



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 01:08 AM UTC

PDB ID : 7YVW / pdb_00007yvw
BMRB ID : 36507
Title : NMR determination of the 2:1 binding motif structure involving cytosine flipping out for the recognition of the CGG/CGG triad DNA
Authors : Furuita, K.; Yamada, T.; Sakurabayashi, S.; Nomura, M.; Kojima, C.; Nakatani, K.
Deposited on : 2022-08-19

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

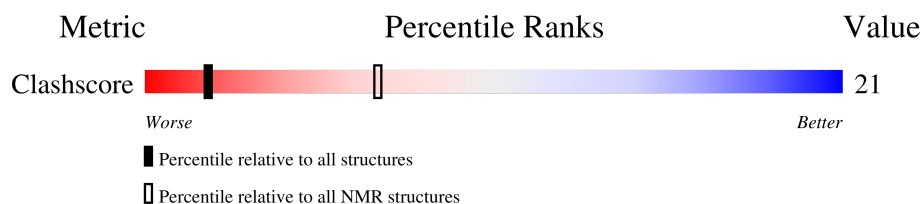
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

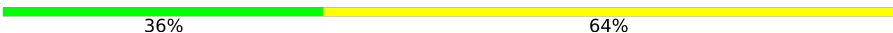
The overall completeness of chemical shifts assignment is 36%.

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 (#Entries)	NMR archive (#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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	11	 18% 82%
2	B	11	 36% 64%

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 832 atoms, of which 310 are hydrogens and 0 are deuteriums.

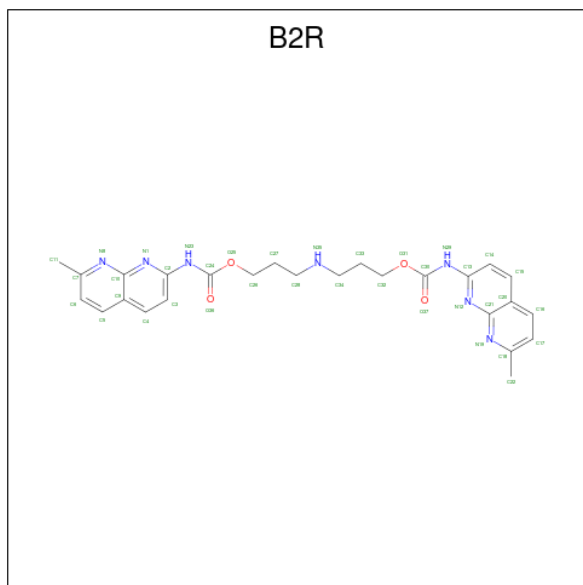
- Molecule 1 is a DNA chain called DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	11	350	108	125	45	62	10	0

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	11	350	108	127	39	66	10	0

- Molecule 3 is 3-[3-[(7-methyl-1,8-naphthyridin-2-yl)carbamoyloxy]propylamino]propyl {N}-(7-methyl-1,8-naphthyridin-2-yl)carbamate (CCD ID: B2R) (formula: C₂₆H₂₉N₇O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
3	A	1	66	26	29	7	4
3	A	1	66	26	29	7	4

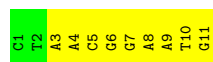
4 Residue-property plots

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.

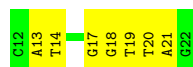
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A: 



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B: 

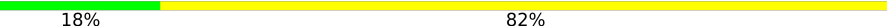


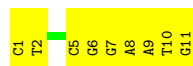
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

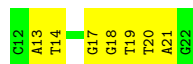
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A: 



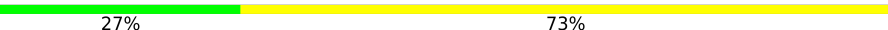
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

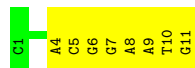
Chain B: 



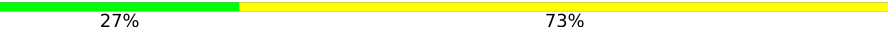
4.2.2 Score per residue for model 2

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

Chain A:  27% 73%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B:  27% 73%



4.2.3 Score per residue for model 3

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

Chain A:  27% 73%



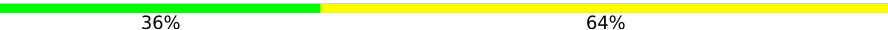
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

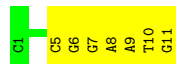
Chain B:  27% 73%



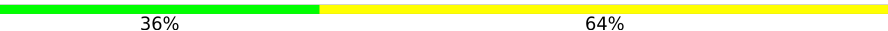
4.2.4 Score per residue for model 4

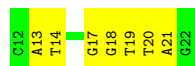
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  36% 64%



