:N3 | 2:18:B:A:N1  | 11       | 0.19          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1  | 8        | 0.19          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 5        | 0.19          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 7        | 0.19          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 11       | 0.19          |
| (6,10)  | 1:4:A:C:N4   | 2:19:B:G:O6  | 14       | 0.19          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 4        | 0.19          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 15       | 0.19          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 3        | 0.19          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 14       | 0.19          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 15       | 0.19          |
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4  | 2        | 0.19          |
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4  | 5        | 0.19          |
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4  | 7        | 0.19          |
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4  | 9        | 0.19          |

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| Key     | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|---------|--------------|--------------|----------|---------------|
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4  | 10       | 0.19          |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1   | 1        | 0.19          |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1   | 3        | 0.19          |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1   | 5        | 0.19          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 4        | 0.19          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 7        | 0.19          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 11       | 0.19          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 12       | 0.19          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 13       | 0.19          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 14       | 0.19          |
| (2,131) | 1:8:A:C:H3'  | 1:9:A:C:H6   | 3        | 0.19          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6  | 5        | 0.18          |
| (6,27)  | 1:8:A:C:N3   | 2:15:B:G:H1  | 3        | 0.18          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 5        | 0.18          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 11       | 0.18          |
| (6,20)  | 2:17:B:A:N6  | 1:6:A:PSU:O2 | 7        | 0.18          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2 | 7        | 0.18          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2 | 10       | 0.18          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2 | 11       | 0.18          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1  | 3        | 0.18          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1  | 4        | 0.18          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1  | 12       | 0.18          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1  | 13       | 0.18          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4  | 9        | 0.18          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 1        | 0.18          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 4        | 0.18          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 5        | 0.18          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 6        | 0.18          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 7        | 0.18          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 10       | 0.18          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 11       | 0.18          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1   | 12       | 0.18          |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1   | 10       | 0.18          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 2        | 0.18          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 3        | 0.18          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6  | 5        | 0.18          |
| (2,164) | 1:11:A:G:H2' | 1:11:A:G:H8  | 1        | 0.18          |
| (6,27)  | 1:8:A:C:N3   | 2:15:B:G:H1  | 10       | 0.17          |
| (6,25)  | 1:8:A:C:H41  | 2:15:B:G:O6  | 15       | 0.17          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4  | 6        | 0.17          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4  | 15       | 0.17          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1   | 4        | 0.17          |

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| Key     | Atom-1       | Atom-2           | Model ID | Violation (Å) |
|---------|--------------|------------------|----------|---------------|
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 8        | 0.17          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 9        | 0.17          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 11       | 0.17          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 15       | 0.17          |
| (6,19)  | 2:17:B:A:H61 | 1:6:A:PSU:O2     | 11       | 0.17          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2     | 2        | 0.17          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2     | 8        | 0.17          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2     | 12       | 0.17          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1      | 6        | 0.17          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1      | 7        | 0.17          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1      | 14       | 0.17          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1      | 15       | 0.17          |
| (6,6)   | 2:20:B:U:N3  | 1:3:A:A:N1       | 9        | 0.17          |
| (6,5)   | 2:20:B:U:H3  | 1:3:A:A:N1       | 8        | 0.17          |
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4      | 3        | 0.17          |
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4      | 6        | 0.17          |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1       | 2        | 0.17          |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1       | 8        | 0.17          |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1       | 11       | 0.17          |
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1       | 15       | 0.17          |
| (5,2)   | 1:9:A:C:H5   | 3:101:B:YB3:H28A | 7        | 0.17          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6      | 6        | 0.17          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6      | 15       | 0.17          |
| (2,164) | 1:11:A:G:H2' | 1:11:A:G:H8      | 12       | 0.17          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6      | 12       | 0.16          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6      | 13       | 0.16          |
| (6,30)  | 1:9:A:C:N4   | 2:13:B:G:O6      | 3        | 0.16          |
| (6,30)  | 1:9:A:C:N4   | 2:13:B:G:O6      | 7        | 0.16          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4      | 2        | 0.16          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4      | 5        | 0.16          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4      | 14       | 0.16          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 3        | 0.16          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 7        | 0.16          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 13       | 0.16          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2     | 9        | 0.16          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1      | 1        | 0.16          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1      | 2        | 0.16          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1      | 5        | 0.16          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1      | 10       | 0.16          |
| (6,7)   | 1:3:A:A:H61  | 2:20:B:U:O4      | 1        | 0.16          |
| (6,5)   | 2:20:B:U:H3  | 1:3:A:A:N1       | 13       | 0.16          |
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4      | 15       | 0.16          |

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| Key     | Atom-1       | Atom-2           | Model ID | Violation (Å) |
|---------|--------------|------------------|----------|---------------|
| (6,1)   | 2:22:B:U:H3  | 1:1:A:A:N1       | 7        | 0.16          |
| (5,2)   | 1:9:A:C:H5   | 3:101:B:YB3:H28A | 4        | 0.16          |
| (5,2)   | 1:9:A:C:H5   | 3:101:B:YB3:H28A | 12       | 0.16          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6      | 1        | 0.16          |
| (2,331) | 2:22:B:U:H2' | 2:22:B:U:H6      | 10       | 0.16          |
| (6,30)  | 1:9:A:C:N4   | 2:13:B:G:O6      | 1        | 0.15          |
| (6,27)  | 1:8:A:C:N3   | 2:15:B:G:H1      | 2        | 0.15          |
| (6,27)  | 1:8:A:C:N3   | 2:15:B:G:H1      | 14       | 0.15          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 2        | 0.15          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 6        | 0.15          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 10       | 0.15          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 12       | 0.15          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 14       | 0.15          |
| (6,19)  | 2:17:B:A:H61 | 1:6:A:PSU:O2     | 3        | 0.15          |
| (6,19)  | 2:17:B:A:H61 | 1:6:A:PSU:O2     | 4        | 0.15          |
| (6,15)  | 2:18:B:A:H61 | 1:5:A:PSU:O2     | 15       | 0.15          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1      | 9        | 0.15          |
| (6,11)  | 1:4:A:C:N3   | 2:19:B:G:H1      | 11       | 0.15          |
| (6,9)   | 1:4:A:C:H41  | 2:19:B:G:O6      | 6        | 0.15          |
| (6,9)   | 1:4:A:C:H41  | 2:19:B:G:O6      | 8        | 0.15          |
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4      | 11       | 0.15          |
| (6,3)   | 1:1:A:A:H61  | 2:22:B:U:O4      | 12       | 0.15          |
| (6,35)  | 1:10:A:U:H3  | 2:12:B:G:O6      | 9        | 0.14          |
| (6,30)  | 1:9:A:C:N4   | 2:13:B:G:O6      | 14       | 0.14          |
| (6,27)  | 1:8:A:C:N3   | 2:15:B:G:H1      | 7        | 0.14          |
| (6,27)  | 1:8:A:C:N3   | 2:15:B:G:H1      | 8        | 0.14          |
| (6,27)  | 1:8:A:C:N3   | 2:15:B:G:H1      | 9        | 0.14          |
| (6,27)  | 1:8:A:C:N3   | 2:15:B:G:H1      | 12       | 0.14          |
| (6,27)  | 1:8:A:C:N3   | 2:15:B:G:H1      | 13       | 0.14          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4      | 4        | 0.14          |
| (6,23)  | 1:7:A:A:H61  | 2:16:B:U:O4      | 12       | 0.14          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 1        | 0.14          |
| (6,21)  | 2:16:B:U:H3  | 1:7:A:A:N1       | 5        | 0.14          |
| (6,19)  | 2:17:B:A:H61 | 1:6:A:PSU:O2     | 1        | 0.14          |
| (6,19)  | 2:17:B:A:H61 | 1:6:A:PSU:O2     | 5        | 0.14          |
| (6,19)  | 2:17:B:A:H61 | 1:6:A:PSU:O2     | 12       | 0.14          |
| (6,9)   | 1:4:A:C:H41  | 2:19:B:G:O6      | 12       | 0.14          |
| (6,9)   | 1:4:A:C:H41  | 2:19:B:G:O6      | 15       | 0.14          |
| (6,5)   | 2:20:B:U:H3  | 1:3:A:A:N1       | 2        | 0.14          |
| (6,5)   | 2:20:B:U:H3  | 1:3:A:A:N1       | 3        | 0.14          |
| (6,5)   | 2:20:B:U:H3  | 1:3:A:A:N1       | 5        | 0.14          |
| (6,5)   | 2:20:B:U:H3  | 1:3:A:A:N1       | 6        | 0.14          |

