



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 10:22 AM UTC

PDB ID : 5J4P / pdb\_00005j4p  
BMRB ID : 30055  
Title : DIY G-Quadruplexes: Solution structure of d(GGTTTGGTTTGGTTTGG) in sodium  
Authors : Dvorkin, S.A.; Webba da Silva, M.  
Deposited on : 2016-04-01

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

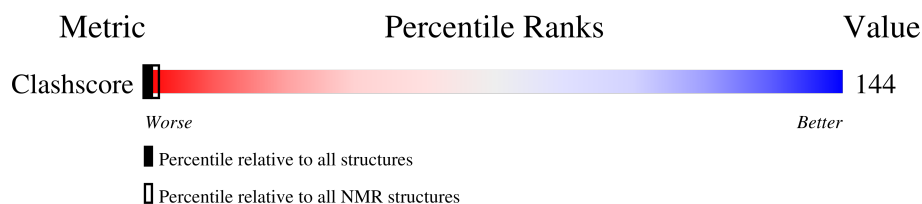
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 47%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

| Mol | Chain | Length | Quality of chain                                                                             |
|-----|-------|--------|----------------------------------------------------------------------------------------------|
| 1   | A     | 18     |  83% 17% |

## 2 Ensemble composition and analysis ⓘ

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 581 atoms, of which 208 are hydrogens and 0 are deuteriums.

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

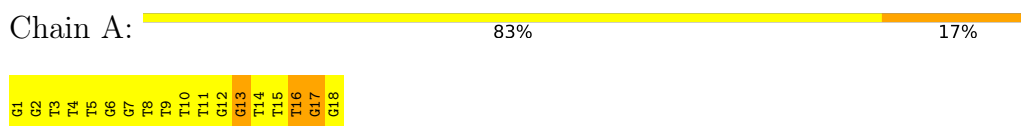
| Mol | Chain | Residues | Atoms |     |     |    |     |    | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|----|-------|
|     |       |          | Total | C   | H   | N  | O   | P  |       |
| 1   | A     | 18       | 581   | 180 | 208 | 60 | 116 | 17 | 0     |

## 4 Residue-property plots

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

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

- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')

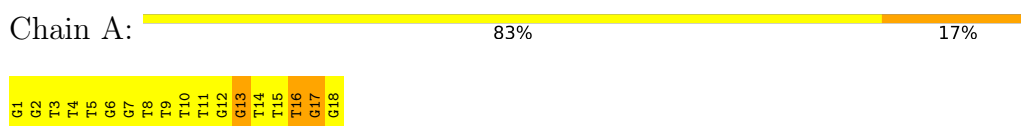


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

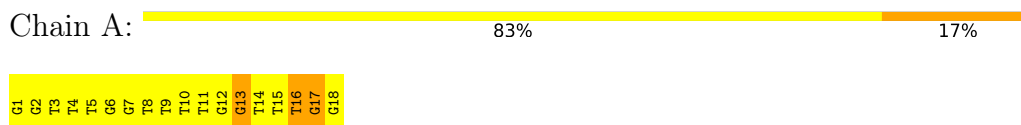
#### 4.2.1 Score per residue for model 1

- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')



#### 4.2.2 Score per residue for model 2

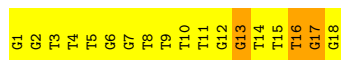
- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')



### 4.2.3 Score per residue for model 3

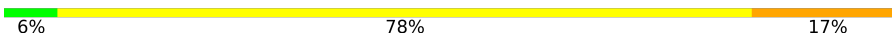
- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')

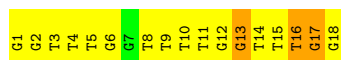
Chain A:  83% 17%



### 4.2.4 Score per residue for model 4

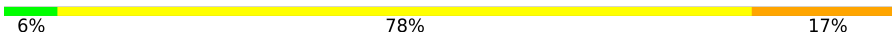
- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')

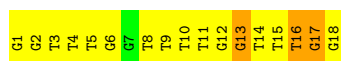
Chain A:  6% 78% 17%



### 4.2.5 Score per residue for model 5

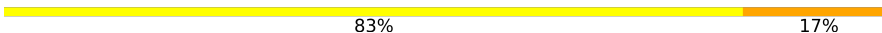
- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')

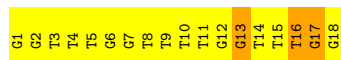
Chain A:  6% 78% 17%



### 4.2.6 Score per residue for model 6

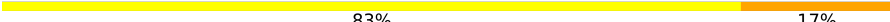
- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')

Chain A:  83% 17%



### 4.2.7 Score per residue for model 7

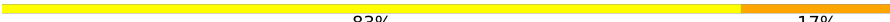
- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')

Chain A:  83% 17%

|    |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| G1 | G2 | T3 | T4 | T5 | G6 | G7 | T8 | T9 | T10 | T11 | G12 | G13 | T14 | T15 | T16 | G17 | G18 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

#### 4.2.8 Score per residue for model 8

- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')

Chain A:  83% 17%

|    |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| G1 | G2 | T3 | T4 | T5 | G6 | G7 | T8 | T9 | T10 | T11 | G12 | G13 | T14 | T15 | T16 | G17 | G18 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

#### 4.2.9 Score per residue for model 9

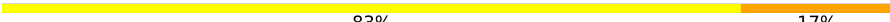
- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')

Chain A:  6% 78% 17%

|    |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| G1 | G2 | T3 | T4 | T5 | G6 | G7 | T8 | T9 | T10 | T11 | G12 | G13 | T14 | T15 | T16 | G17 | G18 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

#### 4.2.10 Score per residue for model 10

- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*G)-3')

Chain A:  83% 17%

|    |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| G1 | G2 | T3 | T4 | T5 | G6 | G7 | T8 | T9 | T10 | T11 | G12 | G13 | T14 | T15 | T16 | G17 | G18 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| Xplor-NIH     | structure calculation |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 193            |
| Number of shifts mapped to atoms             | 193            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 47%            |



## 6 Model quality [i](#)

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

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

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 3.0±0.0   |
| All | All   | 0         | 30        |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 13  | DG   | Sidechain | 10             |
| 1   | A     | 16  | DT   | Sidechain | 10             |
| 1   | A     | 17  | DG   | Sidechain | 10             |

### 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     | 373   | 208      | 210      | 84±5    |
| All | All   | 3730  | 2080     | 2100     | 842     |

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 144.

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

| Atom-1         | Atom-2        | Clash(Å) | Distance(Å) | Models |       |
|----------------|---------------|----------|-------------|--------|-------|
|                |               |          |             | Worst  | Total |
| 1:A:5:DT:C4    | 1:A:15:DT:H1' | 0.81     | 2.11        | 2      | 10    |
| 1:A:13:DG:H4'  | 1:A:14:DT:OP1 | 0.78     | 1.79        | 1      | 10    |
| 1:A:5:DT:O4    | 1:A:15:DT:H1' | 0.77     | 1.79        | 2      | 10    |
| 1:A:13:DG:C6   | 1:A:14:DT:C4  | 0.76     | 2.74        | 10     | 10    |
| 1:A:6:DG:H1'   | 1:A:7:DG:O4'  | 0.75     | 1.81        | 10     | 4     |
| 1:A:4:DT:H72   | 1:A:14:DT:O2  | 0.73     | 1.84        | 4      | 4     |
| 1:A:6:DG:H4'   | 1:A:7:DG:OP1  | 0.72     | 1.82        | 10     | 4     |
| 1:A:12:DG:H4'  | 1:A:13:DG:OP1 | 0.71     | 1.84        | 2      | 10    |
| 1:A:14:DT:C6   | 1:A:15:DT:H2' | 0.71     | 2.21        | 3      | 10    |
| 1:A:13:DG:H2'  | 1:A:16:DT:H72 | 0.69     | 1.63        | 3      | 10    |
| 1:A:13:DG:C6   | 1:A:14:DT:N3  | 0.69     | 2.60        | 2      | 10    |
| 1:A:9:DT:H5'   | 1:A:10:DT:C5  | 0.68     | 2.23        | 8      | 10    |
| 1:A:1:DG:C5    | 1:A:10:DT:C4  | 0.68     | 2.82        | 8      | 10    |
| 1:A:14:DT:C1'  | 1:A:15:DT:H5' | 0.67     | 2.19        | 1      | 10    |
| 1:A:4:DT:H1'   | 1:A:5:DT:H73  | 0.67     | 1.65        | 2      | 10    |
| 1:A:14:DT:C5   | 1:A:15:DT:H2' | 0.66     | 2.25        | 3      | 10    |
| 1:A:1:DG:O4'   | 1:A:10:DT:H71 | 0.64     | 1.93        | 3      | 10    |
| 1:A:5:DT:OP1   | 1:A:5:DT:H3'  | 0.63     | 1.94        | 2      | 1     |
| 1:A:9:DT:H5'   | 1:A:10:DT:C4  | 0.63     | 2.28        | 4      | 10    |
| 1:A:14:DT:H1'  | 1:A:15:DT:C5' | 0.62     | 2.24        | 1      | 10    |
| 1:A:6:DG:H2'   | 1:A:6:DG:N3   | 0.62     | 2.09        | 1      | 8     |
| 1:A:11:DT:H4'  | 1:A:12:DG:C4  | 0.61     | 2.30        | 1      | 3     |
| 1:A:14:DT:H72  | 1:A:16:DT:C2  | 0.61     | 2.30        | 3      | 10    |
| 1:A:14:DT:H1'  | 1:A:15:DT:H5' | 0.60     | 1.73        | 10     | 10    |
| 1:A:1:DG:H4'   | 1:A:2:DG:OP1  | 0.60     | 1.96        | 2      | 4     |
| 1:A:4:DT:C2    | 1:A:5:DT:H72  | 0.59     | 2.32        | 4      | 10    |
| 1:A:8:DT:H1'   | 1:A:9:DT:O5'  | 0.59     | 1.96        | 4      | 10    |
| 1:A:4:DT:O2    | 1:A:5:DT:C7   | 0.59     | 2.51        | 8      | 10    |
| 1:A:13:DG:H1'  | 1:A:14:DT:O5' | 0.59     | 1.97        | 3      | 10    |
| 1:A:15:DT:H73  | 1:A:17:DG:C5  | 0.58     | 2.33        | 8      | 10    |
| 1:A:1:DG:H2''  | 1:A:2:DG:H5'' | 0.58     | 1.76        | 2      | 10    |
| 1:A:15:DT:H2'' | 1:A:16:DT:O5' | 0.57     | 1.99        | 3      | 10    |
| 1:A:14:DT:O4   | 1:A:17:DG:C6  | 0.57     | 2.58        | 3      | 10    |
| 1:A:4:DT:H1'   | 1:A:5:DT:C7   | 0.57     | 2.29        | 2      | 10    |
| 1:A:4:DT:C2    | 1:A:5:DT:C7   | 0.57     | 2.88        | 1      | 10    |
| 1:A:13:DG:C5   | 1:A:14:DT:C4  | 0.56     | 2.94        | 1      | 10    |
| 1:A:4:DT:C4'   | 1:A:5:DT:C5'  | 0.56     | 2.84        | 1      | 9     |
| 1:A:4:DT:C7    | 1:A:14:DT:O2  | 0.55     | 2.54        | 3      | 10    |
| 1:A:15:DT:H2'' | 1:A:16:DT:O2  | 0.55     | 2.02        | 4      | 10    |
| 1:A:3:DT:C6    | 1:A:4:DT:O4   | 0.54     | 2.60        | 4      | 10    |
| 1:A:1:DG:N7    | 1:A:10:DT:C4  | 0.54     | 2.75        | 8      | 10    |
| 1:A:1:DG:H1'   | 1:A:2:DG:O5'  | 0.54     | 2.03        | 2      | 4     |

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| Atom-1         | Atom-2        | Clash(Å) | Distance(Å) | Models |       |
|----------------|---------------|----------|-------------|--------|-------|
|                |               |          |             | Worst  | Total |
| 1:A:9:DT:H1'   | 1:A:11:DT:C4  | 0.54     | 2.38        | 4      | 7     |
| 1:A:4:DT:H73   | 1:A:14:DT:O2  | 0.54     | 2.03        | 8      | 6     |
| 1:A:9:DT:C5'   | 1:A:10:DT:C4  | 0.53     | 2.91        | 3      | 10    |
| 1:A:14:DT:C4   | 1:A:15:DT:C2  | 0.52     | 2.97        | 10     | 10    |
| 1:A:4:DT:H4'   | 1:A:5:DT:C5'  | 0.52     | 2.34        | 1      | 10    |
| 1:A:1:DG:H2'   | 1:A:1:DG:N3   | 0.52     | 2.19        | 4      | 7     |
| 1:A:6:DG:H2'   | 1:A:7:DG:C8   | 0.52     | 2.39        | 3      | 3     |
| 1:A:17:DG:H1'  | 1:A:18:DG:O4' | 0.52     | 2.04        | 1      | 10    |
| 1:A:1:DG:C8    | 1:A:10:DT:H73 | 0.52     | 2.39        | 4      | 7     |
| 1:A:13:DG:C5   | 1:A:14:DT:C5  | 0.52     | 2.97        | 10     | 10    |
| 1:A:7:DG:C6    | 1:A:8:DT:N3   | 0.52     | 2.78        | 2      | 7     |
| 1:A:6:DG:C6    | 1:A:7:DG:C6   | 0.51     | 2.98        | 8      | 4     |
| 1:A:1:DG:H2''  | 1:A:2:DG:C5'  | 0.51     | 2.35        | 4      | 10    |
| 1:A:14:DT:C2'  | 1:A:15:DT:H5' | 0.51     | 2.34        | 1      | 10    |
| 1:A:17:DG:H5'  | 1:A:17:DG:N3  | 0.51     | 2.20        | 1      | 10    |
| 1:A:1:DG:H1'   | 1:A:2:DG:C5'  | 0.51     | 2.36        | 10     | 4     |
| 1:A:5:DT:C4    | 1:A:15:DT:C1' | 0.50     | 2.92        | 2      | 10    |
| 1:A:14:DT:H73  | 1:A:17:DG:N2  | 0.50     | 2.22        | 3      | 10    |
| 1:A:6:DG:C5    | 1:A:7:DG:C5   | 0.49     | 3.00        | 10     | 4     |
| 1:A:1:DG:N7    | 1:A:10:DT:O4  | 0.48     | 2.45        | 2      | 6     |
| 1:A:12:DG:C5   | 1:A:13:DG:C5  | 0.48     | 3.01        | 3      | 10    |
| 1:A:1:DG:C6    | 1:A:10:DT:N3  | 0.48     | 2.81        | 1      | 7     |
| 1:A:13:DG:O6   | 1:A:14:DT:C4  | 0.48     | 2.67        | 4      | 10    |
| 1:A:8:DT:H2'   | 1:A:9:DT:C6   | 0.47     | 2.44        | 4      | 10    |
| 1:A:5:DT:H6    | 1:A:5:DT:O5'  | 0.47     | 1.92        | 4      | 4     |
| 1:A:11:DT:H5'' | 1:A:12:DG:OP1 | 0.47     | 2.09        | 10     | 7     |
| 1:A:3:DT:C1'   | 1:A:4:DT:C4   | 0.47     | 2.97        | 1      | 10    |
| 1:A:4:DT:H3'   | 1:A:4:DT:OP2  | 0.47     | 2.10        | 2      | 4     |
| 1:A:5:DT:C5    | 1:A:15:DT:C2  | 0.47     | 3.02        | 3      | 10    |
| 1:A:13:DG:H2'  | 1:A:16:DT:C7  | 0.47     | 2.38        | 4      | 10    |
| 1:A:1:DG:N3    | 1:A:1:DG:H5'  | 0.47     | 2.24        | 8      | 4     |
| 1:A:4:DT:C4'   | 1:A:5:DT:H5'  | 0.46     | 2.41        | 1      | 6     |
| 1:A:3:DT:H1'   | 1:A:4:DT:C4   | 0.46     | 2.46        | 1      | 4     |
| 1:A:14:DT:C4   | 1:A:15:DT:N1  | 0.45     | 2.85        | 1      | 10    |
| 1:A:14:DT:H2'' | 1:A:15:DT:H5' | 0.45     | 1.89        | 1      | 10    |
| 1:A:5:DT:C6    | 1:A:15:DT:C2  | 0.45     | 3.05        | 4      | 9     |
| 1:A:9:DT:H1'   | 1:A:11:DT:O4  | 0.45     | 2.12        | 4      | 5     |
| 1:A:6:DG:C4'   | 1:A:7:DG:OP1  | 0.45     | 2.62        | 10     | 4     |
| 1:A:17:DG:C2'  | 1:A:18:DG:C8  | 0.44     | 3.01        | 1      | 8     |
| 1:A:15:DT:H2'' | 1:A:16:DT:C2  | 0.44     | 2.47        | 3      | 10    |
| 1:A:5:DT:C2    | 1:A:15:DT:C4  | 0.44     | 3.06        | 3      | 9     |