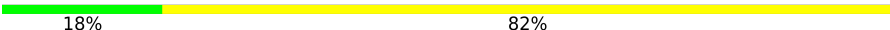
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

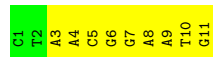
Chain B:  36% 64%



4.2.5 Score per residue for model 5

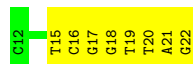
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  18% 82%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

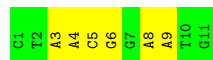
Chain B:  27% 73%



4.2.6 Score per residue for model 6

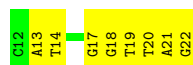
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  45% 55%



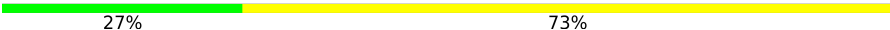
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B:  27% 73%



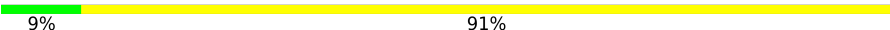
4.2.7 Score per residue for model 7

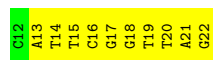
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  27% 73%



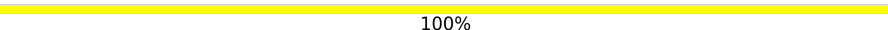
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B:  9% 91%



4.2.8 Score per residue for model 8

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

Chain A:  100%

G1
T2
A3
A4
C5
G6
G7
A8
A9
T10
G11

- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B:  27% 73%

G12
A13
T14
T15
C16
G17
G18
T19
T20
A21
G22

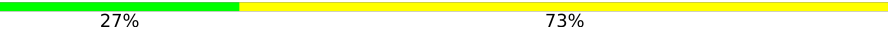
4.2.9 Score per residue for model 9

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

Chain A:  18% 82%

G1
T2
A3
A4
C5
G6
G7
A8
A9
T10
G11

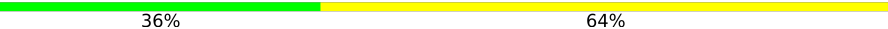
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B:  27% 73%

G12
A13
T14
T15
C16
G17
G18
T19
T20
A21
G22

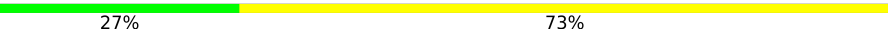
4.2.10 Score per residue for model 10

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

Chain A:  36% 64%

G1
C5
G6
G7
A8
A9
T10
G11

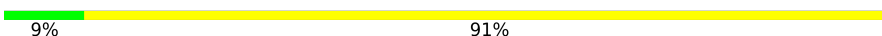
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B:  27% 73%

G12
A13
T14
T15
C16
G17
G18
T19
T20
A21
G22

4.2.11 Score per residue for model 11

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

Chain A:  9% 91%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

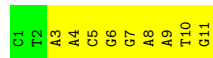
Chain B:  27% 73%



4.2.12 Score per residue for model 12

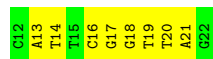
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  18% 82%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B:  27% 73%



4.2.13 Score per residue for model 13

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

Chain A:  27% 73%



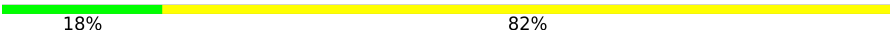
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

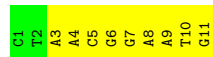
Chain B:  36% 64%



4.2.14 Score per residue for model 14

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

Chain A:  18% 82%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

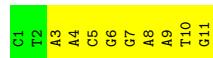
Chain B:  18% 82%



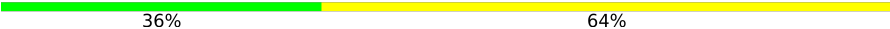
4.2.15 Score per residue for model 15

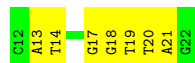
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  18% 82%



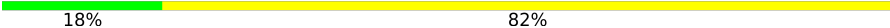
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

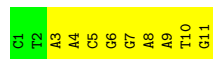
Chain B:  36% 64%



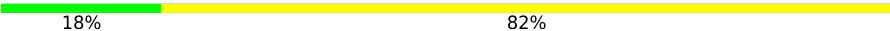
4.2.16 Score per residue for model 16

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

Chain A:  18% 82%



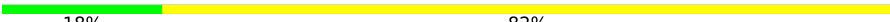
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

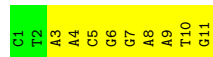
Chain B:  18% 82%



4.2.17 Score per residue for model 17

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

Chain A:  18% 82%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

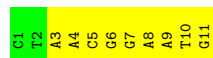
Chain B:  18% 82%



4.2.18 Score per residue for model 18

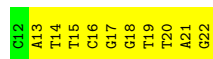
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  18% 82%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