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| Key     | Atom-1        | Atom-2           | Model ID | Violation (Å) |
|---------|---------------|------------------|----------|---------------|
| (6,5)   | 2:20:B:U:H3   | 1:3:A:A:N1       | 7        | 0.14          |
| (6,5)   | 2:20:B:U:H3   | 1:3:A:A:N1       | 12       | 0.14          |
| (6,5)   | 2:20:B:U:H3   | 1:3:A:A:N1       | 14       | 0.14          |
| (6,5)   | 2:20:B:U:H3   | 1:3:A:A:N1       | 15       | 0.14          |
| (6,3)   | 1:1:A:A:H61   | 2:22:B:U:O4      | 13       | 0.14          |
| (2,164) | 1:11:A:G:H2'  | 1:11:A:G:H8      | 11       | 0.14          |
| (2,164) | 1:11:A:G:H2'  | 1:11:A:G:H8      | 14       | 0.14          |
| (6,30)  | 1:9:A:C:N4    | 2:13:B:G:O6      | 5        | 0.13          |
| (6,30)  | 1:9:A:C:N4    | 2:13:B:G:O6      | 10       | 0.13          |
| (6,30)  | 1:9:A:C:N4    | 2:13:B:G:O6      | 12       | 0.13          |
| (6,27)  | 1:8:A:C:N3    | 2:15:B:G:H1      | 6        | 0.13          |
| (6,19)  | 2:17:B:A:H61  | 1:6:A:PSU:O2     | 2        | 0.13          |
| (6,19)  | 2:17:B:A:H61  | 1:6:A:PSU:O2     | 10       | 0.13          |
| (6,19)  | 2:17:B:A:H61  | 1:6:A:PSU:O2     | 13       | 0.13          |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 3        | 0.13          |
| (6,5)   | 2:20:B:U:H3   | 1:3:A:A:N1       | 4        | 0.13          |
| (6,5)   | 2:20:B:U:H3   | 1:3:A:A:N1       | 11       | 0.13          |
| (6,3)   | 1:1:A:A:H61   | 2:22:B:U:O4      | 1        | 0.13          |
| (5,2)   | 1:9:A:C:H5    | 3:101:B:YB3:H28A | 10       | 0.13          |
| (2,164) | 1:11:A:G:H2'  | 1:11:A:G:H8      | 7        | 0.13          |
| (2,164) | 1:11:A:G:H2'  | 1:11:A:G:H8      | 8        | 0.13          |
| (2,164) | 1:11:A:G:H2'  | 1:11:A:G:H8      | 9        | 0.13          |
| (6,35)  | 1:10:A:U:H3   | 2:12:B:G:O6      | 7        | 0.12          |
| (6,30)  | 1:9:A:C:N4    | 2:13:B:G:O6      | 9        | 0.12          |
| (6,30)  | 1:9:A:C:N4    | 2:13:B:G:O6      | 13       | 0.12          |
| (6,30)  | 1:9:A:C:N4    | 2:13:B:G:O6      | 15       | 0.12          |
| (6,27)  | 1:8:A:C:N3    | 2:15:B:G:H1      | 1        | 0.12          |
| (6,27)  | 1:8:A:C:N3    | 2:15:B:G:H1      | 4        | 0.12          |
| (6,19)  | 2:17:B:A:H61  | 1:6:A:PSU:O2     | 15       | 0.12          |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 1        | 0.12          |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 4        | 0.12          |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 10       | 0.12          |
| (6,5)   | 2:20:B:U:H3   | 1:3:A:A:N1       | 9        | 0.12          |
| (6,5)   | 2:20:B:U:H3   | 1:3:A:A:N1       | 10       | 0.12          |
| (6,3)   | 1:1:A:A:H61   | 2:22:B:U:O4      | 14       | 0.12          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 2        | 0.12          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 3        | 0.12          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 8        | 0.12          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 10       | 0.12          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 15       | 0.12          |
| (2,164) | 1:11:A:G:H2'  | 1:11:A:G:H8      | 10       | 0.12          |
| (2,164) | 1:11:A:G:H2'  | 1:11:A:G:H8      | 15       | 0.12          |

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| Key     | Atom-1        | Atom-2           | Model ID | Violation (Å) |
|---------|---------------|------------------|----------|---------------|
| (2,53)  | 1:3:A:A:H8    | 1:2:A:U:H4'      | 13       | 0.12          |
| (6,30)  | 1:9:A:C:N4    | 2:13:B:G:O6      | 6        | 0.11          |
| (6,27)  | 1:8:A:C:N3    | 2:15:B:G:H1      | 5        | 0.11          |
| (6,27)  | 1:8:A:C:N3    | 2:15:B:G:H1      | 11       | 0.11          |
| (6,19)  | 2:17:B:A:H61  | 1:6:A:PSU:O2     | 6        | 0.11          |
| (6,19)  | 2:17:B:A:H61  | 1:6:A:PSU:O2     | 9        | 0.11          |
| (6,19)  | 2:17:B:A:H61  | 1:6:A:PSU:O2     | 14       | 0.11          |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 2        | 0.11          |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 5        | 0.11          |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 7        | 0.11          |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 9        | 0.11          |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 13       | 0.11          |
| (6,5)   | 2:20:B:U:H3   | 1:3:A:A:N1       | 1        | 0.11          |
| (6,3)   | 1:1:A:A:H61   | 2:22:B:U:O4      | 4        | 0.11          |
| (6,3)   | 1:1:A:A:H61   | 2:22:B:U:O4      | 8        | 0.11          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 4        | 0.11          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 5        | 0.11          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 7        | 0.11          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 11       | 0.11          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 12       | 0.11          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 13       | 0.11          |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 14       | 0.11          |
| (2,164) | 1:11:A:G:H2'  | 1:11:A:G:H8      | 13       | 0.11          |
| (2,137) | 1:8:A:C:H3'   | 1:9:A:C:H6       | 5        | 0.11          |
| (2,137) | 1:8:A:C:H3'   | 1:9:A:C:H6       | 14       | 0.11          |
| (2,97)  | 1:6:A:PSU:H2' | 2:17:B:A:H2      | 12       | 0.11          |
| (2,97)  | 1:6:A:PSU:H2' | 2:17:B:A:H2      | 15       | 0.11          |
| (2,53)  | 1:3:A:A:H8    | 1:2:A:U:H4'      | 4        | 0.11          |
| (2,53)  | 1:3:A:A:H8    | 1:2:A:U:H4'      | 12       | 0.11          |
| (6,30)  | 1:9:A:C:N4    | 2:13:B:G:O6      | 11       | 0.1           |
| (6,29)  | 1:9:A:C:H41   | 2:13:B:G:O6      | 3        | 0.1           |
| (6,9)   | 1:4:A:C:H41   | 2:19:B:G:O6      | 11       | 0.1           |
| (5,2)   | 1:8:A:C:H6    | 3:101:B:YB3:H28A | 15       | 0.1           |
| (2,232) | 2:15:B:G:H5'' | 2:15:B:G:H4'     | 9        | 0.1           |
| (2,169) | 1:11:A:G:H4'  | 1:11:A:G:H8      | 5        | 0.1           |
| (2,154) | 1:9:A:C:H5    | 1:10:A:U:H6      | 7        | 0.1           |
| (2,137) | 1:8:A:C:H3'   | 1:9:A:C:H6       | 1        | 0.1           |
| (2,137) | 1:8:A:C:H3'   | 1:9:A:C:H6       | 12       | 0.1           |
| (2,53)  | 1:3:A:A:H8    | 1:2:A:U:H4'      | 9        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

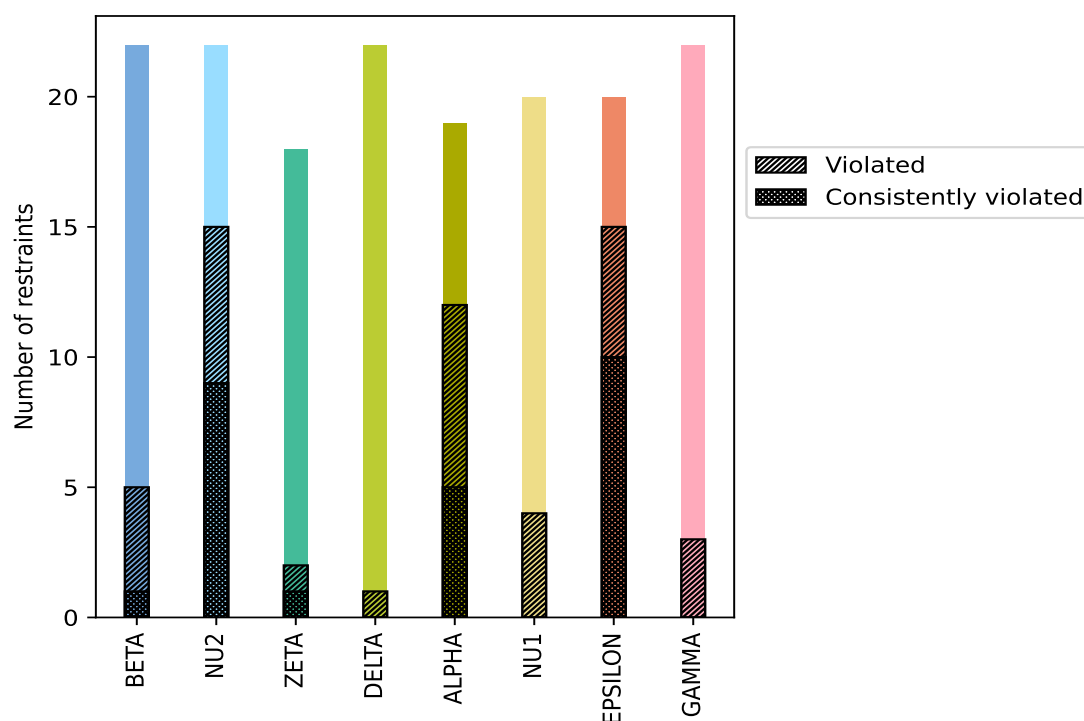
### 10.1 Summary of dihedral-angle violations ⓘ