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| Atom-1        | Atom-2        | Clash(Å) | Distance(Å) | Models |       |
|---------------|---------------|----------|-------------|--------|-------|
|               |               |          |             | Worst  | Total |
| 1:A:1:DG:C2'  | 1:A:2:DG:H5'' | 0.44     | 2.42        | 2      | 7     |
| 1:A:9:DT:O3'  | 1:A:11:DT:H72 | 0.44     | 2.13        | 4      | 6     |
| 1:A:14:DT:O4  | 1:A:15:DT:C5  | 0.44     | 2.71        | 10     | 9     |
| 1:A:6:DG:C2'  | 1:A:7:DG:C8   | 0.44     | 3.00        | 3      | 2     |
| 1:A:7:DG:C5   | 1:A:8:DT:C4   | 0.44     | 3.05        | 2      | 1     |
| 1:A:17:DG:N3  | 1:A:17:DG:H2' | 0.44     | 2.27        | 10     | 10    |
| 1:A:8:DT:C2'  | 1:A:9:DT:O5'  | 0.44     | 2.66        | 1      | 10    |
| 1:A:8:DT:H2'' | 1:A:9:DT:O5'  | 0.44     | 2.13        | 1      | 4     |
| 1:A:6:DG:C4   | 1:A:7:DG:C8   | 0.43     | 3.06        | 1      | 4     |
| 1:A:16:DT:C2' | 1:A:17:DG:O5' | 0.43     | 2.66        | 4      | 10    |
| 1:A:8:DT:C4   | 1:A:9:DT:C2   | 0.43     | 3.06        | 4      | 4     |
| 1:A:8:DT:C1'  | 1:A:9:DT:O5'  | 0.43     | 2.67        | 4      | 6     |
| 1:A:1:DG:C8   | 1:A:10:DT:C7  | 0.43     | 3.02        | 4      | 5     |
| 1:A:6:DG:H2'' | 1:A:7:DG:O5'  | 0.43     | 2.14        | 2      | 1     |
| 1:A:2:DG:C5   | 1:A:4:DT:H71  | 0.43     | 2.49        | 10     | 3     |
| 1:A:7:DG:C6   | 1:A:8:DT:C2   | 0.43     | 3.07        | 2      | 1     |
| 1:A:8:DT:C7   | 1:A:9:DT:C4   | 0.43     | 3.02        | 4      | 6     |
| 1:A:14:DT:C7  | 1:A:16:DT:C2  | 0.42     | 3.02        | 4      | 10    |
| 1:A:4:DT:O2   | 1:A:5:DT:H73  | 0.42     | 2.15        | 1      | 4     |
| 1:A:14:DT:H73 | 1:A:17:DG:C2  | 0.42     | 2.50        | 2      | 3     |
| 1:A:7:DG:C8   | 1:A:8:DT:H72  | 0.42     | 2.49        | 2      | 1     |
| 1:A:14:DT:O4  | 1:A:15:DT:C6  | 0.41     | 2.72        | 3      | 2     |
| 1:A:9:DT:O3'  | 1:A:11:DT:C7  | 0.41     | 2.67        | 1      | 6     |
| 1:A:13:DG:N7  | 1:A:14:DT:C5  | 0.41     | 2.88        | 10     | 5     |
| 1:A:8:DT:C5   | 1:A:9:DT:N3   | 0.41     | 2.88        | 3      | 3     |
| 1:A:1:DG:H1'  | 1:A:2:DG:H5'' | 0.41     | 1.93        | 8      | 9     |
| 1:A:4:DT:O4'  | 1:A:5:DT:H5'  | 0.41     | 2.15        | 1      | 3     |
| 1:A:14:DT:O4  | 1:A:15:DT:C4  | 0.41     | 2.73        | 10     | 1     |
| 1:A:14:DT:H72 | 1:A:16:DT:N1  | 0.41     | 2.30        | 3      | 2     |
| 1:A:9:DT:O5'  | 1:A:10:DT:C4  | 0.41     | 2.74        | 8      | 2     |
| 1:A:7:DG:O6   | 1:A:18:DG:O6  | 0.41     | 2.38        | 8      | 1     |
| 1:A:15:DT:H73 | 1:A:17:DG:C4  | 0.41     | 2.51        | 8      | 1     |
| 1:A:17:DG:C1' | 1:A:18:DG:O5' | 0.40     | 2.69        | 2      | 5     |
| 1:A:6:DG:N3   | 1:A:6:DG:C2'  | 0.40     | 2.84        | 1      | 2     |
| 1:A:12:DG:C4  | 1:A:13:DG:C8  | 0.40     | 3.09        | 2      | 1     |
| 1:A:15:DT:C2' | 1:A:16:DT:O5' | 0.40     | 2.68        | 3      | 2     |
| 1:A:17:DG:C1' | 1:A:18:DG:C8  | 0.40     | 3.05        | 8      | 3     |

## 6.3 Torsion angles [i](#)

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

There are no protein molecules in this entry.

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

There are no protein molecules in this entry.

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 47% for the well-defined parts and 47% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *S173\_cs.txt*

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

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 193 |
| Number of shifts mapped to atoms        | 193 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

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

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

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 47%, i.e. 163 atoms were assigned a chemical shift out of a possible 348. 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   | 115/216 (53%) | 115/126 (91%)  | 0/90 (0%)       | 0/0 (—%)        |
| Base    | 48/132 (36%)  | 48/78 (62%)    | 0/28 (0%)       | 0/26 (0%)       |
| Overall | 163/348 (47%) | 163/204 (80%)  | 0/118 (0%)      | 0/26 (0%)       |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 47%, i.e. 163 atoms were assigned a chemical shift out of a possible 348. 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   | 115/216 (53%) | 115/126 (91%)  | 0/90 (0%)       | 0/0 (—%)        |
| Base    | 48/132 (36%)  | 48/78 (62%)    | 0/28 (0%)       | 0/26 (0%)       |
| Overall | 163/348 (47%) | 163/204 (80%)  | 0/118 (0%)      | 0/26 (0%)       |

#### 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                                | 618   |
| Intra-residue ( $ i-j =0$ )                              | 390   |
| Sequential ( $ i-j =1$ )                                 | 149   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 46    |
| Long range ( $ i-j \geq 5$ )                             | 33    |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 34.3  |
| Number of long range restraints per residue <sup>1</sup> | 1.8   |

<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)  | 16.9                                   | 0.2     |
| 0.2-0.5 (Medium) | 5.4                                    | 0.46    |
| >0.5 (Large)     | 49.0                                   | 5.42    |



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

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

## 9 Distance violation analysis ⓘ

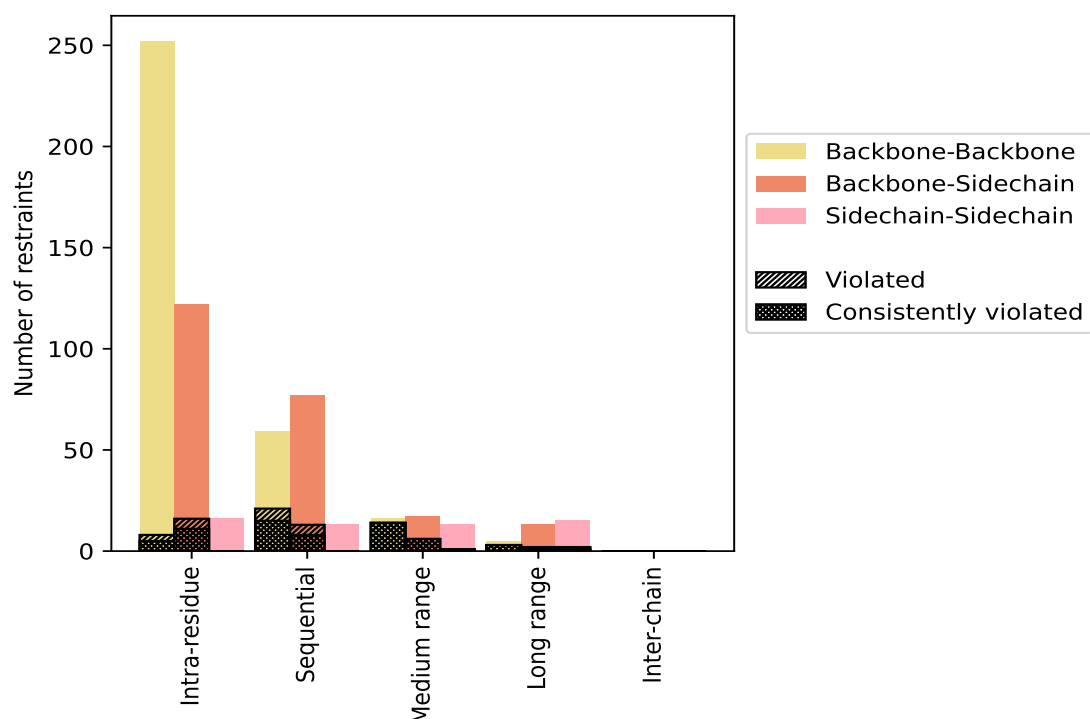
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count               | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                      |                      |
|------------------------------------------------------------|---------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|----------------------|
|                                                            |                     |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>       | % <sup>1</sup>       |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">390</a> | <a href="#">63.1</a>  | <a href="#">24</a>    | <a href="#">6.2</a>  | <a href="#">3.9</a>  | <a href="#">16</a>                 | <a href="#">4.1</a>  | <a href="#">2.6</a>  |
| Backbone-Backbone                                          | 252                 | 40.8                  | 8                     | 3.2                  | 1.3                  | 5                                  | 2.0                  | 0.8                  |
| Backbone-Sidechain                                         | 122                 | 19.7                  | 16                    | 13.1                 | 2.6                  | 11                                 | 9.0                  | 1.8                  |
| Sidechain-Sidechain                                        | 16                  | 2.6                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">149</a> | <a href="#">24.1</a>  | <a href="#">34</a>    | <a href="#">22.8</a> | <a href="#">5.5</a>  | <a href="#">23</a>                 | <a href="#">15.4</a> | <a href="#">3.7</a>  |
| Backbone-Backbone                                          | 59                  | 9.5                   | 21                    | 35.6                 | 3.4                  | 15                                 | 25.4                 | 2.4                  |
| Backbone-Sidechain                                         | 77                  | 12.5                  | 13                    | 16.9                 | 2.1                  | 8                                  | 10.4                 | 1.3                  |
| Sidechain-Sidechain                                        | 13                  | 2.1                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">46</a>  | <a href="#">7.4</a>   | <a href="#">21</a>    | <a href="#">45.7</a> | <a href="#">3.4</a>  | <a href="#">20</a>                 | <a href="#">43.5</a> | <a href="#">3.2</a>  |
| Backbone-Backbone                                          | 16                  | 2.6                   | 14                    | 87.5                 | 2.3                  | 14                                 | 87.5                 | 2.3                  |
| Backbone-Sidechain                                         | 17                  | 2.8                   | 6                     | 35.3                 | 1.0                  | 6                                  | 35.3                 | 1.0                  |
| Sidechain-Sidechain                                        | 13                  | 2.1                   | 1                     | 7.7                  | 0.2                  | 0                                  | 0.0                  | 0.0                  |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">33</a>  | <a href="#">5.3</a>   | <a href="#">7</a>     | <a href="#">21.2</a> | <a href="#">1.1</a>  | <a href="#">5</a>                  | <a href="#">15.2</a> | <a href="#">0.8</a>  |
| Backbone-Backbone                                          | 5                   | 0.8                   | 3                     | 60.0                 | 0.5                  | 3                                  | 60.0                 | 0.5                  |
| Backbone-Sidechain                                         | 13                  | 2.1                   | 2                     | 15.4                 | 0.3                  | 1                                  | 7.7                  | 0.2                  |
| Sidechain-Sidechain                                        | 15                  | 2.4                   | 2                     | 13.3                 | 0.3                  | 1                                  | 6.7                  | 0.2                  |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Backbone-Sidechain                                         | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| Sidechain-Sidechain                                        | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                  |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a>  |
| <a href="#">Total</a>                                      | <a href="#">618</a> | <a href="#">100.0</a> | <a href="#">86</a>    | <a href="#">13.9</a> | <a href="#">13.9</a> | <a href="#">64</a>                 | <a href="#">10.4</a> | <a href="#">10.4</a> |
| Backbone-Backbone                                          | 332                 | 53.7                  | 46                    | 13.9                 | 7.4                  | 37                                 | 11.1                 | 6.0                  |
| Backbone-Sidechain                                         | 229                 | 37.1                  | 37                    | 16.2                 | 6.0                  | 26                                 | 11.4                 | 4.2                  |
| Sidechain-Sidechain                                        | 57                  | 9.2                   | 3                     | 5.3                  | 0.5                  | 1                                  | 1.8                  | 0.2                  |