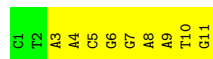
Chain B:  9% 91%



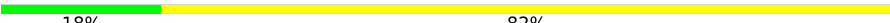
4.2.19 Score per residue for model 19

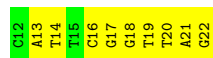
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  18% 82%



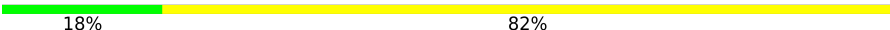
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

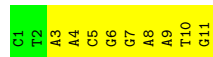
Chain B:  18% 82%



4.2.20 Score per residue for model 20

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

Chain A:  18% 82%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

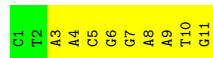
Chain B:  18% 82%



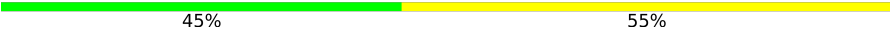
4.2.21 Score per residue for model 21

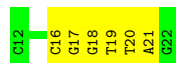
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  18% 82%



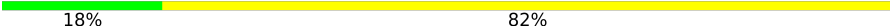
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

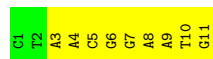
Chain B:  45% 55%



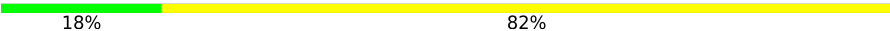
4.2.22 Score per residue for model 22

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

Chain A:  18% 82%



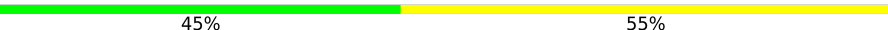
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

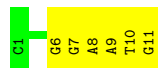
Chain B:  18% 82%



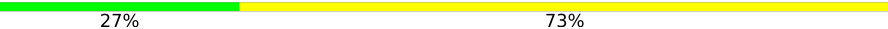
4.2.23 Score per residue for model 23

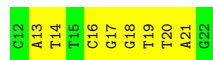
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  45% 55%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

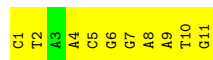
Chain B:  27% 73%



4.2.24 Score per residue for model 24

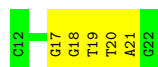
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  9% 91%



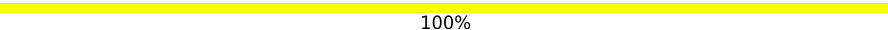
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

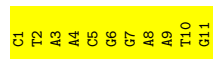
Chain B:  55% 45%



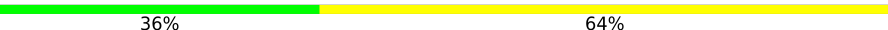
4.2.25 Score per residue for model 25

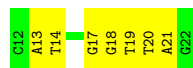
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  100%



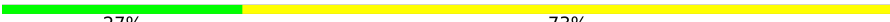
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B:  36% 64%



4.2.26 Score per residue for model 26

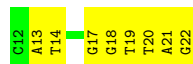
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  27% 73%



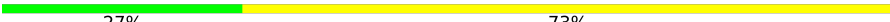
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

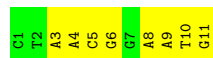
Chain B:  27% 73%



4.2.27 Score per residue for model 27

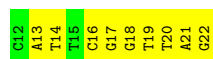
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  27% 73%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B:  18% 82%



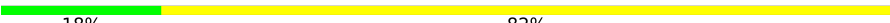
4.2.28 Score per residue for model 28

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

Chain A:  27% 73%



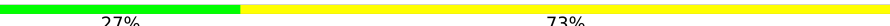
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

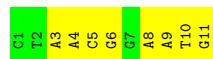
Chain B:  18% 82%



4.2.29 Score per residue for model 29

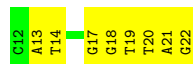
- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*CP*GP*GP*AP*AP*TP*G)-3')

Chain A:  27% 73%



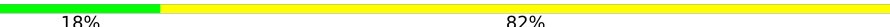
- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

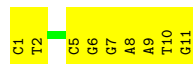
Chain B:  27% 73%



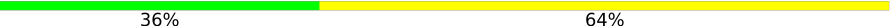
4.2.30 Score per residue for model 30

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

Chain A:  18% 82%



- Molecule 2: DNA (5'-D(*CP*AP*TP*TP*CP*GP*GP*TP*TP*AP*G)-3')

Chain B:  36% 64%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 30 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
CNS	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	174
Number of shifts mapped to atoms	174
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	36%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B2R

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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	225	125	125	8±2
2	B	223	127	127	8±2
3	A	74	58	0	1±1
All	All	15660	9300	7560	479

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 21.