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| BETA       | 22    | 13.3           | 5                     | 22.7           | 3.0            | 1                                  | 4.5            | 0.6            |
| NU2        | 22    | 13.3           | 15                    | 68.2           | 9.1            | 9                                  | 40.9           | 5.5            |
| ZETA       | 18    | 10.9           | 2                     | 11.1           | 1.2            | 1                                  | 5.6            | 0.6            |
| DELTA      | 22    | 13.3           | 1                     | 4.5            | 0.6            | 0                                  | 0.0            | 0.0            |
| ALPHA      | 19    | 11.5           | 12                    | 63.2           | 7.3            | 5                                  | 26.3           | 3.0            |
| NU1        | 20    | 12.1           | 4                     | 20.0           | 2.4            | 0                                  | 0.0            | 0.0            |
| EPSILON    | 20    | 12.1           | 15                    | 75.0           | 9.1            | 10                                 | 50.0           | 6.1            |
| GAMMA      | 22    | 13.3           | 3                     | 13.6           | 1.8            | 0                                  | 0.0            | 0.0            |
| Total      | 165   | 100.0          | 57                    | 34.5           | 34.5           | 26                                 | 15.8           | 15.8           |

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

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations ⓘ



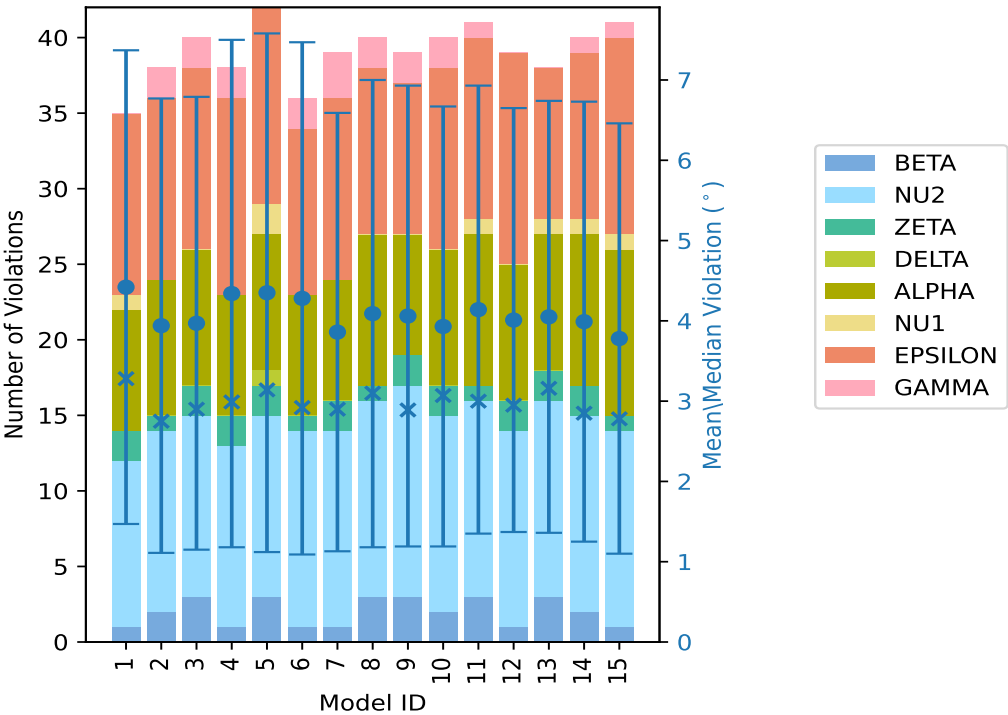
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

| Model ID | Number of violations |     |      |       |       |     |         |       |    | Total | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|------|-------|-------|-----|---------|-------|----|-------|----------|---------|--------|------------|
|          | BETA                 | NU2 | ZETA | DELTA | ALPHA | NU1 | EPSILON | GAMMA |    |       |          |         |        |            |
| 1        | 1                    | 11  | 2    | 0     | 8     | 1   | 12      | 0     | 35 | 4.42  | 11.03    | 2.95    | 3.28   |            |
| 2        | 2                    | 12  | 1    | 0     | 9     | 0   | 12      | 2     | 38 | 3.94  | 11.0     | 2.83    | 2.75   |            |
| 3        | 3                    | 12  | 2    | 0     | 9     | 0   | 12      | 2     | 40 | 3.97  | 11.33    | 2.82    | 2.9    |            |
| 4        | 1                    | 12  | 2    | 0     | 8     | 0   | 13      | 2     | 38 | 4.34  | 13.69    | 3.16    | 2.99   |            |
| 5        | 3                    | 12  | 2    | 1     | 9     | 2   | 13      | 0     | 42 | 4.35  | 14.32    | 3.23    | 3.14   |            |
| 6        | 1                    | 13  | 1    | 0     | 8     | 0   | 11      | 2     | 36 | 4.28  | 12.38    | 3.19    | 2.92   |            |
| 7        | 1                    | 13  | 2    | 0     | 8     | 0   | 12      | 3     | 39 | 3.86  | 10.48    | 2.73    | 2.9    |            |
| 8        | 3                    | 13  | 1    | 0     | 10    | 0   | 11      | 2     | 40 | 4.09  | 11.86    | 2.91    | 3.1    |            |
| 9        | 3                    | 14  | 2    | 0     | 8     | 0   | 10      | 2     | 39 | 4.06  | 11.32    | 2.87    | 2.89   |            |
| 10       | 2                    | 13  | 2    | 0     | 9     | 0   | 12      | 2     | 40 | 3.93  | 11.23    | 2.74    | 3.07   |            |
| 11       | 3                    | 13  | 1    | 0     | 10    | 1   | 12      | 1     | 41 | 4.14  | 10.3     | 2.79    | 3.0    |            |
| 12       | 1                    | 13  | 2    | 0     | 9     | 0   | 14      | 0     | 39 | 4.01  | 10.77    | 2.64    | 2.95   |            |
| 13       | 3                    | 13  | 2    | 0     | 9     | 1   | 10      | 0     | 38 | 4.05  | 11.43    | 2.69    | 3.16   |            |
| 14       | 2                    | 13  | 2    | 0     | 10    | 1   | 11      | 1     | 40 | 3.99  | 10.45    | 2.74    | 2.85   |            |
| 15       | 1                    | 13  | 1    | 0     | 11    | 1   | 13      | 1     | 41 | 3.78  | 10.33    | 2.68    | 2.78   |            |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

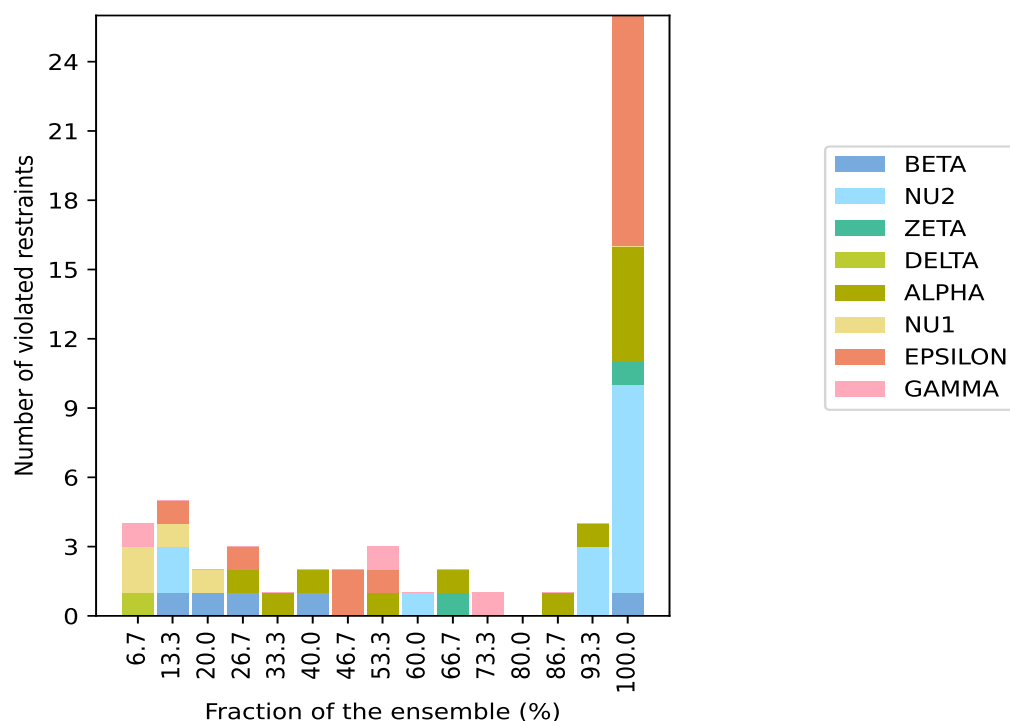
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