<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

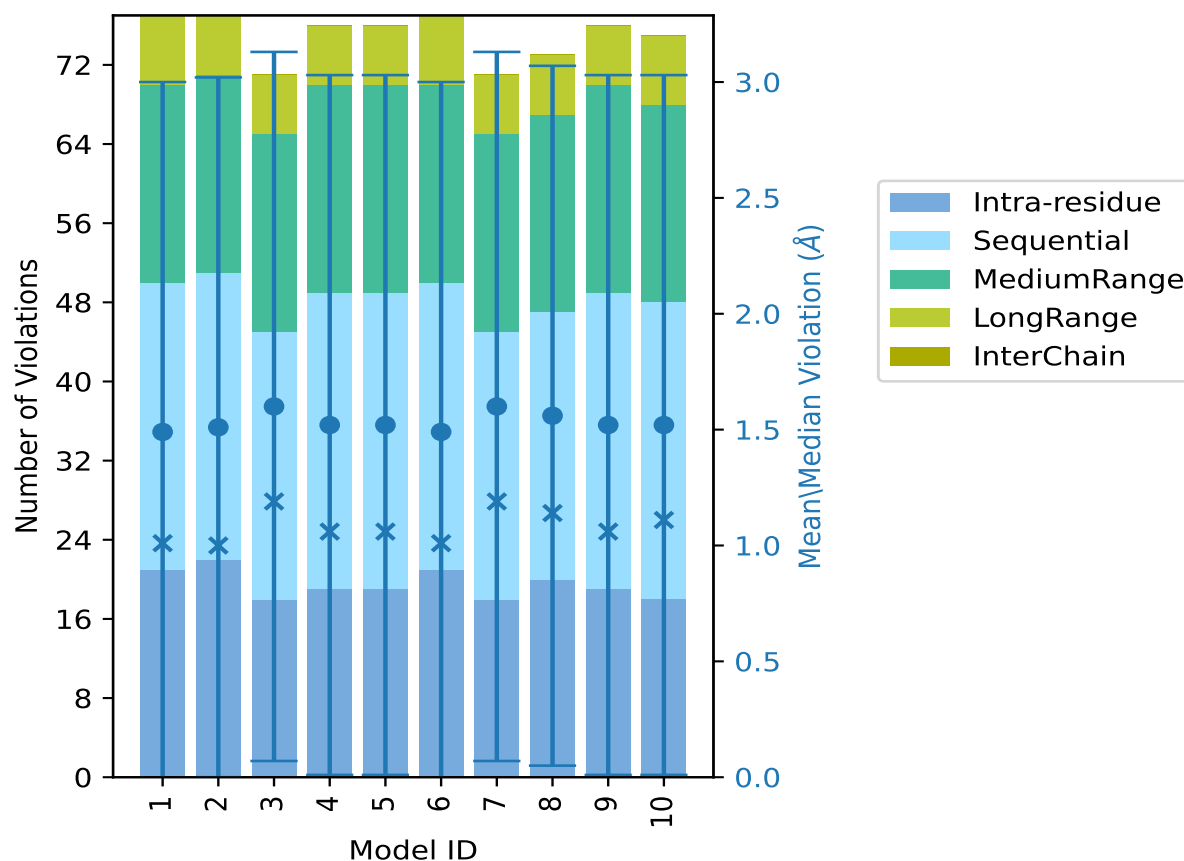
## 9.2 Distance violation statistics for each model [i](#)

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                   | 29              | 20              | 7               | 0               | 77    | 1.49     | 5.36    | 1.51                | 1.01       |
| 2        | 22                   | 29              | 20              | 6               | 0               | 77    | 1.51     | 5.4     | 1.51                | 1.0        |
| 3        | 18                   | 27              | 20              | 6               | 0               | 71    | 1.6      | 5.42    | 1.53                | 1.19       |
| 4        | 19                   | 30              | 21              | 6               | 0               | 76    | 1.52     | 5.42    | 1.51                | 1.06       |
| 5        | 19                   | 30              | 21              | 6               | 0               | 76    | 1.52     | 5.42    | 1.51                | 1.06       |
| 6        | 21                   | 29              | 20              | 7               | 0               | 77    | 1.49     | 5.36    | 1.51                | 1.01       |
| 7        | 18                   | 27              | 20              | 6               | 0               | 71    | 1.6      | 5.42    | 1.53                | 1.19       |
| 8        | 20                   | 27              | 20              | 6               | 0               | 73    | 1.56     | 5.38    | 1.51                | 1.14       |
| 9        | 19                   | 30              | 21              | 6               | 0               | 76    | 1.52     | 5.42    | 1.51                | 1.06       |
| 10       | 18                   | 30              | 20              | 7               | 0               | 75    | 1.52     | 5.37    | 1.51                | 1.11       |

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 532(IR:366, SQ:115, MR:25, LR:26, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |      |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %    |
| 1                             | 1               | 0               | 0               | 0               | 2     | 1                        | 10.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 2                        | 20.0 |
| 3                             | 2               | 1               | 0               | 0               | 6     | 3                        | 30.0 |

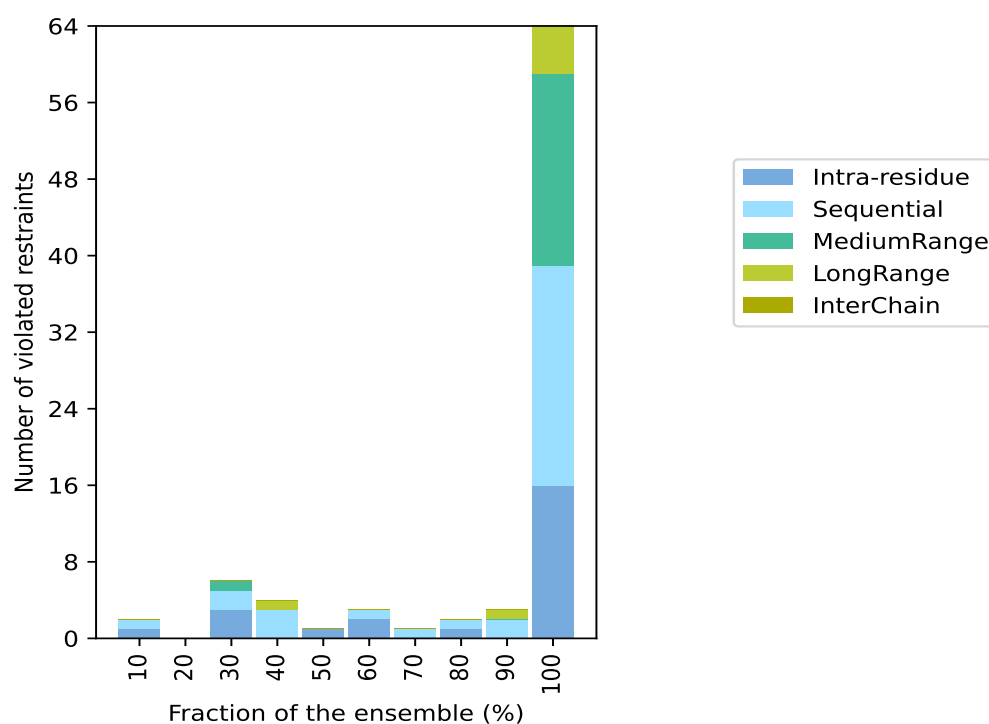
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 3               | 0               | 1               | 0               | 4     | 4                        | 40.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 5                        | 50.0  |
| 2                             | 1               | 0               | 0               | 0               | 3     | 6                        | 60.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 7                        | 70.0  |
| 1                             | 1               | 0               | 0               | 0               | 2     | 8                        | 80.0  |
| 0                             | 2               | 0               | 1               | 0               | 3     | 9                        | 90.0  |
| 16                            | 23              | 20              | 5               | 0               | 64    | 10                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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

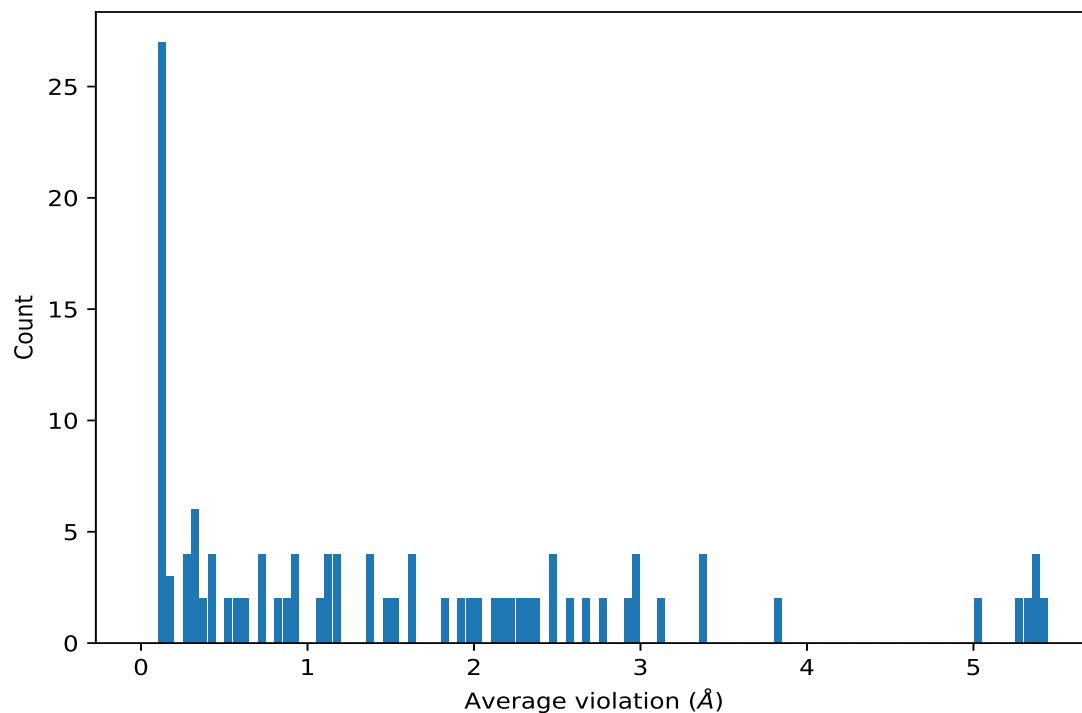


## 9.4 Most violated distance restraints in the ensemble ⓘ

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

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

in the ensemble



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

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

| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 10                  | 5.4      | 0.03                | 5.41       |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 10                  | 5.4      | 0.03                | 5.41       |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 10                  | 5.36     | 0.02                | 5.36       |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 10                  | 5.36     | 0.02                | 5.36       |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 10                  | 5.36     | 0.01                | 5.36       |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 10                  | 5.36     | 0.01                | 5.36       |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 10                  | 5.35     | 0.03                | 5.36       |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 10                  | 5.35     | 0.03                | 5.36       |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 10                  | 5.29     | 0.01                | 5.29       |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 10                  | 5.29     | 0.01                | 5.29       |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 10                  | 5.02     | 0.01                | 5.02       |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 10                  | 5.02     | 0.01                | 5.02       |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 10                  | 3.84     | 0.01                | 3.85       |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 10                  | 3.84     | 0.01                | 3.85       |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 10                  | 3.37     | 0.0                 | 3.37       |

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| Key     | Atom-1        | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,466) | 1:13:A:DG:H1' | 1:16:A:DT:H5'' | 10                  | 3.37     | 0.0                 | 3.37       |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'' | 10                  | 3.35     | 0.02                | 3.35       |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'' | 10                  | 3.35     | 0.02                | 3.35       |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'  | 10                  | 3.12     | 0.16                | 3.06       |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 10                  | 3.12     | 0.16                | 3.06       |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'  | 10                  | 2.95     | 0.12                | 2.96       |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'' | 10                  | 2.95     | 0.12                | 2.96       |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 10                  | 2.95     | 0.01                | 2.95       |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 10                  | 2.95     | 0.01                | 2.95       |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'  | 10                  | 2.93     | 0.15                | 2.94       |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'' | 10                  | 2.93     | 0.15                | 2.94       |
| (1,524) | 1:15:A:DT:H3  | 1:14:A:DT:H5'  | 10                  | 2.8      | 0.03                | 2.8        |
| (1,524) | 1:15:A:DT:H3  | 1:14:A:DT:H5'' | 10                  | 2.8      | 0.03                | 2.8        |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'  | 10                  | 2.67     | 0.15                | 2.62       |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'' | 10                  | 2.67     | 0.15                | 2.62       |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'  | 10                  | 2.59     | 0.0                 | 2.59       |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'' | 10                  | 2.59     | 0.0                 | 2.59       |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 10                  | 2.49     | 0.05                | 2.51       |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 10                  | 2.49     | 0.05                | 2.51       |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 10                  | 2.49     | 0.05                | 2.51       |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 10                  | 2.49     | 0.05                | 2.51       |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 10                  | 2.4      | 0.03                | 2.4        |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 10                  | 2.4      | 0.03                | 2.4        |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 10                  | 2.33     | 0.01                | 2.33       |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 10                  | 2.33     | 0.01                | 2.33       |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 10                  | 2.26     | 0.01                | 2.26       |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 10                  | 2.26     | 0.01                | 2.26       |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 10                  | 2.21     | 0.01                | 2.21       |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 10                  | 2.21     | 0.01                | 2.21       |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 10                  | 2.15     | 0.0                 | 2.15       |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 10                  | 2.15     | 0.0                 | 2.15       |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 10                  | 2.13     | 0.08                | 2.1        |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 10                  | 2.13     | 0.08                | 2.1        |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 10                  | 2.02     | 0.01                | 2.02       |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 10                  | 2.02     | 0.01                | 2.02       |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 10                  | 1.97     | 0.01                | 1.98       |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 10                  | 1.97     | 0.01                | 1.98       |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 10                  | 1.94     | 0.09                | 1.9        |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 10                  | 1.94     | 0.09                | 1.9        |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'  | 10                  | 1.81     | 0.01                | 1.81       |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'' | 10                  | 1.81     | 0.01                | 1.81       |
| (1,459) | 1:13:A:DG:H8  | 1:14:A:DT:H5'  | 10                  | 1.62     | 0.02                | 1.62       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,459) | 1:13:A:DG:H8   | 1:14:A:DT:H5'' | 10                  | 1.62     | 0.02                | 1.62       |
| (1,491) | 1:14:A:DT:H3   | 1:14:A:DT:H5'  | 10                  | 1.6      | 0.01                | 1.6        |
| (1,491) | 1:14:A:DT:H3   | 1:14:A:DT:H5'' | 10                  | 1.6      | 0.01                | 1.6        |
| (1,526) | 1:15:A:DT:H4'  | 1:4:A:DT:H5'   | 10                  | 1.53     | 0.04                | 1.54       |
| (1,526) | 1:15:A:DT:H4'  | 1:4:A:DT:H5''  | 10                  | 1.53     | 0.04                | 1.54       |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5'   | 10                  | 1.46     | 0.03                | 1.45       |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5''  | 10                  | 1.46     | 0.03                | 1.45       |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5'   | 10                  | 1.36     | 0.12                | 1.34       |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5''  | 10                  | 1.36     | 0.12                | 1.34       |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 10                  | 1.35     | 0.06                | 1.36       |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 10                  | 1.35     | 0.06                | 1.36       |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 10                  | 1.17     | 0.04                | 1.19       |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 10                  | 1.17     | 0.04                | 1.19       |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 10                  | 1.17     | 0.04                | 1.19       |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 10                  | 1.17     | 0.04                | 1.19       |
| (1,455) | 1:13:A:DG:H2'  | 1:14:A:DT:H5'  | 10                  | 1.15     | 0.02                | 1.15       |
| (1,455) | 1:13:A:DG:H2'  | 1:14:A:DT:H5'' | 10                  | 1.15     | 0.02                | 1.15       |
| (1,230) | 1:7:A:DG:H1    | 1:10:A:DT:H5'  | 10                  | 1.14     | 0.14                | 1.11       |
| (1,230) | 1:7:A:DG:H1    | 1:10:A:DT:H5'' | 10                  | 1.14     | 0.14                | 1.11       |
| (1,348) | 1:10:A:DT:H5'  | 1:11:A:DT:H5'  | 10                  | 1.05     | 0.03                | 1.06       |
| (1,348) | 1:10:A:DT:H5'  | 1:11:A:DT:H5'' | 10                  | 1.05     | 0.03                | 1.06       |
| (1,156) | 1:5:A:DT:H4'   | 1:5:A:DT:H5'   | 10                  | 0.92     | 0.06                | 0.88       |
| (1,156) | 1:5:A:DT:H4'   | 1:5:A:DT:H5''  | 10                  | 0.92     | 0.06                | 0.88       |
| (1,525) | 1:15:A:DT:H3   | 1:15:A:DT:H5'  | 10                  | 0.92     | 0.01                | 0.91       |
| (1,525) | 1:15:A:DT:H3   | 1:15:A:DT:H5'' | 10                  | 0.92     | 0.01                | 0.91       |
| (1,344) | 1:10:A:DT:H1'  | 1:11:A:DT:H5'  | 10                  | 0.88     | 0.01                | 0.88       |
| (1,344) | 1:10:A:DT:H1'  | 1:11:A:DT:H5'' | 10                  | 0.88     | 0.01                | 0.88       |
| (1,75)  | 1:2:A:DG:H8    | 1:4:A:DT:H5'   | 10                  | 0.83     | 0.16                | 0.72       |
| (1,75)  | 1:2:A:DG:H8    | 1:4:A:DT:H5''  | 10                  | 0.83     | 0.16                | 0.72       |
| (1,308) | 1:9:A:DT:H1'   | 1:8:A:DT:H5'   | 10                  | 0.72     | 0.03                | 0.71       |
| (1,308) | 1:9:A:DT:H1'   | 1:8:A:DT:H5''  | 10                  | 0.72     | 0.03                | 0.71       |
| (1,345) | 1:10:A:DT:H3'  | 1:11:A:DT:H5'  | 10                  | 0.71     | 0.06                | 0.73       |
| (1,345) | 1:10:A:DT:H3'  | 1:11:A:DT:H5'' | 10                  | 0.71     | 0.06                | 0.73       |
| (1,76)  | 1:2:A:DG:H2'   | 1:4:A:DT:H5'   | 10                  | 0.62     | 0.11                | 0.61       |
| (1,76)  | 1:2:A:DG:H2'   | 1:4:A:DT:H5''  | 10                  | 0.62     | 0.11                | 0.61       |
| (1,306) | 1:9:A:DT:H3    | 1:9:A:DT:H5'   | 10                  | 0.56     | 0.01                | 0.56       |
| (1,306) | 1:9:A:DT:H3    | 1:9:A:DT:H5''  | 10                  | 0.56     | 0.01                | 0.56       |
| (1,373) | 1:11:A:DT:H5'  | 1:11:A:DT:H5'' | 10                  | 0.53     | 0.0                 | 0.53       |
| (1,374) | 1:11:A:DT:H5'  | 1:11:A:DT:H5'' | 10                  | 0.53     | 0.0                 | 0.53       |
| (1,119) | 1:4:A:DT:H4'   | 1:4:A:DT:H5'   | 10                  | 0.36     | 0.0                 | 0.36       |
| (1,119) | 1:4:A:DT:H4'   | 1:4:A:DT:H5''  | 10                  | 0.36     | 0.0                 | 0.36       |
| (1,265) | 1:8:A:DT:H3    | 1:8:A:DT:H5'   | 10                  | 0.35     | 0.03                | 0.33       |