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:DC:H2''	1:A:6:DG:OP2	0.83	1.71	4	8
2:B:15:DT:H3'	2:B:16:DC:H5''	0.73	1.59	5	1
2:B:18:DG:C2'	2:B:19:DT:H71	0.72	2.14	13	6
1:A:4:DA:O3'	1:A:5:DC:H2'	0.70	1.87	13	4
2:B:16:DC:OP1	2:B:16:DC:H4'	0.70	1.87	5	1
2:B:18:DG:H2'	2:B:19:DT:H71	0.69	1.64	24	6
1:A:5:DC:H4'	1:A:6:DG:OP1	0.69	1.87	10	16
1:A:5:DC:C4'	1:A:6:DG:H5'	0.68	2.19	14	12
1:A:5:DC:H4'	1:A:6:DG:H5'	0.68	1.66	14	10
2:B:18:DG:H2'	2:B:19:DT:H72	0.67	1.65	26	24

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:19:DT:C2'	2:B:20:DT:H71	0.60	2.27	3	1
2:B:17:DG:OP2	2:B:17:DG:H8	0.59	1.81	6	24
2:B:18:DG:C8	2:B:19:DT:H72	0.59	2.33	12	12
1:A:4:DA:H2''	1:A:5:DC:OP1	0.58	1.97	2	1
3:A:101:B2R:O36	2:B:16:DC:H1'	0.58	1.99	18	6
1:A:5:DC:OP1	1:A:5:DC:H6	0.58	1.82	6	3
1:A:5:DC:O5'	1:A:5:DC:H6	0.57	1.82	1	8
2:B:17:DG:H2''	2:B:18:DG:OP2	0.56	2.00	5	29
1:A:6:DG:OP2	1:A:6:DG:H8	0.55	1.85	2	5
2:B:17:DG:H8	2:B:17:DG:OP2	0.55	1.85	19	1
1:A:6:DG:O5'	1:A:6:DG:H8	0.55	1.84	10	2
1:A:5:DC:O4'	1:A:6:DG:H5'	0.55	2.01	28	8
2:B:18:DG:C2'	2:B:19:DT:H72	0.53	2.33	26	10
1:A:6:DG:H2''	1:A:7:DG:OP2	0.53	2.03	4	8
1:A:5:DC:C6	1:A:5:DC:H5''	0.53	2.39	9	1
2:B:15:DT:H3'	2:B:16:DC:C5'	0.52	2.33	5	1
1:A:5:DC:H5''	1:A:5:DC:H6	0.52	1.64	9	1
1:A:5:DC:H1'	1:A:6:DG:O4'	0.52	2.04	26	4
1:A:6:DG:H2''	1:A:7:DG:C8	0.52	2.40	22	8
2:B:19:DT:H2''	2:B:20:DT:H71	0.51	1.80	3	1
2:B:16:DC:H6	2:B:16:DC:H5''	0.50	1.65	27	1
1:A:4:DA:H2''	3:A:101:B2R:C15	0.50	2.36	25	7
1:A:6:DG:O5'	1:A:6:DG:C8	0.49	2.65	10	1
1:A:3:DA:H2''	1:A:4:DA:OP2	0.49	2.07	13	22
1:A:5:DC:OP1	1:A:5:DC:H4'	0.49	2.08	2	1
2:B:20:DT:H2''	2:B:21:DA:OP2	0.48	2.08	8	30
2:B:19:DT:C6	2:B:20:DT:H72	0.48	2.43	10	3
1:A:7:DG:H2''	1:A:8:DA:OP2	0.48	2.08	10	20
2:B:18:DG:H2''	2:B:19:DT:C6	0.48	2.43	26	5
3:A:102:B2R:O37	2:B:15:DT:H72	0.48	2.08	20	3
1:A:5:DC:H6	1:A:5:DC:O5'	0.48	1.91	19	1
2:B:16:DC:H2''	2:B:17:DG:OP2	0.47	2.09	3	2
1:A:6:DG:P	1:A:6:DG:H8	0.47	2.32	12	4
2:B:18:DG:C2'	2:B:19:DT:C7	0.46	2.94	18	8
2:B:16:DC:O2	2:B:16:DC:O4'	0.46	2.34	21	6
2:B:21:DA:H2''	2:B:22:DG:O5'	0.46	2.09	19	14
2:B:18:DG:H8	2:B:18:DG:O5'	0.45	1.95	4	2
1:A:8:DA:H2''	1:A:9:DA:OP2	0.45	2.12	10	30
2:B:17:DG:OP2	2:B:17:DG:C8	0.45	2.68	8	7
2:B:14:DT:H2''	2:B:15:DT:OP2	0.45	2.12	7	11
2:B:16:DC:O5'	2:B:16:DC:H6	0.44	1.95	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:18:DG:H2''	2:B:19:DT:H71	0.44	1.85	13	1
2:B:16:DC:H5''	2:B:16:DC:C6	0.44	2.46	27	1
1:A:5:DC:OP1	1:A:5:DC:C6	0.44	2.68	6	3
1:A:10:DT:H2''	1:A:11:DG:OP2	0.43	2.13	2	28
3:A:101:B2R:C14	3:A:102:B2R:O36	0.43	2.67	27	1
1:A:5:DC:H4'	1:A:6:DG:C5'	0.43	2.44	28	1
1:A:6:DG:H22	3:A:101:B2R:C11	0.42	2.27	19	3
1:A:5:DC:O2	1:A:5:DC:O4'	0.42	2.35	24	1
2:B:13:DA:C2'	2:B:14:DT:H71	0.42	2.44	2	24
1:A:1:DC:H2'	1:A:2:DT:H72	0.42	1.92	25	3
1:A:1:DC:H2''	1:A:2:DT:O5'	0.41	2.15	1	5
1:A:4:DA:H2''	1:A:5:DC:H2'	0.41	1.92	28	1
3:A:102:B2R:O37	2:B:15:DT:H71	0.41	2.15	30	1
2:B:16:DC:OP1	2:B:16:DC:C4'	0.41	2.65	5	1
1:A:5:DC:O5'	1:A:5:DC:C6	0.41	2.73	30	1
1:A:6:DG:H8	1:A:6:DG:P	0.41	2.38	18	1
2:B:18:DG:O5'	2:B:18:DG:C8	0.40	2.74	4	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