| Number of violated restraints |     |      |       |       |     |         |       |       | Fraction of the ensemble |       |
|-------------------------------|-----|------|-------|-------|-----|---------|-------|-------|--------------------------|-------|
| BETA                          | NU2 | ZETA | DELTA | ALPHA | NU1 | EPSILON | GAMMA | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0    | 1     | 0     | 2   | 0       | 1     | 4     | 1                        | 6.7   |
| 1                             | 2   | 0    | 0     | 0     | 1   | 1       | 0     | 5     | 2                        | 13.3  |
| 1                             | 0   | 0    | 0     | 0     | 1   | 0       | 0     | 2     | 3                        | 20.0  |
| 1                             | 0   | 0    | 0     | 1     | 0   | 1       | 0     | 3     | 4                        | 26.7  |
| 0                             | 0   | 0    | 0     | 1     | 0   | 0       | 0     | 1     | 5                        | 33.3  |
| 1                             | 0   | 0    | 0     | 1     | 0   | 0       | 0     | 2     | 6                        | 40.0  |
| 0                             | 0   | 0    | 0     | 0     | 0   | 2       | 0     | 2     | 7                        | 46.7  |
| 0                             | 0   | 0    | 0     | 1     | 0   | 1       | 1     | 3     | 8                        | 53.3  |
| 0                             | 1   | 0    | 0     | 0     | 0   | 0       | 0     | 1     | 9                        | 60.0  |
| 0                             | 0   | 1    | 0     | 1     | 0   | 0       | 0     | 2     | 10                       | 66.7  |
| 0                             | 0   | 0    | 0     | 0     | 0   | 0       | 1     | 1     | 11                       | 73.3  |
| 0                             | 0   | 0    | 0     | 0     | 0   | 0       | 0     | 0     | 12                       | 80.0  |
| 0                             | 0   | 0    | 0     | 1     | 0   | 0       | 0     | 1     | 13                       | 86.7  |
| 0                             | 3   | 0    | 0     | 1     | 0   | 0       | 0     | 4     | 14                       | 93.3  |
| 1                             | 9   | 1    | 0     | 5     | 0   | 10      | 0     | 26    | 15                       | 100.0 |

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

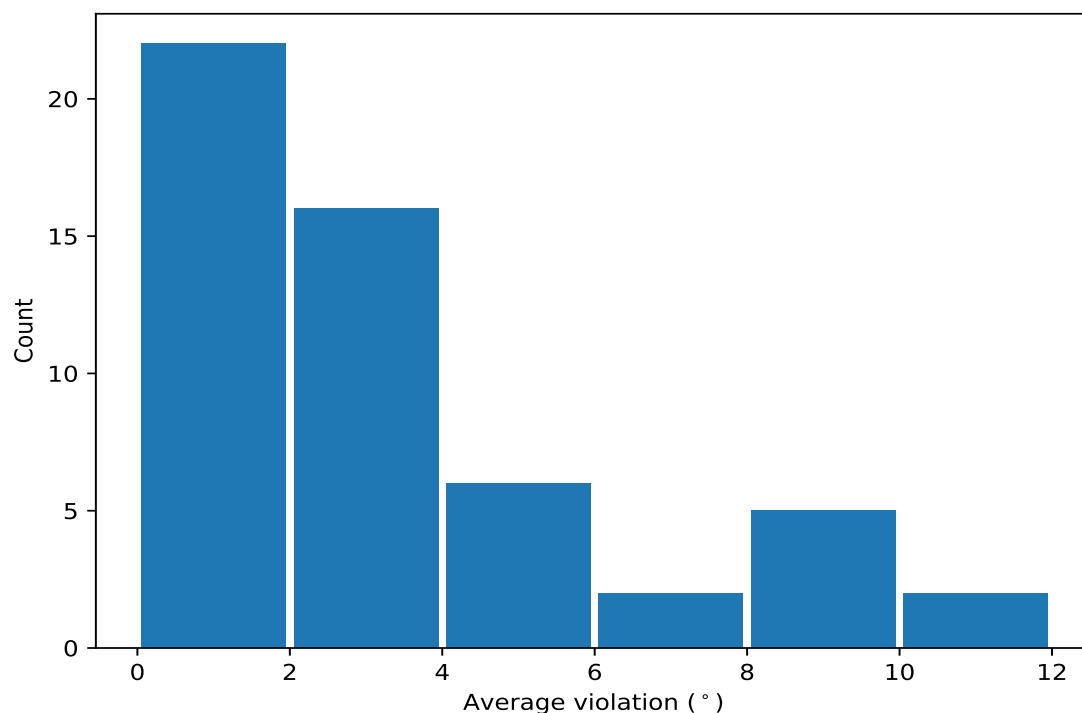
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



### 10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|---------------|---------------|---------------|--------------|---------------------|-------|-----------------|--------|
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 15                  | 10.85 | 1.31            | 11.0   |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 15                  | 10.35 | 0.83            | 10.43  |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 15                  | 8.75  | 0.98            | 8.56   |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 15                  | 8.65  | 0.85            | 8.51   |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 15                  | 8.49  | 0.62            | 8.36   |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 15                  | 8.48  | 0.62            | 8.31   |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 15                  | 8.45  | 1.04            | 8.59   |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 15                  | 7.1   | 1.02            | 6.96   |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 15                  | 5.86  | 0.96            | 5.74   |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 15                  | 5.8   | 1.61            | 6.01   |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 15                  | 5.09  | 0.66            | 4.96   |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 15                  | 4.63  | 1.07            | 4.79   |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 15                  | 4.13  | 0.59            | 4.06   |

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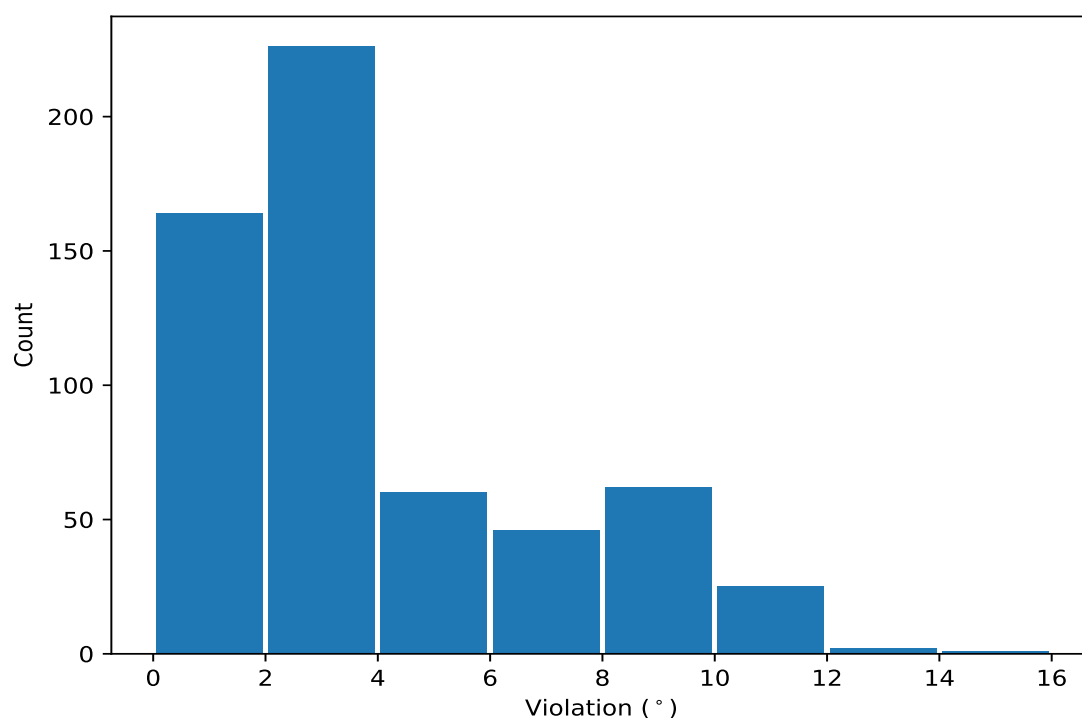
| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|---------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5'  | 15                  | 4.03 | 0.79            | 3.94   |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4'  | 15                  | 3.8  | 0.25            | 3.74   |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P    | 15                  | 3.26 | 0.91            | 3.44   |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'   | 15                  | 3.21 | 0.18            | 3.28   |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4'  | 15                  | 3.18 | 0.34            | 3.32   |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P    | 15                  | 3.04 | 0.82            | 3.1    |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 15                  | 2.69 | 0.29            | 2.82   |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 15                  | 2.69 | 0.26            | 2.71   |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 15                  | 2.61 | 0.3             | 2.66   |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 15                  | 2.58 | 0.87            | 2.4    |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 15                  | 2.53 | 0.35            | 2.44   |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 15                  | 1.76 | 0.3             | 1.7    |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 15                  | 1.73 | 0.41            | 1.7    |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 14                  | 2.09 | 0.59            | 2.18   |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 14                  | 1.89 | 0.59            | 1.71   |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 14                  | 1.61 | 0.32            | 1.7    |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 14                  | 1.56 | 0.27            | 1.55   |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 13                  | 2.06 | 0.55            | 1.96   |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 11                  | 1.96 | 0.62            | 1.94   |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5'  | 10                  | 3.2  | 0.41            | 3.25   |
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 10                  | 1.9  | 0.41            | 1.88   |
| (1,51)  | 1:7:A:A:C1'   | 1:7:A:A:C2'   | 1:7:A:A:C3'   | 1:7:A:A:C4'   | 9                   | 1.25 | 0.15            | 1.24   |
| (1,129) | 2:17:B:A:O3'  | 2:18:B:A:P    | 2:18:B:A:O5'  | 2:18:B:A:C5'  | 8                   | 2.01 | 0.62            | 1.9    |
| (1,21)  | 1:3:A:A:C4'   | 1:3:A:A:C3'   | 1:3:A:A:O3'   | 1:4:A:C:P     | 8                   | 1.63 | 0.39            | 1.64   |
| (1,115) | 2:16:B:U:O5'  | 2:16:B:U:C5'  | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 8                   | 1.57 | 0.27            | 1.5    |
| (1,60)  | 1:8:A:C:C4'   | 1:8:A:C:C3'   | 1:8:A:C:O3'   | 1:9:A:C:P     | 7                   | 2.28 | 0.71            | 2.27   |
| (1,53)  | 1:7:A:A:C4'   | 1:7:A:A:C3'   | 1:7:A:A:O3'   | 1:8:A:C:P     | 7                   | 1.7  | 0.78            | 1.31   |
| (1,70)  | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5'  | 1:10:A:U:C4'  | 6                   | 1.94 | 0.44            | 1.91   |
| (1,145) | 2:19:B:G:O3'  | 2:20:B:U:P    | 2:20:B:U:O5'  | 2:20:B:U:C5'  | 6                   | 1.2  | 0.09            | 1.24   |
| (1,121) | 2:16:B:U:O3'  | 2:17:B:A:P    | 2:17:B:A:O5'  | 2:17:B:A:C5'  | 5                   | 1.76 | 0.4             | 1.66   |
| (1,13)  | 1:2:A:U:C4'   | 1:2:A:U:C3'   | 1:2:A:U:O3'   | 1:3:A:A:P     | 4                   | 1.76 | 0.66            | 1.52   |
| (1,153) | 2:20:B:U:O3'  | 2:21:B:C:P    | 2:21:B:C:O5'  | 2:21:B:C:C5'  | 4                   | 1.66 | 0.5             | 1.4    |
| (1,98)  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5'  | 2:14:B:A:C4'  | 4                   | 1.65 | 0.79            | 1.2    |
| (1,76)  | 1:11:A:G:P    | 1:11:A:G:O5'  | 1:11:A:G:C5'  | 1:11:A:G:C4'  | 3                   | 2.61 | 0.94            | 2.86   |
| (1,67)  | 1:9:A:C:O4'   | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 3                   | 1.21 | 0.23            | 1.06   |
| (1,80)  | 1:11:A:G:O4'  | 1:11:A:G:C1'  | 1:11:A:G:C2'  | 1:11:A:G:C3'  | 2                   | 7.29 | 2.63            | 7.29   |
| (1,29)  | 1:4:A:C:C4'   | 1:4:A:C:C3'   | 1:4:A:C:O3'   | 1:5:A:PSU:P   | 2                   | 1.83 | 0.23            | 1.83   |
| (1,56)  | 1:8:A:C:P     | 1:8:A:C:O5'   | 1:8:A:C:C5'   | 1:8:A:C:C4'   | 2                   | 1.45 | 0.12            | 1.45   |
| (1,93)  | 2:13:B:G:C1'  | 2:13:B:G:C2'  | 2:13:B:G:C3'  | 2:13:B:G:C4'  | 2                   | 1.32 | 0.17            | 1.32   |
| (1,43)  | 1:6:A:PSU:C1' | 1:6:A:PSU:C2' | 1:6:A:PSU:C3' | 1:6:A:PSU:C4' | 2                   | 1.3  | 0.07            | 1.3    |