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| Key     | Atom-1         | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,265) | 1:8:A:DT:H3    | 1:8:A:DT:H5''  | 10                  | 0.35     | 0.03                | 0.33       |
| (1,68)  | 1:2:A:DG:H3'   | 1:3:A:DT:H5'   | 10                  | 0.35     | 0.08                | 0.36       |
| (1,68)  | 1:2:A:DG:H3'   | 1:3:A:DT:H5''  | 10                  | 0.35     | 0.08                | 0.36       |
| (1,220) | 1:7:A:DG:H2'   | 1:8:A:DT:H5'   | 10                  | 0.32     | 0.06                | 0.29       |
| (1,220) | 1:7:A:DG:H2'   | 1:8:A:DT:H5''  | 10                  | 0.32     | 0.06                | 0.29       |
| (1,601) | 1:17:A:DG:H21  | 1:14:A:DT:H2'' | 10                  | 0.16     | 0.0                 | 0.16       |
| (1,413) | 1:12:A:DG:H8   | 1:12:A:DG:H3'  | 10                  | 0.14     | 0.01                | 0.15       |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 10                  | 0.13     | 0.0                 | 0.13       |
| (1,90)  | 1:3:A:DT:H6    | 1:3:A:DT:H2''  | 10                  | 0.13     | 0.0                 | 0.13       |
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 10                  | 0.13     | 0.01                | 0.12       |
| (1,87)  | 1:3:A:DT:H5''  | 1:3:A:DT:H2''  | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,487) | 1:14:A:DT:H6   | 1:15:A:DT:H1'  | 10                  | 0.12     | 0.0                 | 0.12       |
| (1,219) | 1:7:A:DG:H1'   | 1:8:A:DT:H1'   | 10                  | 0.12     | 0.01                | 0.12       |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,254) | 1:8:A:DT:H6    | 1:8:A:DT:H4'   | 10                  | 0.11     | 0.01                | 0.12       |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 10                  | 0.11     | 0.0                 | 0.11       |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5'   | 9                   | 0.16     | 0.04                | 0.15       |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5''  | 9                   | 0.16     | 0.04                | 0.15       |
| (1,618) | 1:18:A:DG:H1   | 1:7:A:DG:H8    | 9                   | 0.12     | 0.01                | 0.11       |
| (1,608) | 1:18:A:DG:H8   | 1:17:A:DG:H1'  | 9                   | 0.1      | 0.0                 | 0.1        |
| (1,181) | 1:6:A:DG:H5'   | 1:6:A:DG:H2''  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'' | 8                   | 0.14     | 0.02                | 0.14       |
| (1,99)  | 1:3:A:DT:H5'   | 1:4:A:DT:H5'   | 7                   | 0.25     | 0.05                | 0.27       |
| (1,99)  | 1:3:A:DT:H5'   | 1:4:A:DT:H5''  | 7                   | 0.25     | 0.05                | 0.27       |
| (1,99)  | 1:3:A:DT:H5''  | 1:4:A:DT:H5'   | 7                   | 0.25     | 0.05                | 0.27       |
| (1,99)  | 1:3:A:DT:H5''  | 1:4:A:DT:H5''  | 7                   | 0.25     | 0.05                | 0.27       |
| (1,10)  | 1:1:A:DG:H8    | 1:1:A:DG:H3'   | 6                   | 0.12     | 0.0                 | 0.12       |
| (1,108) | 1:4:A:DT:H1'   | 1:4:A:DT:H5''  | 6                   | 0.11     | 0.01                | 0.12       |
| (1,339) | 1:10:A:DT:H6   | 1:9:A:DT:H3'   | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,544) | 1:16:A:DT:H6   | 1:16:A:DT:H2'  | 5                   | 0.1      | 0.0                 | 0.1        |
| (1,135) | 1:4:A:DT:H2''  | 1:5:A:DT:H5'   | 4                   | 0.41     | 0.06                | 0.38       |
| (1,135) | 1:4:A:DT:H2''  | 1:5:A:DT:H5''  | 4                   | 0.41     | 0.06                | 0.38       |
| (1,134) | 1:4:A:DT:H2'   | 1:5:A:DT:H5'   | 4                   | 0.4      | 0.07                | 0.36       |
| (1,134) | 1:4:A:DT:H2'   | 1:5:A:DT:H5''  | 4                   | 0.4      | 0.07                | 0.36       |
| (1,102) | 1:3:A:DT:H6    | 1:15:A:DT:H4'  | 4                   | 0.12     | 0.0                 | 0.12       |
| (1,296) | 1:9:A:DT:H5'   | 1:10:A:DT:H2'' | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,372) | 1:11:A:DT:H5'  | 1:11:A:DT:H2'' | 3                   | 0.15     | 0.0                 | 0.15       |
| (1,411) | 1:12:A:DG:H8   | 1:12:A:DG:H2'  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,415) | 1:12:A:DG:H8   | 1:12:A:DG:H5'' | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,62)  | 1:2:A:DG:H8    | 1:1:A:DG:H2'   | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,217) | 1:7:A:DG:H8    | 1:6:A:DG:H4'   | 3                   | 0.1      | 0.0                 | 0.1        |