6.3.3 RNA [i](#)

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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	B2R	A	101	-	40,40,40	1.02±0.02	0±0 (0±0%)
3	B2R	A	102	-	40,40,40	0.94±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	B2R	A	101	-	53,53,53	1.31±0.02	8±1 (14±1%)
3	B2R	A	102	-	53,53,53	1.21±0.02	6±1 (12±1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B2R	A	102	-	-	0±0,20,20,20	0±0,4,4,4
3	B2R	A	101	-	-	0±0,20,20,20	0±0,4,4,4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	101	B2R	C15-C20	2.13	1.37	1.42	28	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	101	B2R	C16-C20	2.01	1.37	1.42	28	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	101	B2R	C16-C20-C21	3.32	120.98	117.86	26	30
3	A	102	B2R	C14-C13-N29	2.88	114.50	123.02	17	30
3	A	101	B2R	O31-C30-N29	2.67	105.17	109.35	23	30
3	A	102	B2R	O31-C30-N29	2.64	105.22	109.35	20	30
3	A	101	B2R	C17-C16-C20	2.62	116.93	120.84	30	30
3	A	101	B2R	O25-C24-N23	2.57	105.32	109.35	9	30
3	A	102	B2R	O25-C24-N23	2.52	105.41	109.35	23	29
3	A	101	B2R	C15-C20-C21	2.44	120.16	117.86	30	20
3	A	102	B2R	C17-C16-C20	2.37	117.30	120.84	14	30
3	A	102	B2R	C3-C2-N23	2.35	116.09	123.02	27	20
3	A	101	B2R	C3-C2-N23	2.34	116.11	123.02	18	17
3	A	101	B2R	C14-C15-C20	2.30	117.41	120.84	17	25
3	A	101	B2R	C3-C4-C9	2.26	117.46	120.84	3	30
3	A	102	B2R	C3-C4-C9	2.25	117.48	120.84	10	26
3	A	102	B2R	C6-C5-C9	2.21	117.55	120.84	12	30
3	A	101	B2R	C14-C13-N29	2.14	116.68	123.02	9	3
3	A	101	B2R	C6-C5-C9	2.09	117.72	120.84	11	10

There are no chirality outliers.