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

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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



### 10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|--------------|----------|---------------|
| (1,78)  | 1:11:A:G:C5'  | 1:11:A:G:C4'  | 1:11:A:G:C3'  | 1:11:A:G:O3' | 5        | 14.32         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 4        | 13.69         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 6        | 12.38         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 5        | 11.87         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 8        | 11.86         |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 4        | 11.63         |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 13       | 11.43         |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 3        | 11.33         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 9        | 11.32         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 3        | 11.23         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 10       | 11.23         |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 1        | 11.03         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 2        | 11.0          |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 12       | 10.77         |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 2        | 10.72         |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 8        | 10.71         |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 1        | 10.52         |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 7        | 10.48         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 14       | 10.45         |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 6        | 10.43         |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 5        | 10.42         |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|--------------|----------|---------------|
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 10       | 10.4          |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 15       | 10.33         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 11       | 10.3          |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 11       | 10.24         |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 7        | 10.18         |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 14       | 10.15         |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 4        | 10.12         |
| (1,80)  | 1:11:A:G:O4'  | 1:11:A:G:C1'  | 1:11:A:G:C2'  | 1:11:A:G:C3' | 5        | 9.92          |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 10       | 9.89          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 9        | 9.88          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 9        | 9.85          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 6        | 9.79          |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 9        | 9.75          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 12       | 9.6           |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 12       | 9.58          |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 15       | 9.55          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 2        | 9.54          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 8        | 9.45          |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 12       | 9.43          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 10       | 9.38          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 6        | 9.37          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 11       | 9.33          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 1        | 9.32          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 15       | 9.32          |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 8        | 9.29          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 14       | 9.28          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 11       | 9.22          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 13       | 9.19          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 3        | 9.1           |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 13       | 9.03          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 4        | 9.02          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 11       | 8.95          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 1        | 8.86          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 3        | 8.86          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 7        | 8.7           |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 10       | 8.67          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 8        | 8.64          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 6        | 8.63          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 15       | 8.59          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 5        | 8.59          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 11       | 8.56          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 3        | 8.55          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 4        | 8.55          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 7        | 8.53          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 5        | 8.51          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 1        | 8.51          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 4        | 8.5           |
| (1,37)  | 1:5:A:PSU:C4' | 1:5:A:PSU:C3' | 1:5:A:PSU:O3' | 1:6:A:PSU:P  | 5        | 8.49          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 14       | 8.49          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 15       | 8.44          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 12       | 8.44          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|--------------|----------|---------------|
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 6        | 8.41          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 14       | 8.39          |
| (1,89)  | 2:12:B:G:O3'  | 2:13:B:G:P    | 2:13:B:G:O5'  | 2:13:B:G:C5' | 1        | 8.39          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 5        | 8.38          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 2        | 8.38          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 8        | 8.36          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 13       | 8.36          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 8        | 8.33          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 1        | 8.31          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 5        | 8.3           |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 2        | 8.24          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 9        | 8.22          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 3        | 8.18          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 1        | 8.15          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 6        | 8.12          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 2        | 8.07          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 9        | 8.04          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 14       | 8.0           |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 7        | 7.99          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 13       | 7.99          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 4        | 7.98          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 7        | 7.98          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 3        | 7.97          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 6        | 7.97          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 14       | 7.97          |
| (1,7)   | 1:1:A:A:O3'   | 1:2:A:U:P     | 1:2:A:U:O5'   | 1:2:A:U:C5'  | 11       | 7.96          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 6        | 7.86          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 10       | 7.85          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 13       | 7.81          |
| (1,111) | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 2:15:B:G:O3'  | 2:16:B:U:P   | 15       | 7.78          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 9        | 7.78          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 4        | 7.75          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 11       | 7.74          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 13       | 7.67          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 7        | 7.66          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 15       | 7.66          |
| (1,103) | 2:14:B:A:C4'  | 2:14:B:A:C3'  | 2:14:B:A:O3'  | 2:15:B:G:P   | 2        | 7.59          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 8        | 7.52          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 9        | 7.49          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 7        | 7.43          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 13       | 7.4           |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 14       | 7.34          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 12       | 7.32          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 1        | 7.28          |
| (1,119) | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2:16:B:U:O3'  | 2:17:B:A:P   | 4        | 7.25          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 14       | 7.25          |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 12       | 7.13          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 6        | 7.12          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 15       | 6.96          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 3        | 6.92          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 2        | 6.76          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|--------------|----------|---------------|
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 13       | 6.71          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 1        | 6.7           |
| (1,69)  | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5' | 10       | 6.64          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 12       | 6.55          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 11       | 6.54          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 8        | 6.53          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 5        | 6.43          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 11       | 6.33          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 4        | 6.25          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 9        | 6.09          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 2        | 6.07          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 12       | 6.01          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 11       | 6.0           |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 5        | 5.97          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 3        | 5.96          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 10       | 5.88          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 7        | 5.76          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 11       | 5.74          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 15       | 5.73          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 10       | 5.59          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 2        | 5.56          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 15       | 5.52          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 7        | 5.48          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 8        | 5.46          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 6        | 5.41          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 9        | 5.37          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 12       | 5.34          |