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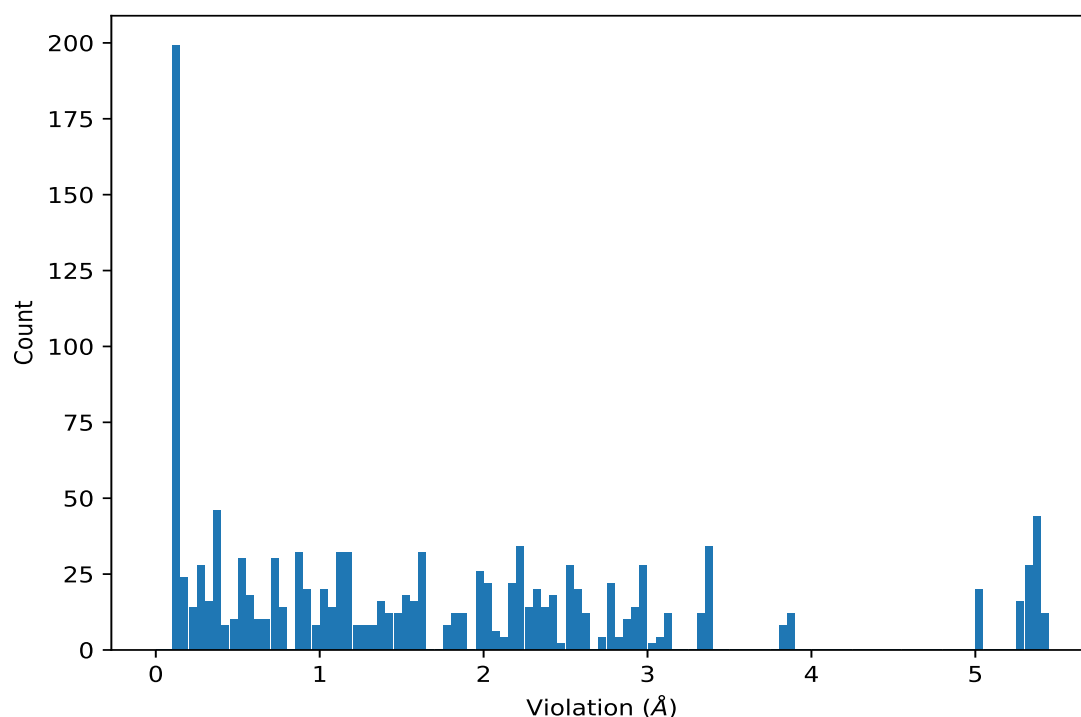
| Key     | Atom-1       | Atom-2       | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|--------------|--------------|---------------------|----------|---------------------|------------|
| (1,495) | 1:14:A:DT:H3 | 1:16:A:DT:H3 | 3                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 3        | 5.42          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 3        | 5.42          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 4        | 5.42          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 4        | 5.42          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 5        | 5.42          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 5        | 5.42          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 7        | 5.42          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 7        | 5.42          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 9        | 5.42          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 9        | 5.42          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 2        | 5.4           |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 2        | 5.4           |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 3        | 5.38          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 3        | 5.38          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 7        | 5.38          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 7        | 5.38          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 8        | 5.38          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 8        | 5.38          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 4        | 5.38          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 4        | 5.38          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 5        | 5.38          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 5        | 5.38          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 9        | 5.38          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 9        | 5.38          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 4        | 5.37          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 4        | 5.37          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 5        | 5.37          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 5        | 5.37          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 9        | 5.37          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 9        | 5.37          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 4        | 5.37          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 4        | 5.37          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 5        | 5.37          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 5        | 5.37          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 9        | 5.37          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 9        | 5.37          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 10       | 5.37          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 10       | 5.37          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 3        | 5.37          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 3        | 5.37          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 7        | 5.37          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 7        | 5.37          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 2        | 5.36          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 2        | 5.36          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 3        | 5.36          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 3        | 5.36          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 7        | 5.36          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 7        | 5.36          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 2        | 5.36          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 2        | 5.36          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 8        | 5.36          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 8        | 5.36          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 1        | 5.36          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 1        | 5.36          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'  | 6        | 5.36          |
| (1,555) | 1:16:A:DT:H2'' | 1:14:A:DT:H5'' | 6        | 5.36          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 10       | 5.35          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 10       | 5.35          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 2        | 5.35          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 2        | 5.35          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 1        | 5.34          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 1        | 5.34          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 6        | 5.34          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 6        | 5.34          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 8        | 5.34          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 8        | 5.34          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'  | 10       | 5.34          |
| (1,558) | 1:16:A:DT:H5'' | 1:14:A:DT:H5'' | 10       | 5.34          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 1        | 5.33          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 1        | 5.33          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'  | 6        | 5.33          |
| (1,556) | 1:16:A:DT:H4'  | 1:14:A:DT:H5'' | 6        | 5.33          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 10       | 5.33          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 10       | 5.33          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 1        | 5.32          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 1        | 5.32          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 6        | 5.32          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 6        | 5.32          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'  | 8        | 5.32          |
| (1,520) | 1:15:A:DT:H6   | 1:14:A:DT:H5'' | 8        | 5.32          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 3        | 5.31          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 3        | 5.31          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 7        | 5.31          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 7        | 5.31          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 8        | 5.3           |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 8        | 5.3           |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 1        | 5.29          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 1        | 5.29          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 4        | 5.29          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 4        | 5.29          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 5        | 5.29          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 5        | 5.29          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 6        | 5.29          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 6        | 5.29          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 9        | 5.29          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 9        | 5.29          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 2        | 5.28          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 2        | 5.28          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'  | 10       | 5.28          |
| (1,465) | 1:13:A:DG:H4'  | 1:16:A:DT:H5'' | 10       | 5.28          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 2        | 5.03          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 2        | 5.03          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 3        | 5.02          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 3        | 5.02          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 4        | 5.02          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 4        | 5.02          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 5        | 5.02          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 5        | 5.02          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 7        | 5.02          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 7        | 5.02          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 9        | 5.02          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 9        | 5.02          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 1        | 5.01          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 1        | 5.01          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 6        | 5.01          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 6        | 5.01          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 8        | 5.01          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 8        | 5.01          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'  | 10       | 5.01          |
| (1,557) | 1:16:A:DT:H5'  | 1:14:A:DT:H5'' | 10       | 5.01          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 2        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 2        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 3        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 3        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 4        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 4        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 5        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 5        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 7        | 3.85          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 7        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 9        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 9        | 3.85          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 1        | 3.83          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 1        | 3.83          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 6        | 3.83          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 6        | 3.83          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 8        | 3.83          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 8        | 3.83          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'  | 10       | 3.83          |
| (1,517) | 1:15:A:DT:H2'' | 1:14:A:DT:H5'' | 10       | 3.83          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 2        | 3.38          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'' | 2        | 3.38          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 3        | 3.38          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'' | 3        | 3.38          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 7        | 3.38          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'' | 7        | 3.38          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 8        | 3.38          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'' | 8        | 3.38          |
| (1,554) | 1:16:A:DT:H1'  | 1:14:A:DT:H5'  | 4        | 3.37          |
| (1,554) | 1:16:A:DT:H1'  | 1:14:A:DT:H5'' | 4        | 3.37          |
| (1,554) | 1:16:A:DT:H1'  | 1:14:A:DT:H5'  | 5        | 3.37          |
| (1,554) | 1:16:A:DT:H1'  | 1:14:A:DT:H5'' | 5        | 3.37          |
| (1,554) | 1:16:A:DT:H1'  | 1:14:A:DT:H5'  | 9        | 3.37          |
| (1,554) | 1:16:A:DT:H1'  | 1:14:A:DT:H5'' | 9        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 1        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'' | 1        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 4        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'' | 4        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 5        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'' | 5        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 6        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'' | 6        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 9        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'' | 9        | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'  | 10       | 3.37          |
| (1,466) | 1:13:A:DG:H1'  | 1:16:A:DT:H5'' | 10       | 3.37          |
| (1,554) | 1:16:A:DT:H1'  | 1:14:A:DT:H5'  | 3        | 3.36          |
| (1,554) | 1:16:A:DT:H1'  | 1:14:A:DT:H5'' | 3        | 3.36          |
| (1,554) | 1:16:A:DT:H1'  | 1:14:A:DT:H5'  | 7        | 3.36          |
| (1,554) | 1:16:A:DT:H1'  | 1:14:A:DT:H5'' | 7        | 3.36          |
| (1,27)  | 1:1:A:DG:H8    | 1:10:A:DT:H5'  | 1        | 3.36          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 1        | 3.36          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'  | 6        | 3.36          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 6        | 3.36          |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'  | 2        | 3.34          |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'' | 2        | 3.34          |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'  | 8        | 3.34          |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'' | 8        | 3.34          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'  | 2        | 3.34          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 2        | 3.34          |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'  | 10       | 3.33          |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'' | 10       | 3.33          |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'  | 1        | 3.32          |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'' | 1        | 3.32          |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'  | 6        | 3.32          |
| (1,554) | 1:16:A:DT:H1' | 1:14:A:DT:H5'' | 6        | 3.32          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'  | 4        | 3.11          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'' | 4        | 3.11          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'  | 5        | 3.11          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'' | 5        | 3.11          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'  | 9        | 3.11          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'' | 9        | 3.11          |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'  | 4        | 3.1           |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'' | 4        | 3.1           |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'  | 5        | 3.1           |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'' | 5        | 3.1           |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'  | 9        | 3.1           |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'' | 9        | 3.1           |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'  | 3        | 3.09          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 3        | 3.09          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'  | 7        | 3.09          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 7        | 3.09          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'  | 10       | 3.03          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 10       | 3.03          |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'  | 3        | 2.99          |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'' | 3        | 2.99          |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'  | 7        | 2.99          |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'' | 7        | 2.99          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'  | 8        | 2.99          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 8        | 2.99          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'  | 4        | 2.98          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 4        | 2.98          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'  | 5        | 2.98          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 5        | 2.98          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'  | 9        | 2.98          |
| (1,27)  | 1:1:A:DG:H8   | 1:10:A:DT:H5'' | 9        | 2.98          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'  | 3        | 2.97          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'' | 3        | 2.97          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'  | 7        | 2.97          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'' | 7        | 2.97          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 3        | 2.96          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 3        | 2.96          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 7        | 2.96          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 7        | 2.96          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 2        | 2.95          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 2        | 2.95          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 4        | 2.95          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 4        | 2.95          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 5        | 2.95          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 5        | 2.95          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 9        | 2.95          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 9        | 2.95          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 1        | 2.94          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 1        | 2.94          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 6        | 2.94          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 6        | 2.94          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 8        | 2.94          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 8        | 2.94          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'  | 10       | 2.94          |
| (1,516) | 1:15:A:DT:H1' | 1:14:A:DT:H5'' | 10       | 2.94          |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'  | 10       | 2.93          |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'' | 10       | 2.93          |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'  | 8        | 2.92          |
| (1,304) | 1:9:A:DT:H6   | 1:11:A:DT:H5'' | 8        | 2.92          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'  | 2        | 2.92          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'' | 2        | 2.92          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'  | 10       | 2.9           |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'' | 10       | 2.9           |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'  | 8        | 2.89          |
| (1,298) | 1:9:A:DT:H1'  | 1:11:A:DT:H5'' | 8        | 2.89          |
| (1,524) | 1:15:A:DT:H3  | 1:14:A:DT:H5'  | 2        | 2.87          |
| (1,524) | 1:15:A:DT:H3  | 1:14:A:DT:H5'' | 2        | 2.87          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'  | 1        | 2.87          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'' | 1        | 2.87          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'  | 6        | 2.87          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,26)  | 1:1:A:DG:H1' | 1:10:A:DT:H5'' | 6        | 2.87          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'  | 3        | 2.81          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'' | 3        | 2.81          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'  | 7        | 2.81          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'' | 7        | 2.81          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'  | 4        | 2.8           |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'' | 4        | 2.8           |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'  | 5        | 2.8           |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'' | 5        | 2.8           |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'  | 9        | 2.8           |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'' | 9        | 2.8           |
| (1,304) | 1:9:A:DT:H6  | 1:11:A:DT:H5'  | 2        | 2.8           |
| (1,304) | 1:9:A:DT:H6  | 1:11:A:DT:H5'' | 2        | 2.8           |
| (1,304) | 1:9:A:DT:H6  | 1:11:A:DT:H5'  | 1        | 2.79          |
| (1,304) | 1:9:A:DT:H6  | 1:11:A:DT:H5'' | 1        | 2.79          |
| (1,304) | 1:9:A:DT:H6  | 1:11:A:DT:H5'  | 6        | 2.79          |
| (1,304) | 1:9:A:DT:H6  | 1:11:A:DT:H5'' | 6        | 2.79          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'  | 8        | 2.78          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'' | 8        | 2.78          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'  | 1        | 2.77          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'' | 1        | 2.77          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'  | 6        | 2.77          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'' | 6        | 2.77          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'  | 10       | 2.77          |
| (1,524) | 1:15:A:DT:H3 | 1:14:A:DT:H5'' | 10       | 2.77          |
| (1,298) | 1:9:A:DT:H1' | 1:11:A:DT:H5'  | 2        | 2.75          |
| (1,298) | 1:9:A:DT:H1' | 1:11:A:DT:H5'' | 2        | 2.75          |
| (1,298) | 1:9:A:DT:H1' | 1:11:A:DT:H5'  | 1        | 2.73          |
| (1,298) | 1:9:A:DT:H1' | 1:11:A:DT:H5'' | 1        | 2.73          |
| (1,298) | 1:9:A:DT:H1' | 1:11:A:DT:H5'  | 6        | 2.73          |
| (1,298) | 1:9:A:DT:H1' | 1:11:A:DT:H5'' | 6        | 2.73          |
| (1,26)  | 1:1:A:DG:H1' | 1:10:A:DT:H5'  | 4        | 2.62          |
| (1,26)  | 1:1:A:DG:H1' | 1:10:A:DT:H5'' | 4        | 2.62          |
| (1,26)  | 1:1:A:DG:H1' | 1:10:A:DT:H5'  | 5        | 2.62          |
| (1,26)  | 1:1:A:DG:H1' | 1:10:A:DT:H5'' | 5        | 2.62          |
| (1,26)  | 1:1:A:DG:H1' | 1:10:A:DT:H5'  | 9        | 2.62          |
| (1,26)  | 1:1:A:DG:H1' | 1:10:A:DT:H5'' | 9        | 2.62          |
| (1,550) | 1:16:A:DT:H6 | 1:16:A:DT:H5'  | 4        | 2.6           |
| (1,550) | 1:16:A:DT:H6 | 1:16:A:DT:H5'' | 4        | 2.6           |
| (1,550) | 1:16:A:DT:H6 | 1:16:A:DT:H5'  | 5        | 2.6           |
| (1,550) | 1:16:A:DT:H6 | 1:16:A:DT:H5'' | 5        | 2.6           |
| (1,550) | 1:16:A:DT:H6 | 1:16:A:DT:H5'  | 9        | 2.6           |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'' | 9        | 2.6           |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'  | 1        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'' | 1        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'  | 2        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'' | 2        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'  | 3        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'' | 3        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'  | 6        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'' | 6        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'  | 7        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'' | 7        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'  | 8        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'' | 8        | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'  | 10       | 2.59          |
| (1,550) | 1:16:A:DT:H6  | 1:16:A:DT:H5'' | 10       | 2.59          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'  | 10       | 2.58          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'' | 10       | 2.58          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'  | 3        | 2.57          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'' | 3        | 2.57          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'  | 7        | 2.57          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'' | 7        | 2.57          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 1        | 2.53          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 1        | 2.53          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 6        | 2.53          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 6        | 2.53          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 8        | 2.53          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 8        | 2.53          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 1        | 2.53          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 1        | 2.53          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 6        | 2.53          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 6        | 2.53          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 8        | 2.53          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 8        | 2.53          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 10       | 2.52          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 10       | 2.52          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 10       | 2.52          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 10       | 2.52          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 2        | 2.51          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 2        | 2.51          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 3        | 2.51          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 3        | 2.51          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 7        | 2.51          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 7        | 2.51          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 2        | 2.51          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 2        | 2.51          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 3        | 2.51          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 3        | 2.51          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 7        | 2.51          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 7        | 2.51          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'  | 8        | 2.45          |
| (1,26)  | 1:1:A:DG:H1'  | 1:10:A:DT:H5'' | 8        | 2.45          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 4        | 2.43          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 4        | 2.43          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 5        | 2.43          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 5        | 2.43          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 9        | 2.43          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 9        | 2.43          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 4        | 2.41          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 4        | 2.41          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 5        | 2.41          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 5        | 2.41          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 9        | 2.41          |
| (1,303) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 9        | 2.41          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 4        | 2.41          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 4        | 2.41          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 5        | 2.41          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 5        | 2.41          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'  | 9        | 2.41          |
| (1,302) | 1:9:A:DT:H5'' | 1:11:A:DT:H5'' | 9        | 2.41          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 3        | 2.4           |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 3        | 2.4           |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 7        | 2.4           |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 7        | 2.4           |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 2        | 2.39          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 2        | 2.39          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 8        | 2.38          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 8        | 2.38          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 10       | 2.37          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 10       | 2.37          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 1        | 2.36          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 1        | 2.36          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'  | 6        | 2.36          |
| (1,559) | 1:16:A:DT:H6  | 1:14:A:DT:H5'' | 6        | 2.36          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 2        | 2.34          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 2        | 2.34          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 4        | 2.34          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 4        | 2.34          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 5        | 2.34          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 5        | 2.34          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 9        | 2.34          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 9        | 2.34          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 3        | 2.33          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 3        | 2.33          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 7        | 2.33          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 7        | 2.33          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 1        | 2.31          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 1        | 2.31          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 6        | 2.31          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 6        | 2.31          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 8        | 2.31          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 8        | 2.31          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'  | 10       | 2.31          |
| (1,518) | 1:15:A:DT:H2' | 1:14:A:DT:H5'' | 10       | 2.31          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 10       | 2.28          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 10       | 2.28          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 3        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 3        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 4        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 4        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 5        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 5        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 7        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 7        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 8        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 8        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 9        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 9        | 2.26          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 1        | 2.24          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 1        | 2.24          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 2        | 2.24          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 2        | 2.24          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5'   | 6        | 2.24          |
| (1,263) | 1:8:A:DT:H6   | 1:9:A:DT:H5''  | 6        | 2.24          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 1        | 2.24          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 1        | 2.24          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 6        | 2.24          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 6        | 2.24          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 1        | 2.22          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 1        | 2.22          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 2        | 2.22          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 2        | 2.22          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 6        | 2.22          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 6        | 2.22          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 8        | 2.22          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 8        | 2.22          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 3        | 2.21          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 3        | 2.21          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 7        | 2.21          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 7        | 2.21          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 10       | 2.21          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 10       | 2.21          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 10       | 2.21          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 10       | 2.21          |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 4        | 2.2           |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 4        | 2.2           |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 5        | 2.2           |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 5        | 2.2           |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 8        | 2.2           |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 8        | 2.2           |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'  | 9        | 2.2           |
| (1,551) | 1:16:A:DT:H3' | 1:15:A:DT:H5'' | 9        | 2.2           |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 2        | 2.17          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 2        | 2.17          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 2        | 2.16          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 2        | 2.16          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 3        | 2.16          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 3        | 2.16          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 7        | 2.16          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 7        | 2.16          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 1        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 1        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 4        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 4        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 5        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 5        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 6        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 6        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 8        | 2.15          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 8        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 9        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 9        | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'  | 10       | 2.15          |
| (1,519) | 1:15:A:DT:H3' | 1:14:A:DT:H5'' | 10       | 2.15          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 3        | 2.1           |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 3        | 2.1           |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 7        | 2.1           |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 7        | 2.1           |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 4        | 2.07          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 4        | 2.07          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 5        | 2.07          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 5        | 2.07          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 9        | 2.07          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 9        | 2.07          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 3        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 3        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 4        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 4        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 5        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 5        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 7        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 7        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 8        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 8        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 9        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 9        | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 10       | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 10       | 2.02          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 1        | 2.01          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 1        | 2.01          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 6        | 2.01          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 6        | 2.01          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5'   | 2        | 2.01          |
| (1,225) | 1:7:A:DG:H8   | 1:8:A:DT:H5''  | 2        | 2.01          |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'  | 2        | 2.0           |
| (1,552) | 1:16:A:DT:H1' | 1:15:A:DT:H5'' | 2        | 2.0           |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 3        | 1.98          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 3        | 1.98          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 4        | 1.98          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 4        | 1.98          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 5        | 1.98          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 5        | 1.98          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 7        | 1.98          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 7        | 1.98          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 9        | 1.98          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 9        | 1.98          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 10       | 1.97          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 10       | 1.97          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 4        | 1.97          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 4        | 1.97          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 5        | 1.97          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 5        | 1.97          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 9        | 1.97          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 9        | 1.97          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 1        | 1.96          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 1        | 1.96          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 2        | 1.96          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 2        | 1.96          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 6        | 1.96          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 6        | 1.96          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'  | 8        | 1.96          |
| (1,515) | 1:15:A:DT:H6  | 1:15:A:DT:H5'' | 8        | 1.96          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 1        | 1.9           |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 1        | 1.9           |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 6        | 1.9           |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 6        | 1.9           |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 10       | 1.89          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 10       | 1.89          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 8        | 1.88          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 8        | 1.88          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 3        | 1.85          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 3        | 1.85          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5'   | 7        | 1.85          |
| (1,496) | 1:14:A:DT:H1' | 1:5:A:DT:H5''  | 7        | 1.85          |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'  | 4        | 1.82          |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'' | 4        | 1.82          |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'  | 5        | 1.82          |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'' | 5        | 1.82          |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'  | 9        | 1.82          |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'' | 9        | 1.82          |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'  | 2        | 1.81          |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'' | 2        | 1.81          |
| (1,486) | 1:14:A:DT:H6  | 1:14:A:DT:H5'  | 3        | 1.81          |