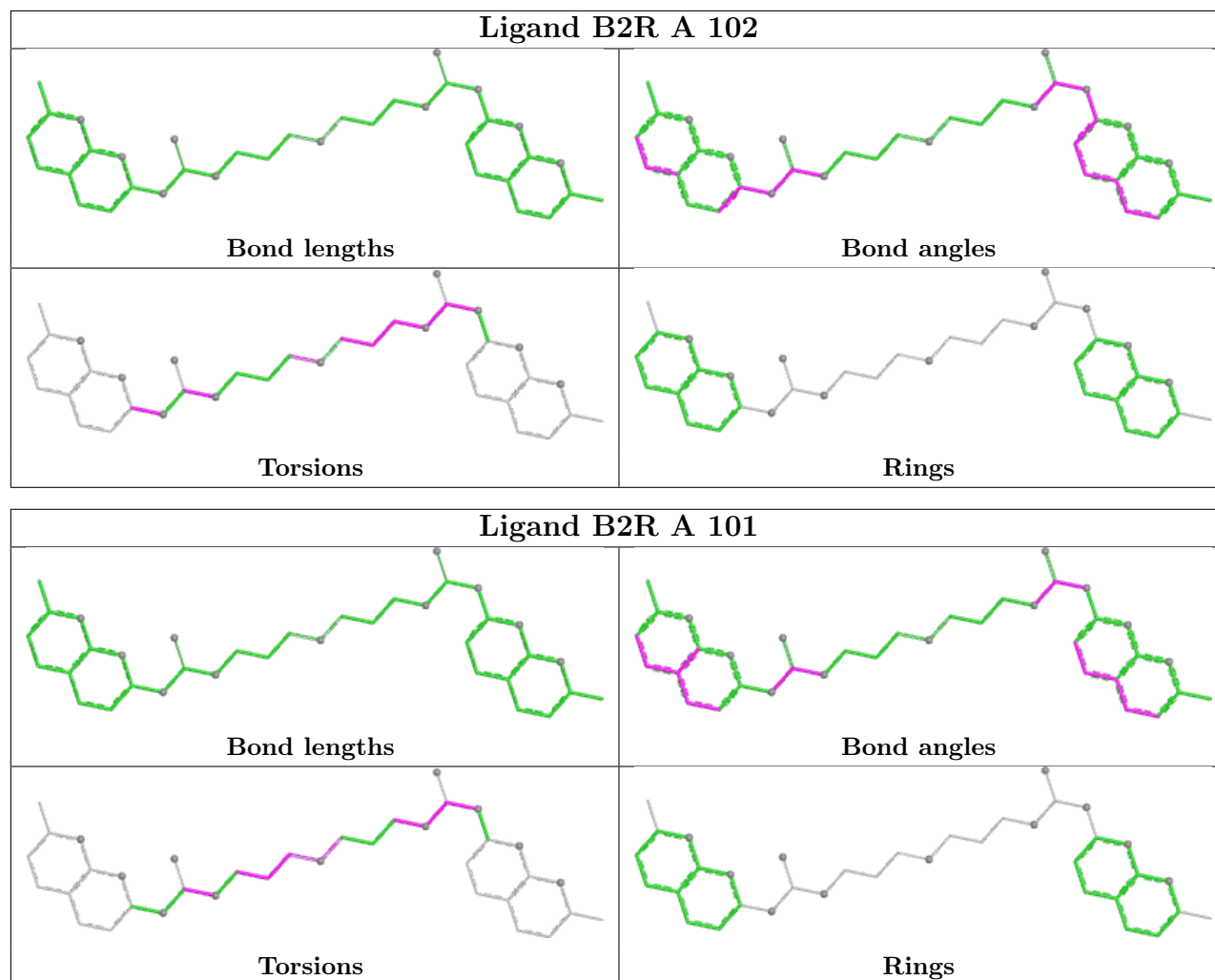
All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
3	A	102	B2R	O36-C24-N23-C2	1

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 36% for the well-defined parts and 36% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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

Total number of shifts	174
Number of shifts mapped to atoms	174
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 36%, i.e. 156 atoms were assigned a chemical shift out of a possible 434. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	100/264 (38%)	100/154 (65%)	0/110 (0%)	0/0 (—%)
Base	56/170 (33%)	56/104 (54%)	0/38 (0%)	0/28 (0%)
Overall	156/434 (36%)	156/258 (60%)	0/148 (0%)	0/28 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 36%, i.e. 156 atoms were assigned a chemical shift out of a possible 434. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	100/264 (38%)	100/154 (65%)	0/110 (0%)	0/0 (—%)
Base	56/170 (33%)	56/104 (54%)	0/38 (0%)	0/28 (0%)
Overall	156/434 (36%)	156/258 (60%)	0/148 (0%)	0/28 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	4	DA	H1'	4.81	4.86 – 7.31	-5.2

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	286
Intra-residue ($ i-j =0$)	137
Sequential ($ i-j =1$)	87
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	4
Hydrogen bond restraints	58
Disulfide bond restraints	0
Total dihedral-angle restraints	177
Number of unmapped restraints	0
Number of restraints per residue	19.3
Number of long range restraints per residue ¹	0.0

¹Long 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)	25.6	0.2
0.2-0.5 (Medium)	23.9	0.5
>0.5 (Large)	17.2	7.9

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	46.9	5.74
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