| (1,62)  | 1:8:A:C:O3'   | 1:9:A:C:P     | 1:9:A:C:O5'   | 1:9:A:C:C5'  | 10       | 5.31          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 1        | 5.28          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 14       | 5.27          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 9        | 5.22          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 13       | 5.18          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 3        | 5.15          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P   | 7        | 5.12          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 9        | 5.07          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 2        | 5.04          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 15       | 4.99          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 4        | 4.99          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 9        | 4.96          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 10       | 4.96          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 13       | 4.94          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 4        | 4.91          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 8        | 4.9           |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 3        | 4.85          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 14       | 4.82          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 14       | 4.81          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 12       | 4.8           |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 15       | 4.79          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 6        | 4.72          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 5        | 4.66          |
| (1,80)  | 1:11:A:G:O4'  | 1:11:A:G:C1'  | 1:11:A:G:C2'  | 1:11:A:G:C3' | 1        | 4.66          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|--------------|----------|---------------|
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 11       | 4.64          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 12       | 4.63          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 15       | 4.59          |
| (1,159) | 2:21:B:C:C4'  | 2:21:B:C:C3'  | 2:21:B:C:O3'  | 2:22:B:U:P   | 5        | 4.55          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 14       | 4.48          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 13       | 4.46          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 3        | 4.42          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 7        | 4.4           |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P   | 14       | 4.33          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 8        | 4.31          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 7        | 4.3           |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 4        | 4.27          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 8        | 4.27          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 1        | 4.21          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 5        | 4.19          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5' | 6        | 4.18          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 2        | 4.17          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 8        | 4.16          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 13       | 4.15          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 8        | 4.08          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 10       | 4.06          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 14       | 4.03          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 5        | 3.96          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 15       | 3.96          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 7        | 3.96          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P   | 9        | 3.95          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 9        | 3.94          |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P   | 11       | 3.92          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 6        | 3.92          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 13       | 3.92          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 11       | 3.91          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P   | 11       | 3.9           |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 14       | 3.88          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5' | 2        | 3.87          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P   | 3        | 3.85          |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5' | 9        | 3.84          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 10       | 3.84          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 10       | 3.83          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5' | 4        | 3.83          |
| (1,106) | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4' | 1        | 3.8           |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P   | 13       | 3.79          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P   | 10       | 3.78          |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P   | 3        | 3.78          |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5' | 5        | 3.77          |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P   | 12       | 3.77          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 1        | 3.76          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 2        | 3.76          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 11       | 3.76          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 12       | 3.76          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4' | 6        | 3.74          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 9        | 3.74          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|--------------|----------|---------------|
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 4        | 3.71          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 12       | 3.7           |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P   | 2        | 3.69          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P   | 14       | 3.63          |
| (1,60)  | 1:8:A:C:C4'   | 1:8:A:C:C3'   | 1:8:A:C:O3'   | 1:9:A:C:P    | 5        | 3.63          |
| (1,76)  | 1:11:A:G:P    | 1:11:A:G:O5'  | 1:11:A:G:C5'  | 1:11:A:G:C4' | 11       | 3.61          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 7        | 3.57          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 1        | 3.55          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4' | 11       | 3.53          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 2        | 3.53          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 10       | 3.53          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 5        | 3.53          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 3        | 3.5           |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'  | 13       | 3.5           |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P   | 15       | 3.49          |
| (1,109) | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 2:15:B:G:C4' | 3        | 3.46          |
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P   | 12       | 3.45          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P   | 12       | 3.44          |
| (1,53)  | 1:7:A:A:C4'   | 1:7:A:A:C3'   | 1:7:A:A:O3'   | 1:8:A:C:P    | 8        | 3.44          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P   | 13       | 3.41          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4' | 3        | 3.41          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4' | 7        | 3.41          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4' | 1        | 3.4           |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'  | 14       | 3.4           |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4' | 8        | 3.39          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'  | 10       | 3.39          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4' | 13       | 3.35          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'  | 6        | 3.34          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'  | 7        | 3.34          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P   | 5        | 3.33          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4' | 5        | 3.32          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5' | 3        | 3.31          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P    | 15       | 3.31          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4' | 7        | 3.3           |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P   | 10       | 3.29          |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5' | 12       | 3.28          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'  | 1        | 3.28          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'  | 5        | 3.28          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'  | 15       | 3.28          |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P   | 1        | 3.27          |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5' | 1        | 3.26          |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5' | 13       | 3.26          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4' | 10       | 3.25          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5' | 4        | 3.25          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'  | 8        | 3.25          |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5' | 4        | 3.24          |
| (1,129) | 2:17:B:A:O3'  | 2:18:B:A:P    | 2:18:B:A:O5'  | 2:18:B:A:C5' | 2        | 3.23          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'  | 3        | 3.21          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4' | 15       | 3.2           |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5' | 11       | 3.17          |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5' | 8        | 3.14          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|---------------|----------|---------------|
| (1,135) | 2:18:B:A:C4'  | 2:18:B:A:C3'  | 2:18:B:A:O3'  | 2:19:B:G:P    | 6        | 3.14          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 4        | 3.12          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 10       | 3.1           |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P    | 8        | 3.1           |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 8        | 3.1           |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P    | 9        | 3.09          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5'  | 13       | 3.06          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 10       | 3.04          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'   | 9        | 3.04          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 12       | 3.02          |
| (1,98)  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5'  | 2:14:B:A:C4'  | 8        | 3.01          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 1        | 3.01          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 11       | 3.0           |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 11       | 3.0           |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P    | 4        | 2.99          |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P    | 5        | 2.99          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 5        | 2.98          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'   | 4        | 2.98          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 3        | 2.96          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 10       | 2.96          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 15       | 2.95          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 15       | 2.95          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'   | 11       | 2.95          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'   | 12       | 2.95          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 5        | 2.94          |
| (1,97)  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5'  | 6        | 2.94          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 1        | 2.94          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 12       | 2.94          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 14       | 2.92          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 5        | 2.92          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 7        | 2.92          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 8        | 2.91          |