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| Key     | Atom-1       | Atom-2         | Model ID | Violation (Å) |
|---------|--------------|----------------|----------|---------------|
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'' | 3        | 1.81          |
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'  | 7        | 1.81          |
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'' | 7        | 1.81          |
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'  | 1        | 1.79          |
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'' | 1        | 1.79          |
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'  | 6        | 1.79          |
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'' | 6        | 1.79          |
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'  | 8        | 1.79          |
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'' | 8        | 1.79          |
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'  | 10       | 1.79          |
| (1,486) | 1:14:A:DT:H6 | 1:14:A:DT:H5'' | 10       | 1.79          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'  | 4        | 1.65          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'' | 4        | 1.65          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'  | 5        | 1.65          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'' | 5        | 1.65          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'  | 9        | 1.65          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'' | 9        | 1.65          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'  | 2        | 1.63          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'' | 2        | 1.63          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'  | 8        | 1.62          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'' | 8        | 1.62          |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'  | 3        | 1.61          |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'' | 3        | 1.61          |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'  | 7        | 1.61          |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'' | 7        | 1.61          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'  | 3        | 1.61          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'' | 3        | 1.61          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'  | 7        | 1.61          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'' | 7        | 1.61          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'  | 10       | 1.61          |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'' | 10       | 1.61          |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'  | 1        | 1.6           |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'' | 1        | 1.6           |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'  | 2        | 1.6           |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'' | 2        | 1.6           |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'  | 6        | 1.6           |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'' | 6        | 1.6           |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'  | 10       | 1.6           |
| (1,491) | 1:14:A:DT:H3 | 1:14:A:DT:H5'' | 10       | 1.6           |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'  | 1        | 1.6           |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'' | 1        | 1.6           |
| (1,459) | 1:13:A:DG:H8 | 1:14:A:DT:H5'  | 6        | 1.6           |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,459) | 1:13:A:DG:H8  | 1:14:A:DT:H5'' | 6        | 1.6           |
| (1,491) | 1:14:A:DT:H3  | 1:14:A:DT:H5'  | 4        | 1.59          |
| (1,491) | 1:14:A:DT:H3  | 1:14:A:DT:H5'' | 4        | 1.59          |
| (1,491) | 1:14:A:DT:H3  | 1:14:A:DT:H5'  | 5        | 1.59          |
| (1,491) | 1:14:A:DT:H3  | 1:14:A:DT:H5'' | 5        | 1.59          |
| (1,491) | 1:14:A:DT:H3  | 1:14:A:DT:H5'  | 8        | 1.59          |
| (1,491) | 1:14:A:DT:H3  | 1:14:A:DT:H5'' | 8        | 1.59          |
| (1,491) | 1:14:A:DT:H3  | 1:14:A:DT:H5'  | 9        | 1.59          |
| (1,491) | 1:14:A:DT:H3  | 1:14:A:DT:H5'' | 9        | 1.59          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5'   | 8        | 1.58          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5''  | 8        | 1.58          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5'   | 1        | 1.57          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5''  | 1        | 1.57          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5'   | 6        | 1.57          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5''  | 6        | 1.57          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5'   | 10       | 1.57          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5''  | 10       | 1.57          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5'   | 3        | 1.54          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5''  | 3        | 1.54          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5'   | 7        | 1.54          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5''  | 7        | 1.54          |
| (1,78)  | 1:2:A:DG:H3'  | 1:4:A:DT:H5'   | 2        | 1.53          |
| (1,78)  | 1:2:A:DG:H3'  | 1:4:A:DT:H5''  | 2        | 1.53          |
| (1,290) | 1:9:A:DT:H6   | 1:9:A:DT:H5'   | 4        | 1.51          |
| (1,290) | 1:9:A:DT:H6   | 1:9:A:DT:H5''  | 4        | 1.51          |
| (1,290) | 1:9:A:DT:H6   | 1:9:A:DT:H5'   | 5        | 1.51          |
| (1,290) | 1:9:A:DT:H6   | 1:9:A:DT:H5''  | 5        | 1.51          |
| (1,290) | 1:9:A:DT:H6   | 1:9:A:DT:H5'   | 9        | 1.51          |
| (1,290) | 1:9:A:DT:H6   | 1:9:A:DT:H5''  | 9        | 1.51          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5'   | 4        | 1.5           |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5''  | 4        | 1.5           |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5'   | 5        | 1.5           |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5''  | 5        | 1.5           |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5'   | 9        | 1.5           |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5''  | 9        | 1.5           |
| (1,78)  | 1:2:A:DG:H3'  | 1:4:A:DT:H5'   | 4        | 1.47          |
| (1,78)  | 1:2:A:DG:H3'  | 1:4:A:DT:H5''  | 4        | 1.47          |
| (1,78)  | 1:2:A:DG:H3'  | 1:4:A:DT:H5'   | 5        | 1.47          |
| (1,78)  | 1:2:A:DG:H3'  | 1:4:A:DT:H5''  | 5        | 1.47          |
| (1,78)  | 1:2:A:DG:H3'  | 1:4:A:DT:H5'   | 9        | 1.47          |
| (1,78)  | 1:2:A:DG:H3'  | 1:4:A:DT:H5''  | 9        | 1.47          |
| (1,526) | 1:15:A:DT:H4' | 1:4:A:DT:H5'   | 2        | 1.46          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,526) | 1:15:A:DT:H4'  | 1:4:A:DT:H5''  | 2        | 1.46          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5'   | 3        | 1.46          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5''  | 3        | 1.46          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5'   | 7        | 1.46          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5''  | 7        | 1.46          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5'   | 2        | 1.44          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5''  | 2        | 1.44          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5'   | 1        | 1.43          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5''  | 1        | 1.43          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5'   | 6        | 1.43          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5''  | 6        | 1.43          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5'   | 8        | 1.43          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5''  | 8        | 1.43          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5'   | 10       | 1.43          |
| (1,290) | 1:9:A:DT:H6    | 1:9:A:DT:H5''  | 10       | 1.43          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 8        | 1.41          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 8        | 1.41          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 10       | 1.4           |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 10       | 1.4           |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 3        | 1.39          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 3        | 1.39          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 7        | 1.39          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 7        | 1.39          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 4        | 1.36          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 4        | 1.36          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 5        | 1.36          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 5        | 1.36          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 9        | 1.36          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 9        | 1.36          |
| (1,230) | 1:7:A:DG:H1    | 1:10:A:DT:H5'  | 1        | 1.35          |
| (1,230) | 1:7:A:DG:H1    | 1:10:A:DT:H5'' | 1        | 1.35          |
| (1,230) | 1:7:A:DG:H1    | 1:10:A:DT:H5'  | 6        | 1.35          |
| (1,230) | 1:7:A:DG:H1    | 1:10:A:DT:H5'' | 6        | 1.35          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5'   | 1        | 1.34          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5''  | 1        | 1.34          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5'   | 6        | 1.34          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5''  | 6        | 1.34          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5'   | 10       | 1.34          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5''  | 10       | 1.34          |
| (1,230) | 1:7:A:DG:H1    | 1:10:A:DT:H5'  | 2        | 1.3           |
| (1,230) | 1:7:A:DG:H1    | 1:10:A:DT:H5'' | 2        | 1.3           |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 2        | 1.27          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 2        | 1.27          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 1        | 1.26          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 1        | 1.26          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'  | 6        | 1.26          |
| (1,349) | 1:10:A:DT:H5'' | 1:11:A:DT:H5'' | 6        | 1.26          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5'   | 8        | 1.26          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5''  | 8        | 1.26          |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 1        | 1.22          |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 1        | 1.22          |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 6        | 1.22          |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 6        | 1.22          |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 1        | 1.22          |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 1        | 1.22          |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 6        | 1.22          |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 6        | 1.22          |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 8        | 1.2           |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 8        | 1.2           |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 10       | 1.2           |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 10       | 1.2           |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 8        | 1.2           |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 8        | 1.2           |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 10       | 1.2           |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 10       | 1.2           |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 2        | 1.19          |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 2        | 1.19          |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 3        | 1.19          |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 3        | 1.19          |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 7        | 1.19          |
| (1,301) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 7        | 1.19          |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 2        | 1.19          |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 2        | 1.19          |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 3        | 1.19          |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 3        | 1.19          |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'  | 7        | 1.19          |
| (1,300) | 1:9:A:DT:H5'   | 1:11:A:DT:H5'' | 7        | 1.19          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5'   | 3        | 1.19          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5''  | 3        | 1.19          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5'   | 7        | 1.19          |
| (1,78)  | 1:2:A:DG:H3'   | 1:4:A:DT:H5''  | 7        | 1.19          |
| (1,455) | 1:13:A:DG:H2'  | 1:14:A:DT:H5'  | 4        | 1.18          |
| (1,455) | 1:13:A:DG:H2'  | 1:14:A:DT:H5'' | 4        | 1.18          |
| (1,455) | 1:13:A:DG:H2'  | 1:14:A:DT:H5'  | 5        | 1.18          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'' | 5        | 1.18          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'  | 9        | 1.18          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'' | 9        | 1.18          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'  | 2        | 1.16          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'' | 2        | 1.16          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'  | 3        | 1.15          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'' | 3        | 1.15          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'  | 7        | 1.15          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'' | 7        | 1.15          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'  | 8        | 1.14          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'' | 8        | 1.14          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'  | 1        | 1.13          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'' | 1        | 1.13          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'  | 6        | 1.13          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'' | 6        | 1.13          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'  | 10       | 1.13          |
| (1,455) | 1:13:A:DG:H2' | 1:14:A:DT:H5'' | 10       | 1.13          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'  | 8        | 1.13          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'' | 8        | 1.13          |
| (1,301) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'  | 4        | 1.11          |
| (1,301) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'' | 4        | 1.11          |
| (1,301) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'  | 5        | 1.11          |
| (1,301) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'' | 5        | 1.11          |
| (1,301) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'  | 9        | 1.11          |
| (1,301) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'' | 9        | 1.11          |
| (1,300) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'  | 4        | 1.11          |
| (1,300) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'' | 4        | 1.11          |
| (1,300) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'  | 5        | 1.11          |
| (1,300) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'' | 5        | 1.11          |
| (1,300) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'  | 9        | 1.11          |
| (1,300) | 1:9:A:DT:H5'  | 1:11:A:DT:H5'' | 9        | 1.11          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'  | 3        | 1.11          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'' | 3        | 1.11          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'  | 7        | 1.11          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'' | 7        | 1.11          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'  | 10       | 1.11          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'' | 10       | 1.11          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'  | 4        | 1.08          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'' | 4        | 1.08          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'  | 5        | 1.08          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'' | 5        | 1.08          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'  | 9        | 1.08          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'' | 9        | 1.08          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'  | 8        | 1.06          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'' | 8        | 1.06          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'  | 10       | 1.06          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'' | 10       | 1.06          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'  | 3        | 1.05          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'' | 3        | 1.05          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'  | 7        | 1.05          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'' | 7        | 1.05          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5'   | 4        | 1.04          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5''  | 4        | 1.04          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5'   | 5        | 1.04          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5''  | 5        | 1.04          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5'   | 9        | 1.04          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5''  | 9        | 1.04          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'  | 1        | 1.01          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'' | 1        | 1.01          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'  | 6        | 1.01          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'' | 6        | 1.01          |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'  | 2        | 1.0           |
| (1,348) | 1:10:A:DT:H5' | 1:11:A:DT:H5'' | 2        | 1.0           |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5'   | 2        | 1.0           |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5''  | 2        | 1.0           |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5'   | 4        | 1.0           |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5''  | 4        | 1.0           |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5'   | 5        | 1.0           |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5''  | 5        | 1.0           |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5'   | 9        | 1.0           |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5''  | 9        | 1.0           |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5'   | 2        | 0.98          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5''  | 2        | 0.98          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'  | 4        | 0.97          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'' | 4        | 0.97          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'  | 5        | 0.97          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'' | 5        | 0.97          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'  | 9        | 0.97          |