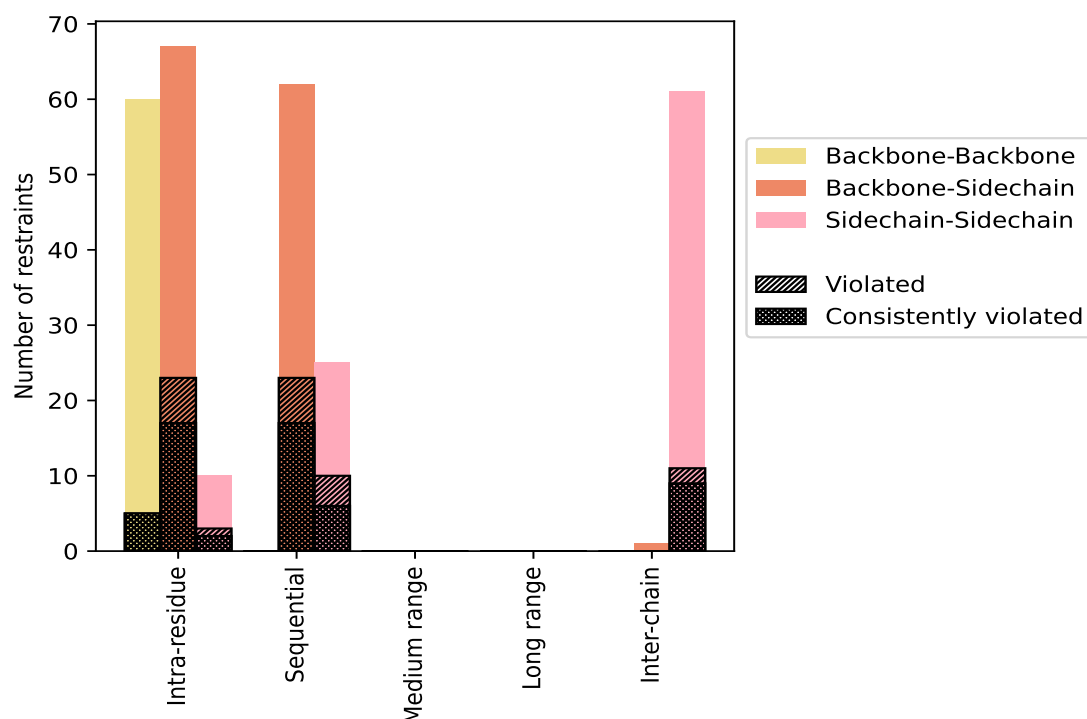
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	137	47.9	31	22.6	10.8	24	17.5	8.4
Backbone-Backbone	60	21.0	5	8.3	1.7	5	8.3	1.7
Backbone-Sidechain	67	23.4	23	34.3	8.0	17	25.4	5.9
Sidechain-Sidechain	10	3.5	3	30.0	1.0	2	20.0	0.7
Sequential (i-j =1)	87	30.4	33	37.9	11.5	23	26.4	8.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	62	21.7	23	37.1	8.0	17	27.4	5.9
Sidechain-Sidechain	25	8.7	10	40.0	3.5	6	24.0	2.1
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
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
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
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
Inter-chain	4	1.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	3	1.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	58	20.3	11	19.0	3.8	9	15.5	3.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	286	100.0	75	26.2	26.2	56	19.6	19.6
Backbone-Backbone	60	21.0	5	8.3	1.7	5	8.3	1.7
Backbone-Sidechain	130	45.5	46	35.4	16.1	34	26.2	11.9
Sidechain-Sidechain	96	33.6	24	25.0	8.4	17	17.7	5.9

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ 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 ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	28	32	0	0	11	71	0.77	6.77	1.57	0.23
2	27	32	0	0	10	69	0.84	7.3	1.7	0.25
3	27	30	0	0	10	67	0.87	7.59	1.8	0.24
4	28	30	0	0	11	69	0.8	6.84	1.57	0.25
5	29	28	0	0	10	67	0.83	6.99	1.62	0.25
6	28	28	0	0	10	66	0.86	7.12	1.72	0.26
7	28	27	0	0	9	64	0.9	7.46	1.81	0.26
8	28	31	0	0	10	69	0.85	7.25	1.7	0.26
9	28	30	0	0	11	69	0.78	7.19	1.55	0.25
10	27	32	0	0	11	70	0.84	7.09	1.73	0.25