| (1,66)  | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 1:9:A:C:C4'   | 2        | 2.91          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 6        | 2.91          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P    | 7        | 2.9           |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 8        | 2.9           |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 12       | 2.89          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 9        | 2.89          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 10       | 2.88          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4'  | 14       | 2.88          |
| (1,13)  | 1:2:A:U:C4'   | 1:2:A:U:C3'   | 1:2:A:U:O3'   | 1:3:A:A:P     | 4        | 2.87          |
| (1,76)  | 1:11:A:G:P    | 1:11:A:G:O5'  | 1:11:A:G:C5'  | 1:11:A:G:C4'  | 13       | 2.86          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 3        | 2.85          |
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 4        | 2.85          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4'  | 4        | 2.84          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 4        | 2.84          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 2        | 2.83          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 14       | 2.82          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 14       | 2.82          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 7        | 2.81          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 11       | 2.81          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|---------------|----------|---------------|
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 9        | 2.79          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 15       | 2.78          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4'  | 12       | 2.77          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 13       | 2.76          |
| (1,45)  | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 1:6:A:PSU:O3' | 1:7:A:A:P     | 3        | 2.74          |
| (1,143) | 2:19:B:G:C4'  | 2:19:B:G:C3'  | 2:19:B:G:O3'  | 2:20:B:U:P    | 5        | 2.71          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 12       | 2.71          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 2        | 2.67          |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P    | 4        | 2.67          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 13       | 2.66          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4'  | 2        | 2.66          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 8        | 2.66          |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5'  | 2        | 2.64          |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P    | 7        | 2.64          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 11       | 2.64          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 5        | 2.63          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 5        | 2.62          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 4        | 2.61          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 3        | 2.61          |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 10       | 2.6           |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 15       | 2.6           |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 15       | 2.59          |
| (1,60)  | 1:8:A:C:C4'   | 1:8:A:C:C3'   | 1:8:A:C:O3'   | 1:9:A:C:P     | 15       | 2.59          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 1        | 2.58          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 4        | 2.57          |
| (1,125) | 2:17:B:A:C1'  | 2:17:B:A:C2'  | 2:17:B:A:C3'  | 2:17:B:A:C4'  | 9        | 2.57          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 13       | 2.55          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 11       | 2.54          |
| (1,153) | 2:20:B:U:O3'  | 2:21:B:C:P    | 2:21:B:C:O5'  | 2:21:B:C:C5'  | 14       | 2.52          |
| (1,70)  | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5'  | 1:10:A:U:C4'  | 13       | 2.52          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 1        | 2.5           |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 6        | 2.5           |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 15       | 2.48          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 4        | 2.47          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 3        | 2.46          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 12       | 2.45          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 6        | 2.45          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P    | 2        | 2.44          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 14       | 2.44          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 11       | 2.43          |
| (1,129) | 2:17:B:A:O3'  | 2:18:B:A:P    | 2:18:B:A:O5'  | 2:18:B:A:C5'  | 1        | 2.43          |
| (1,160) | 2:21:B:C:O3'  | 2:22:B:U:P    | 2:22:B:U:O5'  | 2:22:B:U:C5'  | 14       | 2.42          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 13       | 2.42          |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 11       | 2.41          |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 9        | 2.4           |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 3        | 2.4           |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 7        | 2.4           |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 3        | 2.39          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 14       | 2.39          |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 9        | 2.39          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 9        | 2.38          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|---------------|----------|---------------|
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 2        | 2.37          |
| (1,60)  | 1:8:A:C:C4'   | 1:8:A:C:C3'   | 1:8:A:C:O3'   | 1:9:A:C:P     | 4        | 2.37          |
| (1,121) | 2:16:B:U:O3'  | 2:17:B:A:P    | 2:17:B:A:O5'  | 2:17:B:A:C5'  | 3        | 2.35          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 10       | 2.35          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 11       | 2.35          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 7        | 2.34          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 6        | 2.33          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P    | 6        | 2.32          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 12       | 2.32          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 12       | 2.3           |
| (1,70)  | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5'  | 1:10:A:U:C4'  | 5        | 2.29          |
| (1,129) | 2:17:B:A:O3'  | 2:18:B:A:P    | 2:18:B:A:O5'  | 2:18:B:A:C5'  | 5        | 2.28          |
| (1,60)  | 1:8:A:C:C4'   | 1:8:A:C:C3'   | 1:8:A:C:O3'   | 1:9:A:C:P     | 12       | 2.27          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 8        | 2.26          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 5        | 2.26          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 13       | 2.25          |
| (1,21)  | 1:3:A:A:C4'   | 1:3:A:A:C3'   | 1:3:A:A:O3'   | 1:4:A:C:P     | 2        | 2.25          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 6        | 2.24          |
| (1,60)  | 1:8:A:C:C4'   | 1:8:A:C:C3'   | 1:8:A:C:O3'   | 1:9:A:C:P     | 7        | 2.24          |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 3        | 2.23          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 8        | 2.21          |
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 10       | 2.21          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 9        | 2.21          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 10       | 2.19          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 6        | 2.18          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 12       | 2.17          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 12       | 2.17          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 14       | 2.16          |
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 12       | 2.16          |
| (1,21)  | 1:3:A:A:C4'   | 1:3:A:A:C3'   | 1:3:A:A:O3'   | 1:4:A:C:P     | 12       | 2.16          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 11       | 2.16          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 14       | 2.13          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 8        | 2.13          |
| (1,53)  | 1:7:A:A:C4'   | 1:7:A:A:C3'   | 1:7:A:A:O3'   | 1:8:A:C:P     | 10       | 2.13          |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P    | 8        | 2.12          |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 2        | 2.1           |
| (1,11)  | 1:2:A:U:C1'   | 1:2:A:U:C2'   | 1:2:A:U:C3'   | 1:2:A:U:C4'   | 13       | 2.1           |
| (1,133) | 2:18:B:A:C1'  | 2:18:B:A:C2'  | 2:18:B:A:C3'  | 2:18:B:A:C4'  | 7        | 2.08          |
| (1,121) | 2:16:B:U:O3'  | 2:17:B:A:P    | 2:17:B:A:O5'  | 2:17:B:A:C5'  | 11       | 2.08          |
| (1,29)  | 1:4:A:C:C4'   | 1:4:A:C:C3'   | 1:4:A:C:O3'   | 1:5:A:PSU:P   | 15       | 2.06          |
| (1,129) | 2:17:B:A:O3'  | 2:18:B:A:P    | 2:18:B:A:O5'  | 2:18:B:A:C5'  | 7        | 2.04          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 3        | 2.03          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 5        | 2.02          |
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 13       | 2.0           |
| (1,115) | 2:16:B:U:O5'  | 2:16:B:U:C5'  | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 3        | 1.98          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2        | 1.98          |
| (1,115) | 2:16:B:U:O5'  | 2:16:B:U:C5'  | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 4        | 1.96          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 10       | 1.96          |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 14       | 1.94          |
| (1,117) | 2:16:B:U:C1'  | 2:16:B:U:C2'  | 2:16:B:U:C3'  | 2:16:B:U:C4'  | 2        | 1.93          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 13       | 1.93          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|---------------|----------|---------------|
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 1        | 1.93          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 15       | 1.93          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 9        | 1.92          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 10       | 1.92          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 1        | 1.92          |
| (1,70)  | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5'  | 1:10:A:U:C4'  | 9        | 1.91          |
| (1,70)  | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5'  | 1:10:A:U:C4'  | 11       | 1.91          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 11       | 1.9           |
| (1,70)  | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5'  | 1:10:A:U:C4'  | 14       | 1.89          |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 15       | 1.87          |
| (1,141) | 2:19:B:G:C1'  | 2:19:B:G:C2'  | 2:19:B:G:C3'  | 2:19:B:G:C4'  | 1        | 1.86          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 7        | 1.86          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 15       | 1.85          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 15       | 1.84          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 13       | 1.84          |
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 3        | 1.82          |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P    | 15       | 1.81          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 5        | 1.79          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 1        | 1.78          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 6        | 1.76          |
| (1,129) | 2:17:B:A:O3'  | 2:18:B:A:P    | 2:18:B:A:O5'  | 2:18:B:A:C5'  | 10       | 1.76          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 9        | 1.76          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 9        | 1.76          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 5        | 1.76          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 10       | 1.76          |