| (1,230) | 1:7:A:DG:H1   | 1:10:A:DT:H5'' | 9        | 0.97          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'  | 2        | 0.95          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'' | 2        | 0.95          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'  | 1        | 0.92          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'' | 1        | 0.92          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'  | 6        | 0.92          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'' | 6        | 0.92          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'  | 8        | 0.92          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'' | 8        | 0.92          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'  | 3        | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'' | 3        | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'  | 4        | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'' | 4        | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'  | 5        | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'' | 5        | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'  | 7        | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'' | 7        | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'  | 9        | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'' | 9        | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'  | 10       | 0.91          |
| (1,525) | 1:15:A:DT:H3  | 1:15:A:DT:H5'' | 10       | 0.91          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'  | 2        | 0.89          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'' | 2        | 0.89          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'  | 1        | 0.88          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'' | 1        | 0.88          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'  | 3        | 0.88          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'' | 3        | 0.88          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'  | 6        | 0.88          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'' | 6        | 0.88          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'  | 7        | 0.88          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'' | 7        | 0.88          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5'   | 8        | 0.88          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5''  | 8        | 0.88          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5'   | 10       | 0.88          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5''  | 10       | 0.88          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'  | 4        | 0.87          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'' | 4        | 0.87          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'  | 5        | 0.87          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'' | 5        | 0.87          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'  | 8        | 0.87          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'' | 8        | 0.87          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'  | 9        | 0.87          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'' | 9        | 0.87          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'  | 10       | 0.87          |
| (1,344) | 1:10:A:DT:H1' | 1:11:A:DT:H5'' | 10       | 0.87          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5'   | 1        | 0.87          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5''  | 1        | 0.87          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5'   | 6        | 0.87          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5''  | 6        | 0.87          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5'   | 3        | 0.86          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5''  | 3        | 0.86          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5'   | 7        | 0.86          |
| (1,156) | 1:5:A:DT:H4'  | 1:5:A:DT:H5''  | 7        | 0.86          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5'   | 2        | 0.79          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5''  | 2        | 0.79          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'  | 3        | 0.77          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'' | 3        | 0.77          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'  | 7        | 0.77          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'' | 7        | 0.77          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'  | 8        | 0.76          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'' | 8        | 0.76          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'  | 10       | 0.76          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'' | 10       | 0.76          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5'   | 1        | 0.76          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5''  | 1        | 0.76          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5'   | 6        | 0.76          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5''  | 6        | 0.76          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'  | 4        | 0.73          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'' | 4        | 0.73          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'  | 5        | 0.73          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'' | 5        | 0.73          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'  | 9        | 0.73          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'' | 9        | 0.73          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5'   | 8        | 0.73          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5''  | 8        | 0.73          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5'   | 8        | 0.73          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5''  | 8        | 0.73          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5'   | 10       | 0.72          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5''  | 10       | 0.72          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5'   | 4        | 0.72          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5''  | 4        | 0.72          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5'   | 5        | 0.72          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5''  | 5        | 0.72          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5'   | 9        | 0.72          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5''  | 9        | 0.72          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5'   | 4        | 0.71          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5''  | 4        | 0.71          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5'   | 5        | 0.71          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5''  | 5        | 0.71          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5'   | 9        | 0.71          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5''  | 9        | 0.71          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5'   | 1        | 0.71          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5''  | 1        | 0.71          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5'   | 6        | 0.71          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5''  | 6        | 0.71          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5'   | 10       | 0.71          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5''  | 10       | 0.71          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5'   | 3        | 0.69          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5''  | 3        | 0.69          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5'   | 7        | 0.69          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5''  | 7        | 0.69          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5'   | 2        | 0.68          |
| (1,308) | 1:9:A:DT:H1'  | 1:8:A:DT:H5''  | 2        | 0.68          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5'   | 3        | 0.68          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5''  | 3        | 0.68          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5'   | 7        | 0.68          |
| (1,75)  | 1:2:A:DG:H8   | 1:4:A:DT:H5''  | 7        | 0.68          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'  | 2        | 0.62          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'' | 2        | 0.62          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'  | 1        | 0.61          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'' | 1        | 0.61          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'  | 6        | 0.61          |
| (1,345) | 1:10:A:DT:H3' | 1:11:A:DT:H5'' | 6        | 0.61          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5'   | 1        | 0.61          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5''  | 1        | 0.61          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5'   | 6        | 0.61          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5''  | 6        | 0.61          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5'   | 10       | 0.6           |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5''  | 10       | 0.6           |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5'   | 1        | 0.58          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5''  | 1        | 0.58          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5'   | 6        | 0.58          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5''  | 6        | 0.58          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5'   | 8        | 0.57          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5''  | 8        | 0.57          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5'   | 2        | 0.56          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5''  | 2        | 0.56          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5'   | 10       | 0.56          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5''  | 10       | 0.56          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5'   | 4        | 0.55          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5''  | 4        | 0.55          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5'   | 5        | 0.55          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5''  | 5        | 0.55          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5'   | 9        | 0.55          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5''  | 9        | 0.55          |
| (1,374) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 1        | 0.54          |
| (1,374) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 2        | 0.54          |
| (1,374) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 6        | 0.54          |
| (1,373) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 1        | 0.54          |
| (1,373) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 2        | 0.54          |
| (1,373) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 6        | 0.54          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5'   | 3        | 0.54          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5''  | 3        | 0.54          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5'   | 7        | 0.54          |
| (1,306) | 1:9:A:DT:H3   | 1:9:A:DT:H5''  | 7        | 0.54          |
| (1,374) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 3        | 0.53          |
| (1,374) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 4        | 0.53          |
| (1,374) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 5        | 0.53          |
| (1,374) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 7        | 0.53          |
| (1,374) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 8        | 0.53          |
| (1,374) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 9        | 0.53          |
| (1,374) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 10       | 0.53          |
| (1,373) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 3        | 0.53          |
| (1,373) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 4        | 0.53          |
| (1,373) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 5        | 0.53          |
| (1,373) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 7        | 0.53          |
| (1,373) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 8        | 0.53          |
| (1,373) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 9        | 0.53          |
| (1,373) | 1:11:A:DT:H5' | 1:11:A:DT:H5'' | 10       | 0.53          |
| (1,134) | 1:4:A:DT:H2'  | 1:5:A:DT:H5'   | 2        | 0.53          |
| (1,134) | 1:4:A:DT:H2'  | 1:5:A:DT:H5''  | 2        | 0.53          |
| (1,135) | 1:4:A:DT:H2'' | 1:5:A:DT:H5'   | 2        | 0.51          |
| (1,135) | 1:4:A:DT:H2'' | 1:5:A:DT:H5''  | 2        | 0.51          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5'   | 8        | 0.51          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5''  | 8        | 0.51          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'   | 3        | 0.46          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5''  | 3        | 0.46          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'   | 7        | 0.46          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5''  | 7        | 0.46          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5'   | 3        | 0.45          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5''  | 3        | 0.45          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5'   | 7        | 0.45          |
| (1,76)  | 1:2:A:DG:H2'  | 1:4:A:DT:H5''  | 7        | 0.45          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'   | 8        | 0.45          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'' | 8        | 0.45          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'  | 1        | 0.4           |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'' | 1        | 0.4           |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'  | 6        | 0.4           |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'' | 6        | 0.4           |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'  | 1        | 0.4           |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'' | 1        | 0.4           |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'  | 6        | 0.4           |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'' | 6        | 0.4           |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'  | 8        | 0.39          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'' | 8        | 0.39          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'  | 8        | 0.38          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'' | 8        | 0.38          |
| (1,135) | 1:4:A:DT:H2'' | 1:5:A:DT:H5'  | 4        | 0.38          |
| (1,135) | 1:4:A:DT:H2'' | 1:5:A:DT:H5'' | 4        | 0.38          |
| (1,135) | 1:4:A:DT:H2'' | 1:5:A:DT:H5'  | 5        | 0.38          |
| (1,135) | 1:4:A:DT:H2'' | 1:5:A:DT:H5'' | 5        | 0.38          |
| (1,135) | 1:4:A:DT:H2'' | 1:5:A:DT:H5'  | 9        | 0.38          |
| (1,135) | 1:4:A:DT:H2'' | 1:5:A:DT:H5'' | 9        | 0.38          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'  | 10       | 0.37          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'' | 10       | 0.37          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'  | 10       | 0.37          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'' | 10       | 0.37          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'  | 3        | 0.37          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'' | 3        | 0.37          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'  | 7        | 0.37          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'' | 7        | 0.37          |
| (1,134) | 1:4:A:DT:H2'  | 1:5:A:DT:H5'  | 4        | 0.36          |
| (1,134) | 1:4:A:DT:H2'  | 1:5:A:DT:H5'' | 4        | 0.36          |
| (1,134) | 1:4:A:DT:H2'  | 1:5:A:DT:H5'  | 5        | 0.36          |
| (1,134) | 1:4:A:DT:H2'  | 1:5:A:DT:H5'' | 5        | 0.36          |
| (1,134) | 1:4:A:DT:H2'  | 1:5:A:DT:H5'  | 9        | 0.36          |
| (1,134) | 1:4:A:DT:H2'  | 1:5:A:DT:H5'' | 9        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'  | 1        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'' | 1        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'  | 2        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'' | 2        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'  | 4        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'' | 4        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'  | 5        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'' | 5        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'  | 6        | 0.36          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'' | 6        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'  | 8        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'' | 8        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'  | 9        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'' | 9        | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'  | 10       | 0.36          |
| (1,119) | 1:4:A:DT:H4'  | 1:4:A:DT:H5'' | 10       | 0.36          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'  | 4        | 0.36          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'' | 4        | 0.36          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'  | 5        | 0.36          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'' | 5        | 0.36          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'  | 9        | 0.36          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'' | 9        | 0.36          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'  | 3        | 0.33          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'' | 3        | 0.33          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'  | 4        | 0.33          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'' | 4        | 0.33          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'  | 5        | 0.33          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'' | 5        | 0.33          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'  | 7        | 0.33          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'' | 7        | 0.33          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'  | 9        | 0.33          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'' | 9        | 0.33          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5'  | 2        | 0.33          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5'' | 2        | 0.33          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5'  | 2        | 0.33          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5'' | 2        | 0.33          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'  | 2        | 0.32          |