| (1,129) | 2:17:B:A:O3'  | 2:18:B:A:P    | 2:18:B:A:O5'  | 2:18:B:A:C5'  | 8        | 1.75          |
| (1,115) | 2:16:B:U:O5'  | 2:16:B:U:C5'  | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 8        | 1.74          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 7        | 1.73          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 2        | 1.73          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 12       | 1.73          |
| (1,21)  | 1:3:A:A:C4'   | 1:3:A:A:C3'   | 1:3:A:A:O3'   | 1:4:A:C:P     | 10       | 1.73          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 14       | 1.72          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 5        | 1.7           |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 12       | 1.7           |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 5        | 1.7           |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 8        | 1.7           |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 14       | 1.7           |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 8        | 1.69          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 13       | 1.68          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 10       | 1.68          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 15       | 1.68          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 13       | 1.67          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 2        | 1.67          |
| (1,121) | 2:16:B:U:O3'  | 2:17:B:A:P    | 2:17:B:A:O5'  | 2:17:B:A:C5'  | 10       | 1.66          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 8        | 1.66          |
| (1,60)  | 1:8:A:C:C4'   | 1:8:A:C:C3'   | 1:8:A:C:O3'   | 1:9:A:C:P     | 1        | 1.66          |
| (1,21)  | 1:3:A:A:C4'   | 1:3:A:A:C3'   | 1:3:A:A:O3'   | 1:4:A:C:P     | 1        | 1.66          |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P    | 6        | 1.63          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 3        | 1.62          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 4        | 1.62          |
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 5        | 1.62          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|---------------|----------|---------------|
| (1,21)  | 1:3:A:A:C4'   | 1:3:A:A:C3'   | 1:3:A:A:O3'   | 1:4:A:C:P     | 3        | 1.62          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 9        | 1.6           |
| (1,29)  | 1:4:A:C:C4'   | 1:4:A:C:C3'   | 1:4:A:C:O3'   | 1:5:A:PSU:P   | 12       | 1.6           |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 3        | 1.59          |
| (1,127) | 2:17:B:A:C4'  | 2:17:B:A:C3'  | 2:17:B:A:O3'  | 2:18:B:A:P    | 2        | 1.59          |
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 9        | 1.59          |
| (1,56)  | 1:8:A:C:P     | 1:8:A:C:O5'   | 1:8:A:C:C5'   | 1:8:A:C:C4'   | 3        | 1.57          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 7        | 1.56          |
| (1,51)  | 1:7:A:A:C1'   | 1:7:A:A:C2'   | 1:7:A:A:C3'   | 1:7:A:A:C4'   | 14       | 1.56          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 4        | 1.56          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 7        | 1.56          |
| (1,67)  | 1:9:A:C:O4'   | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 14       | 1.54          |
| (1,13)  | 1:2:A:U:C4'   | 1:2:A:U:C3'   | 1:2:A:U:O3'   | 1:3:A:A:P     | 11       | 1.54          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 15       | 1.52          |
| (1,115) | 2:16:B:U:O5'  | 2:16:B:U:C5'  | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 2        | 1.52          |
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 14       | 1.52          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 4        | 1.51          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 8        | 1.51          |
| (1,13)  | 1:2:A:U:C4'   | 1:2:A:U:C3'   | 1:2:A:U:O3'   | 1:3:A:A:P     | 6        | 1.51          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 11       | 1.5           |
| (1,129) | 2:17:B:A:O3'  | 2:18:B:A:P    | 2:18:B:A:O5'  | 2:18:B:A:C5'  | 3        | 1.5           |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 10       | 1.49          |
| (1,153) | 2:20:B:U:O3'  | 2:21:B:C:P    | 2:21:B:C:O5'  | 2:21:B:C:C5'  | 15       | 1.48          |
| (1,93)  | 2:13:B:G:C1'  | 2:13:B:G:C2'  | 2:13:B:G:C3'  | 2:13:B:G:C4'  | 11       | 1.48          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 9        | 1.48          |
| (1,115) | 2:16:B:U:O5'  | 2:16:B:U:C5'  | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 9        | 1.47          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 3        | 1.47          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 6        | 1.46          |
| (1,53)  | 1:7:A:A:C4'   | 1:7:A:A:C3'   | 1:7:A:A:O3'   | 1:8:A:C:P     | 5        | 1.46          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 6        | 1.45          |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 4        | 1.44          |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 6        | 1.44          |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 2        | 1.44          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 9        | 1.43          |
| (1,51)  | 1:7:A:A:C1'   | 1:7:A:A:C2'   | 1:7:A:A:C3'   | 1:7:A:A:C4'   | 9        | 1.43          |
| (1,121) | 2:16:B:U:O3'  | 2:17:B:A:P    | 2:17:B:A:O5'  | 2:17:B:A:C5'  | 15       | 1.41          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 13       | 1.4           |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 2        | 1.39          |
| (1,110) | 2:15:B:G:O4'  | 2:15:B:G:C1'  | 2:15:B:G:C2'  | 2:15:B:G:C3'  | 15       | 1.39          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 1        | 1.39          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 7        | 1.39          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 10       | 1.38          |
| (1,43)  | 1:6:A:PSU:C1' | 1:6:A:PSU:C2' | 1:6:A:PSU:C3' | 1:6:A:PSU:C4' | 6        | 1.37          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 1        | 1.36          |
| (1,76)  | 1:11:A:G:P    | 1:11:A:G:O5'  | 1:11:A:G:C5'  | 1:11:A:G:C4'  | 8        | 1.35          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 14       | 1.35          |
| (1,88)  | 2:13:B:G:C3'  | 2:13:B:G:O3'  | 2:14:B:A:P    | 2:14:B:A:O5'  | 7        | 1.34          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 14       | 1.34          |
| (1,153) | 2:20:B:U:O3'  | 2:21:B:C:P    | 2:21:B:C:O5'  | 2:21:B:C:C5'  | 9        | 1.33          |
| (1,153) | 2:20:B:U:O3'  | 2:21:B:C:P    | 2:21:B:C:O5'  | 2:21:B:C:C5'  | 11       | 1.33          |
| (1,56)  | 1:8:A:C:P     | 1:8:A:C:O5'   | 1:8:A:C:C5'   | 1:8:A:C:C4'   | 2        | 1.33          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|---------------|----------|---------------|
| (1,115) | 2:16:B:U:O5'  | 2:16:B:U:C5'  | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 7        | 1.32          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 12       | 1.31          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 4        | 1.31          |
| (1,53)  | 1:7:A:A:C4'   | 1:7:A:A:C3'   | 1:7:A:A:O3'   | 1:8:A:C:P     | 3        | 1.31          |
| (1,53)  | 1:7:A:A:C4'   | 1:7:A:A:C3'   | 1:7:A:A:O3'   | 1:8:A:C:P     | 7        | 1.3           |
| (1,19)  | 1:3:A:A:C1'   | 1:3:A:A:C2'   | 1:3:A:A:C3'   | 1:3:A:A:C4'   | 6        | 1.3           |
| (1,115) | 2:16:B:U:O5'  | 2:16:B:U:C5'  | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 6        | 1.29          |
| (1,51)  | 1:7:A:A:C1'   | 1:7:A:A:C2'   | 1:7:A:A:C3'   | 1:7:A:A:C4'   | 13       | 1.29          |
| (1,145) | 2:19:B:G:O3'  | 2:20:B:U:P    | 2:20:B:U:O5'  | 2:20:B:U:C5'  | 6        | 1.28          |
| (1,145) | 2:19:B:G:O3'  | 2:20:B:U:P    | 2:20:B:U:O5'  | 2:20:B:U:C5'  | 14       | 1.28          |
| (1,121) | 2:16:B:U:O3'  | 2:17:B:A:P    | 2:17:B:A:O5'  | 2:17:B:A:C5'  | 12       | 1.28          |
| (1,51)  | 1:7:A:A:C1'   | 1:7:A:A:C2'   | 1:7:A:A:C3'   | 1:7:A:A:C4'   | 7        | 1.28          |
| (1,145) | 2:19:B:G:O3'  | 2:20:B:U:P    | 2:20:B:U:O5'  | 2:20:B:U:C5'  | 8        | 1.27          |
| (1,61)  | 1:9:A:C:C3'   | 1:9:A:C:O3'   | 1:10:A:U:P    | 1:10:A:U:O5'  | 15       | 1.27          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 7        | 1.25          |
| (1,115) | 2:16:B:U:O5'  | 2:16:B:U:C5'  | 2:16:B:U:C4'  | 2:16:B:U:C3'  | 10       | 1.25          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 11       | 1.25          |
| (1,21)  | 1:3:A:A:C4'   | 1:3:A:A:C3'   | 1:3:A:A:O3'   | 1:4:A:C:P     | 5        | 1.25          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 14       | 1.24          |
| (1,51)  | 1:7:A:A:C1'   | 1:7:A:A:C2'   | 1:7:A:A:C3'   | 1:7:A:A:C4'   | 12       | 1.24          |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 4        | 1.23          |
| (1,43)  | 1:6:A:PSU:C1' | 1:6:A:PSU:C2' | 1:6:A:PSU:C3' | 1:6:A:PSU:C4' | 9        | 1.23          |
| (1,21)  | 1:3:A:A:C4'   | 1:3:A:A:C3'   | 1:3:A:A:O3'   | 1:4:A:C:P     | 4        | 1.23          |
| (1,145) | 2:19:B:G:O3'  | 2:20:B:U:P    | 2:20:B:U:O5'  | 2:20:B:U:C5'  | 13       | 1.21          |
| (1,98)  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5'  | 2:14:B:A:C4'  | 10       | 1.21          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 6        | 1.21          |
| (1,98)  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5'  | 2:14:B:A:C4'  | 9        | 1.2           |
| (1,51)  | 1:7:A:A:C1'   | 1:7:A:A:C2'   | 1:7:A:A:C3'   | 1:7:A:A:C4'   | 10       | 1.2           |
| (1,151) | 2:20:B:U:C4'  | 2:20:B:U:C3'  | 2:20:B:U:O3'  | 2:21:B:C:P    | 1        | 1.18          |
| (1,60)  | 1:8:A:C:C4'   | 1:8:A:C:C3'   | 1:8:A:C:O3'   | 1:9:A:C:P     | 2        | 1.18          |
| (1,53)  | 1:7:A:A:C4'   | 1:7:A:A:C3'   | 1:7:A:A:O3'   | 1:8:A:C:P     | 11       | 1.18          |
| (1,101) | 2:14:B:A:C1'  | 2:14:B:A:C2'  | 2:14:B:A:C3'  | 2:14:B:A:C4'  | 5        | 1.17          |
| (1,98)  | 2:14:B:A:P    | 2:14:B:A:O5'  | 2:14:B:A:C5'  | 2:14:B:A:C4'  | 5        | 1.17          |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 7        | 1.16          |
| (1,93)  | 2:13:B:G:C1'  | 2:13:B:G:C2'  | 2:13:B:G:C3'  | 2:13:B:G:C4'  | 15       | 1.15          |
| (1,51)  | 1:7:A:A:C1'   | 1:7:A:A:C2'   | 1:7:A:A:C3'   | 1:7:A:A:C4'   | 8        | 1.14          |
| (1,13)  | 1:2:A:U:C4'   | 1:2:A:U:C3'   | 1:2:A:U:O3'   | 1:3:A:A:P     | 12       | 1.13          |
| (1,51)  | 1:7:A:A:C1'   | 1:7:A:A:C2'   | 1:7:A:A:C3'   | 1:7:A:A:C4'   | 3        | 1.12          |
| (1,21)  | 1:3:A:A:C4'   | 1:3:A:A:C3'   | 1:3:A:A:O3'   | 1:4:A:C:P     | 15       | 1.12          |
| (1,145) | 2:19:B:G:O3'  | 2:20:B:U:P    | 2:20:B:U:O5'  | 2:20:B:U:C5'  | 15       | 1.11          |
| (1,105) | 2:14:B:A:O3'  | 2:15:B:G:P    | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 8        | 1.1           |
| (1,73)  | 1:10:A:U:C1'  | 1:10:A:U:C2'  | 1:10:A:U:C3'  | 1:10:A:U:C4'  | 13       | 1.1           |
| (1,53)  | 1:7:A:A:C4'   | 1:7:A:A:C3'   | 1:7:A:A:O3'   | 1:8:A:C:P     | 14       | 1.1           |
| (1,70)  | 1:10:A:U:P    | 1:10:A:U:O5'  | 1:10:A:U:C5'  | 1:10:A:U:C4'  | 3        | 1.09          |
| (1,149) | 2:20:B:U:C1'  | 2:20:B:U:C2'  | 2:20:B:U:C3'  | 2:20:B:U:C4'  | 11       | 1.08          |
| (1,85)  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 2:12:B:G:C4'  | 8        | 1.07          |
| (1,129) | 2:17:B:A:O3'  | 2:18:B:A:P    | 2:18:B:A:O5'  | 2:18:B:A:C5'  | 15       | 1.06          |
| (1,67)  | 1:9:A:C:O4'   | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 13       | 1.06          |
| (1,145) | 2:19:B:G:O3'  | 2:20:B:U:P    | 2:20:B:U:O5'  | 2:20:B:U:C5'  | 4        | 1.05          |
| (1,86)  | 2:12:B:G:O4'  | 2:12:B:G:C1'  | 2:12:B:G:C2'  | 2:12:B:G:C3'  | 11       | 1.05          |
| (1,67)  | 1:9:A:C:O4'   | 1:9:A:C:C1'   | 1:9:A:C:C2'   | 1:9:A:C:C3'   | 5        | 1.04          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|---------------|----------|---------------|
| (1,51)  | 1:7:A:A:C1'   | 1:7:A:A:C2'   | 1:7:A:A:C3'   | 1:7:A:A:C4'   | 2        | 1.03          |
| (1,41)  | 1:6:A:PSU:O5' | 1:6:A:PSU:C5' | 1:6:A:PSU:C4' | 1:6:A:PSU:C3' | 2        | 1.01          |
| (1,137) | 2:18:B:A:O3'  | 2:19:B:G:P    | 2:19:B:G:O5'  | 2:19:B:G:C5'  | 1        | 1.0           |
| (1,107) | 2:15:B:G:O5'  | 2:15:B:G:C5'  | 2:15:B:G:C4'  | 2:15:B:G:C3'  | 7        | 1.0           |