| (1,265) | 1:8:A:DT:H3   | 1:8:A:DT:H5'' | 2        | 0.32          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'  | 4        | 0.29          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'' | 4        | 0.29          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'  | 5        | 0.29          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'' | 5        | 0.29          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'  | 9        | 0.29          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'' | 9        | 0.29          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'  | 3        | 0.28          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'' | 3        | 0.28          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'  | 7        | 0.28          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'' | 7        | 0.28          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'  | 1        | 0.28          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'' | 1        | 0.28          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'  | 6        | 0.28          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5''  | 6        | 0.28          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'   | 10       | 0.28          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5''  | 10       | 0.28          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5'   | 4        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5''  | 4        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5'   | 4        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5''  | 4        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5'   | 5        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5''  | 5        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5'   | 5        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5''  | 5        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5'   | 9        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5''  | 9        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5'   | 9        | 0.27          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5''  | 9        | 0.27          |
| (1,262) | 1:8:A:DT:H3'  | 1:9:A:DT:H5'   | 4        | 0.22          |
| (1,262) | 1:8:A:DT:H3'  | 1:9:A:DT:H5''  | 4        | 0.22          |
| (1,262) | 1:8:A:DT:H3'  | 1:9:A:DT:H5'   | 5        | 0.22          |
| (1,262) | 1:8:A:DT:H3'  | 1:9:A:DT:H5''  | 5        | 0.22          |
| (1,262) | 1:8:A:DT:H3'  | 1:9:A:DT:H5'   | 9        | 0.22          |
| (1,262) | 1:8:A:DT:H3'  | 1:9:A:DT:H5''  | 9        | 0.22          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5'   | 2        | 0.21          |
| (1,68)  | 1:2:A:DG:H3'  | 1:3:A:DT:H5''  | 2        | 0.21          |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5'   | 2        | 0.2           |
| (1,220) | 1:7:A:DG:H2'  | 1:8:A:DT:H5''  | 2        | 0.2           |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5'   | 10       | 0.2           |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5''  | 10       | 0.2           |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5'   | 10       | 0.2           |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5''  | 10       | 0.2           |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5'   | 1        | 0.19          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5''  | 1        | 0.19          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5'   | 1        | 0.19          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5''  | 1        | 0.19          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5'   | 6        | 0.19          |
| (1,99)  | 1:3:A:DT:H5'  | 1:4:A:DT:H5''  | 6        | 0.19          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5'   | 6        | 0.19          |
| (1,99)  | 1:3:A:DT:H5'' | 1:4:A:DT:H5''  | 6        | 0.19          |
| (1,262) | 1:8:A:DT:H3'  | 1:9:A:DT:H5'   | 10       | 0.17          |
| (1,262) | 1:8:A:DT:H3'  | 1:9:A:DT:H5''  | 10       | 0.17          |
| (1,601) | 1:17:A:DG:H21 | 1:14:A:DT:H2'' | 3        | 0.16          |
| (1,601) | 1:17:A:DG:H21 | 1:14:A:DT:H2'' | 4        | 0.16          |
| (1,601) | 1:17:A:DG:H21 | 1:14:A:DT:H2'' | 5        | 0.16          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,601) | 1:17:A:DG:H21  | 1:14:A:DT:H2'' | 7        | 0.16          |
| (1,601) | 1:17:A:DG:H21  | 1:14:A:DT:H2'' | 8        | 0.16          |
| (1,601) | 1:17:A:DG:H21  | 1:14:A:DT:H2'' | 9        | 0.16          |
| (1,601) | 1:17:A:DG:H21  | 1:14:A:DT:H2'' | 10       | 0.16          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'  | 4        | 0.16          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'' | 4        | 0.16          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'  | 5        | 0.16          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'' | 5        | 0.16          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'  | 9        | 0.16          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'' | 9        | 0.16          |
| (1,181) | 1:6:A:DG:H5'   | 1:6:A:DG:H2''  | 10       | 0.16          |
| (1,601) | 1:17:A:DG:H21  | 1:14:A:DT:H2'' | 1        | 0.15          |
| (1,601) | 1:17:A:DG:H21  | 1:14:A:DT:H2'' | 2        | 0.15          |
| (1,601) | 1:17:A:DG:H21  | 1:14:A:DT:H2'' | 6        | 0.15          |
| (1,413) | 1:12:A:DG:H8   | 1:12:A:DG:H3'  | 3        | 0.15          |
| (1,413) | 1:12:A:DG:H8   | 1:12:A:DG:H3'  | 4        | 0.15          |
| (1,413) | 1:12:A:DG:H8   | 1:12:A:DG:H3'  | 5        | 0.15          |
| (1,413) | 1:12:A:DG:H8   | 1:12:A:DG:H3'  | 7        | 0.15          |
| (1,413) | 1:12:A:DG:H8   | 1:12:A:DG:H3'  | 9        | 0.15          |
| (1,372) | 1:11:A:DT:H5'  | 1:11:A:DT:H2'' | 1        | 0.15          |
| (1,372) | 1:11:A:DT:H5'  | 1:11:A:DT:H2'' | 2        | 0.15          |
| (1,372) | 1:11:A:DT:H5'  | 1:11:A:DT:H2'' | 6        | 0.15          |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5'   | 3        | 0.15          |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5''  | 3        | 0.15          |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5'   | 7        | 0.15          |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5''  | 7        | 0.15          |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5'   | 8        | 0.15          |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5''  | 8        | 0.15          |
| (1,181) | 1:6:A:DG:H5'   | 1:6:A:DG:H2''  | 1        | 0.15          |
| (1,181) | 1:6:A:DG:H5'   | 1:6:A:DG:H2''  | 6        | 0.15          |
| (1,181) | 1:6:A:DG:H5'   | 1:6:A:DG:H2''  | 8        | 0.15          |
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 3        | 0.14          |
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 7        | 0.14          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'  | 3        | 0.14          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'' | 3        | 0.14          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'  | 7        | 0.14          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'' | 7        | 0.14          |
| (1,413) | 1:12:A:DG:H8   | 1:12:A:DG:H3'  | 8        | 0.14          |
| (1,413) | 1:12:A:DG:H8   | 1:12:A:DG:H3'  | 10       | 0.14          |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 2        | 0.14          |
| (1,618) | 1:18:A:DG:H1   | 1:7:A:DG:H8    | 8        | 0.13          |
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 8        | 0.13          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 10       | 0.13          |
| (1,487) | 1:14:A:DT:H6   | 1:15:A:DT:H1'  | 2        | 0.13          |
| (1,487) | 1:14:A:DT:H6   | 1:15:A:DT:H1'  | 3        | 0.13          |
| (1,487) | 1:14:A:DT:H6   | 1:15:A:DT:H1'  | 7        | 0.13          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'  | 2        | 0.13          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'' | 2        | 0.13          |
| (1,219) | 1:7:A:DG:H1'   | 1:8:A:DT:H1'   | 1        | 0.13          |
| (1,219) | 1:7:A:DG:H1'   | 1:8:A:DT:H1'   | 6        | 0.13          |
| (1,219) | 1:7:A:DG:H1'   | 1:8:A:DT:H1'   | 8        | 0.13          |
| (1,181) | 1:6:A:DG:H5'   | 1:6:A:DG:H2''  | 2        | 0.13          |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 1        | 0.13          |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 3        | 0.13          |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 4        | 0.13          |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 5        | 0.13          |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 6        | 0.13          |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 7        | 0.13          |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 8        | 0.13          |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 9        | 0.13          |
| (1,167) | 1:5:A:DT:H3    | 1:16:A:DT:H3   | 10       | 0.13          |
| (1,90)  | 1:3:A:DT:H6    | 1:3:A:DT:H2''  | 1        | 0.13          |
| (1,90)  | 1:3:A:DT:H6    | 1:3:A:DT:H2''  | 2        | 0.13          |
| (1,90)  | 1:3:A:DT:H6    | 1:3:A:DT:H2''  | 3        | 0.13          |
| (1,90)  | 1:3:A:DT:H6    | 1:3:A:DT:H2''  | 6        | 0.13          |
| (1,90)  | 1:3:A:DT:H6    | 1:3:A:DT:H2''  | 7        | 0.13          |
| (1,90)  | 1:3:A:DT:H6    | 1:3:A:DT:H2''  | 10       | 0.13          |
| (1,87)  | 1:3:A:DT:H5''  | 1:3:A:DT:H2''  | 3        | 0.13          |
| (1,87)  | 1:3:A:DT:H5''  | 1:3:A:DT:H2''  | 7        | 0.13          |
| (1,87)  | 1:3:A:DT:H5''  | 1:3:A:DT:H2''  | 8        | 0.13          |
| (1,618) | 1:18:A:DG:H1   | 1:7:A:DG:H8    | 3        | 0.12          |
| (1,618) | 1:18:A:DG:H1   | 1:7:A:DG:H8    | 7        | 0.12          |
| (1,618) | 1:18:A:DG:H1   | 1:7:A:DG:H8    | 10       | 0.12          |
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 1        | 0.12          |
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 2        | 0.12          |
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 4        | 0.12          |
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 5        | 0.12          |
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 6        | 0.12          |
| (1,612) | 1:18:A:DG:H8   | 1:17:A:DG:H4'  | 9        | 0.12          |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 3        | 0.12          |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 7        | 0.12          |
| (1,487) | 1:14:A:DT:H6   | 1:15:A:DT:H1'  | 1        | 0.12          |
| (1,487) | 1:14:A:DT:H6   | 1:15:A:DT:H1'  | 4        | 0.12          |
| (1,487) | 1:14:A:DT:H6   | 1:15:A:DT:H1'  | 5        | 0.12          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,487) | 1:14:A:DT:H6  | 1:15:A:DT:H1' | 6        | 0.12          |
| (1,487) | 1:14:A:DT:H6  | 1:15:A:DT:H1' | 8        | 0.12          |
| (1,487) | 1:14:A:DT:H6  | 1:15:A:DT:H1' | 9        | 0.12          |
| (1,487) | 1:14:A:DT:H6  | 1:15:A:DT:H1' | 10       | 0.12          |
| (1,413) | 1:12:A:DG:H8  | 1:12:A:DG:H3' | 1        | 0.12          |
| (1,413) | 1:12:A:DG:H8  | 1:12:A:DG:H3' | 2        | 0.12          |
| (1,413) | 1:12:A:DG:H8  | 1:12:A:DG:H3' | 6        | 0.12          |
| (1,254) | 1:8:A:DT:H6   | 1:8:A:DT:H4'  | 3        | 0.12          |
| (1,254) | 1:8:A:DT:H6   | 1:8:A:DT:H4'  | 4        | 0.12          |
| (1,254) | 1:8:A:DT:H6   | 1:8:A:DT:H4'  | 5        | 0.12          |
| (1,254) | 1:8:A:DT:H6   | 1:8:A:DT:H4'  | 7        | 0.12          |
| (1,254) | 1:8:A:DT:H6   | 1:8:A:DT:H4'  | 9        | 0.12          |
| (1,219) | 1:7:A:DG:H1'  | 1:8:A:DT:H1'  | 2        | 0.12          |
| (1,219) | 1:7:A:DG:H1'  | 1:8:A:DT:H1'  | 10       | 0.12          |
| (1,181) | 1:6:A:DG:H5'  | 1:6:A:DG:H2'' | 4        | 0.12          |
| (1,181) | 1:6:A:DG:H5'  | 1:6:A:DG:H2'' | 5        | 0.12          |
| (1,181) | 1:6:A:DG:H5'  | 1:6:A:DG:H2'' | 9        | 0.12          |
| (1,108) | 1:4:A:DT:H1'  | 1:4:A:DT:H5'' | 2        | 0.12          |
| (1,108) | 1:4:A:DT:H1'  | 1:4:A:DT:H5'' | 4        | 0.12          |
| (1,108) | 1:4:A:DT:H1'  | 1:4:A:DT:H5'' | 5        | 0.12          |
| (1,108) | 1:4:A:DT:H1'  | 1:4:A:DT:H5'' | 9        | 0.12          |
| (1,102) | 1:3:A:DT:H6   | 1:15:A:DT:H4' | 1        | 0.12          |
| (1,102) | 1:3:A:DT:H6   | 1:15:A:DT:H4' | 6        | 0.12          |
| (1,90)  | 1:3:A:DT:H6   | 1:3:A:DT:H2'' | 4        | 0.12          |
| (1,90)  | 1:3:A:DT:H6   | 1:3:A:DT:H2'' | 5        | 0.12          |
| (1,90)  | 1:3:A:DT:H6   | 1:3:A:DT:H2'' | 8        | 0.12          |
| (1,90)  | 1:3:A:DT:H6   | 1:3:A:DT:H2'' | 9        | 0.12          |
| (1,87)  | 1:3:A:DT:H5'' | 1:3:A:DT:H2'' | 1        | 0.12          |
| (1,87)  | 1:3:A:DT:H5'' | 1:3:A:DT:H2'' | 2        | 0.12          |
| (1,87)  | 1:3:A:DT:H5'' | 1:3:A:DT:H2'' | 4        | 0.12          |
| (1,87)  | 1:3:A:DT:H5'' | 1:3:A:DT:H2'' | 5        | 0.12          |
| (1,87)  | 1:3:A:DT:H5'' | 1:3:A:DT:H2'' | 6        | 0.12          |
| (1,87)  | 1:3:A:DT:H5'' | 1:3:A:DT:H2'' | 9        | 0.12          |
| (1,87)  | 1:3:A:DT:H5'' | 1:3:A:DT:H2'' | 10       | 0.12          |
| (1,10)  | 1:1:A:DG:H8   | 1:1:A:DG:H3'  | 4        | 0.12          |
| (1,10)  | 1:1:A:DG:H8   | 1:1:A:DG:H3'  | 5        | 0.12          |
| (1,10)  | 1:1:A:DG:H8   | 1:1:A:DG:H3'  | 8        | 0.12          |
| (1,10)  | 1:1:A:DG:H8   | 1:1:A:DG:H3'  | 9        | 0.12          |
| (1,618) | 1:18:A:DG:H1  | 1:7:A:DG:H8   | 1        | 0.11          |
| (1,618) | 1:18:A:DG:H1  | 1:7:A:DG:H8   | 4        | 0.11          |
| (1,618) | 1:18:A:DG:H1  | 1:7:A:DG:H8   | 5        | 0.11          |
| (1,618) | 1:18:A:DG:H1  | 1:7:A:DG:H8   | 6        | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,618) | 1:18:A:DG:H1   | 1:7:A:DG:H8    | 9        | 0.11          |
| (1,608) | 1:18:A:DG:H8   | 1:17:A:DG:H1'  | 3        | 0.11          |
| (1,608) | 1:18:A:DG:H8   | 1:17:A:DG:H1'  | 7        | 0.11          |
| (1,608) | 1:18:A:DG:H8   | 1:17:A:DG:H1'  | 8        | 0.11          |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 3        | 0.11          |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 4        | 0.11          |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 5        | 0.11          |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 7        | 0.11          |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 8        | 0.11          |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 9        | 0.11          |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 10       | 0.11          |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 1        | 0.11          |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 2        | 0.11          |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 4        | 0.11          |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 5        | 0.11          |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 6        | 0.11          |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 8        | 0.11          |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 9        | 0.11          |
| (1,553) | 1:16:A:DT:H6   | 1:13:A:DG:H1'  | 10       | 0.11          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'  | 10       | 0.11          |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'' | 10       | 0.11          |
| (1,415) | 1:12:A:DG:H8   | 1:12:A:DG:H5'' | 1        | 0.11          |
| (1,415) | 1:12:A:DG:H8   | 1:12:A:DG:H5'' | 2        | 0.11          |
| (1,415) | 1:12:A:DG:H8   | 1:12:A:DG:H5'' | 6        | 0.11          |
| (1,411) | 1:12:A:DG:H8   | 1:12:A:DG:H2'  | 1        | 0.11          |
| (1,411) | 1:12:A:DG:H8   | 1:12:A:DG:H2'  | 2        | 0.11          |
| (1,411) | 1:12:A:DG:H8   | 1:12:A:DG:H2'  | 6        | 0.11          |
| (1,339) | 1:10:A:DT:H6   | 1:9:A:DT:H3'   | 3        | 0.11          |
| (1,339) | 1:10:A:DT:H6   | 1:9:A:DT:H3'   | 4        | 0.11          |
| (1,339) | 1:10:A:DT:H6   | 1:9:A:DT:H3'   | 5        | 0.11          |
| (1,339) | 1:10:A:DT:H6   | 1:9:A:DT:H3'   | 7        | 0.11          |
| (1,339) | 1:10:A:DT:H6   | 1:9:A:DT:H3'   | 9        | 0.11          |
| (1,296) | 1:9:A:DT:H5'   | 1:10:A:DT:H2'' | 1        | 0.11          |
| (1,296) | 1:9:A:DT:H5'   | 1:10:A:DT:H2'' | 6        | 0.11          |
| (1,296) | 1:9:A:DT:H5'   | 1:10:A:DT:H2'' | 8        | 0.11          |
| (1,296) | 1:9:A:DT:H5'   | 1:10:A:DT:H2'' | 10       | 0.11          |
| (1,254) | 1:8:A:DT:H6    | 1:8:A:DT:H4'   | 8        | 0.11          |
| (1,254) | 1:8:A:DT:H6    | 1:8:A:DT:H4'   | 10       | 0.11          |
| (1,219) | 1:7:A:DG:H1'   | 1:8:A:DT:H1'   | 3        | 0.11          |
| (1,219) | 1:7:A:DG:H1'   | 1:8:A:DT:H1'   | 7        | 0.11          |
| (1,102) | 1:3:A:DT:H6    | 1:15:A:DT:H4'  | 2        | 0.11          |
| (1,102) | 1:3:A:DT:H6    | 1:15:A:DT:H4'  | 10       | 0.11          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,62)  | 1:2:A:DG:H8    | 1:1:A:DG:H2'   | 2        | 0.11          |
| (1,10)  | 1:1:A:DG:H8    | 1:1:A:DG:H3'   | 3        | 0.11          |
| (1,10)  | 1:1:A:DG:H8    | 1:1:A:DG:H3'   | 7        | 0.11          |
| (1,608) | 1:18:A:DG:H8   | 1:17:A:DG:H1'  | 1        | 0.1           |
| (1,608) | 1:18:A:DG:H8   | 1:17:A:DG:H1'  | 4        | 0.1           |
| (1,608) | 1:18:A:DG:H8   | 1:17:A:DG:H1'  | 5        | 0.1           |
| (1,608) | 1:18:A:DG:H8   | 1:17:A:DG:H1'  | 6        | 0.1           |
| (1,608) | 1:18:A:DG:H8   | 1:17:A:DG:H1'  | 9        | 0.1           |
| (1,608) | 1:18:A:DG:H8   | 1:17:A:DG:H1'  | 10       | 0.1           |
| (1,592) | 1:17:A:DG:H1   | 1:17:A:DG:H1'  | 8        | 0.1           |
| (1,587) | 1:17:A:DG:H8   | 1:16:A:DT:H5'  | 10       | 0.1           |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 1        | 0.1           |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 2        | 0.1           |
| (1,586) | 1:17:A:DG:H8   | 1:16:A:DT:H1'  | 6        | 0.1           |
| (1,544) | 1:16:A:DT:H6   | 1:16:A:DT:H2'  | 1        | 0.1           |
| (1,544) | 1:16:A:DT:H6   | 1:16:A:DT:H2'  | 2        | 0.1           |
| (1,544) | 1:16:A:DT:H6   | 1:16:A:DT:H2'  | 6        | 0.1           |
| (1,544) | 1:16:A:DT:H6   | 1:16:A:DT:H2'  | 8        | 0.1           |
| (1,544) | 1:16:A:DT:H6   | 1:16:A:DT:H2'  | 10       | 0.1           |
| (1,495) | 1:14:A:DT:H3   | 1:16:A:DT:H3   | 4        | 0.1           |
| (1,495) | 1:14:A:DT:H3   | 1:16:A:DT:H3   | 5        | 0.1           |
| (1,495) | 1:14:A:DT:H3   | 1:16:A:DT:H3   | 9        | 0.1           |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'  | 8        | 0.1           |
| (1,456) | 1:13:A:DG:H2'' | 1:14:A:DT:H5'' | 8        | 0.1           |
| (1,339) | 1:10:A:DT:H6   | 1:9:A:DT:H3'   | 2        | 0.1           |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5'   | 1        | 0.1           |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5''  | 1        | 0.1           |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5'   | 6        | 0.1           |
| (1,262) | 1:8:A:DT:H3'   | 1:9:A:DT:H5''  | 6        | 0.1           |
| (1,254) | 1:8:A:DT:H6    | 1:8:A:DT:H4'   | 1        | 0.1           |
| (1,254) | 1:8:A:DT:H6    | 1:8:A:DT:H4'   | 2        | 0.1           |
| (1,254) | 1:8:A:DT:H6    | 1:8:A:DT:H4'   | 6        | 0.1           |
| (1,219) | 1:7:A:DG:H1'   | 1:8:A:DT:H1'   | 4        | 0.1           |
| (1,219) | 1:7:A:DG:H1'   | 1:8:A:DT:H1'   | 5        | 0.1           |
| (1,219) | 1:7:A:DG:H1'   | 1:8:A:DT:H1'   | 9        | 0.1           |
| (1,217) | 1:7:A:DG:H8    | 1:6:A:DG:H4'   | 1        | 0.1           |
| (1,217) | 1:7:A:DG:H8    | 1:6:A:DG:H4'   | 6        | 0.1           |
| (1,217) | 1:7:A:DG:H8    | 1:6:A:DG:H4'   | 10       | 0.1           |
| (1,108) | 1:4:A:DT:H1'   | 1:4:A:DT:H5''  | 3        | 0.1           |
| (1,108) | 1:4:A:DT:H1'   | 1:4:A:DT:H5''  | 7        | 0.1           |
| (1,62)  | 1:2:A:DG:H8    | 1:1:A:DG:H2'   | 1        | 0.1           |
| (1,62)  | 1:2:A:DG:H8    | 1:1:A:DG:H2'   | 6        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found