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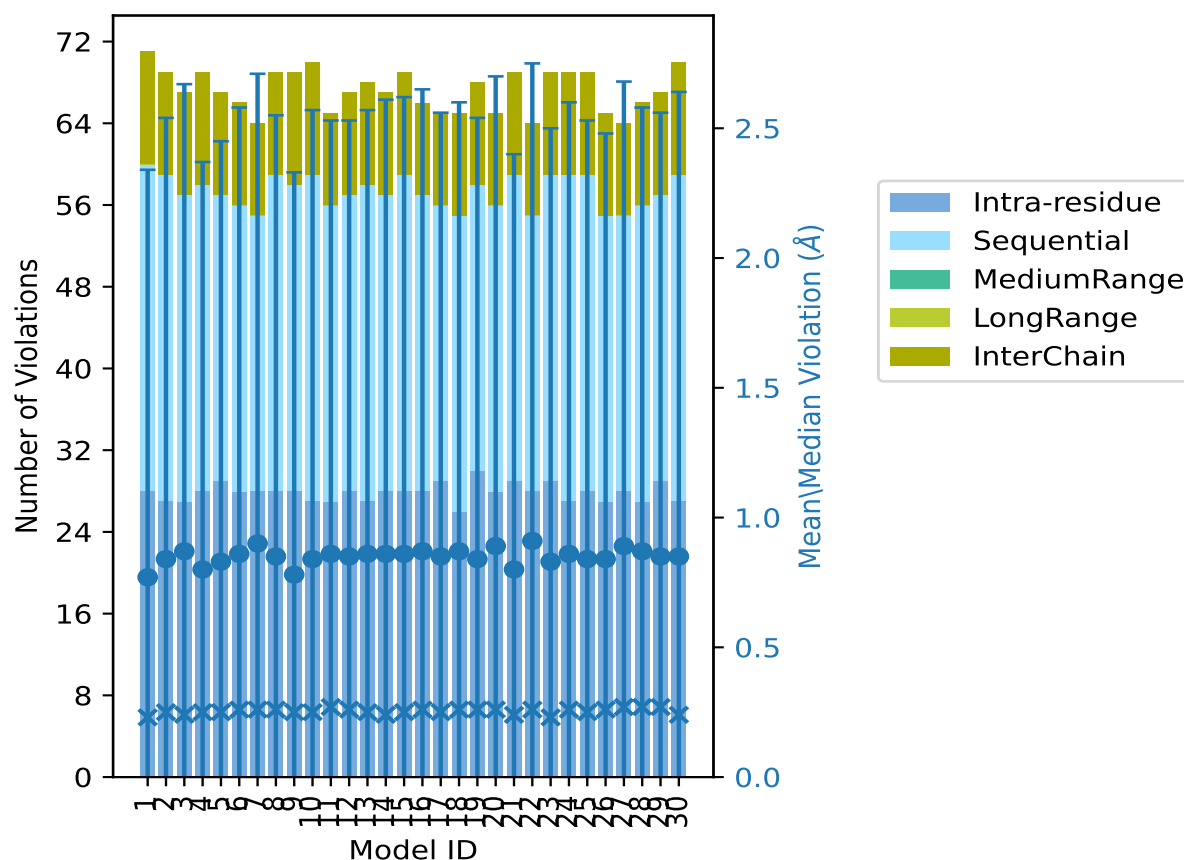
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	27	29	0	0	9	65	0.86	7.05	1.67	0.27
12	28	29	0	0	10	67	0.85	7.56	1.68	0.26
13	27	31	0	0	10	68	0.86	7.37	1.71	0.25
14	28	29	0	0	10	67	0.86	7.38	1.75	0.24
15	28	31	0	0	10	69	0.86	7.9	1.76	0.25
16	28	29	0	0	9	66	0.87	7.42	1.78	0.26
17	29	27	0	0	9	65	0.85	7.42	1.71	0.25
18	26	29	0	0	10	65	0.87	7.28	1.73	0.26
19	30	28	0	0	10	68	0.84	7.33	1.7	0.26
20	28	28	0	0	9	65	0.89	7.55	1.81	0.26
21	29	30	0	0	10	69	0.8	6.94	1.6	0.24
22	28	27	0	0	9	64	0.91	7.59	1.84	0.26
23	29	30	0	0	10	69	0.83	7.21	1.67	0.23
24	27	32	0	0	10	69	0.86	7.36	1.74	0.26
25	28	31	0	0	10	69	0.84	7.27	1.69	0.25
26	27	28	0	0	10	65	0.84	6.98	1.64	0.26
27	28	27	0	0	9	64	0.89	7.49	1.79	0.27
28	27	29	0	0	10	66	0.87	7.2	1.71	0.27
29	29	28	0	0	10	67	0.85	7.58	1.71	0.27
30	27	32	0	0	11	70	0.85	7.6	1.79	0.24

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard 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, 164(IR:106, SQ:54, MR:0, LR:0, IC:4) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	0	0	0	0	1	1	3.3
0	0	0	0	0	0	2	6.7
0	1	0	0	0	1	3	10.0
1	0	0	0	0	1	4	13.3
0	0	0	0	0	0	5	16.7
0	0	0	0	0	0	6	20.0

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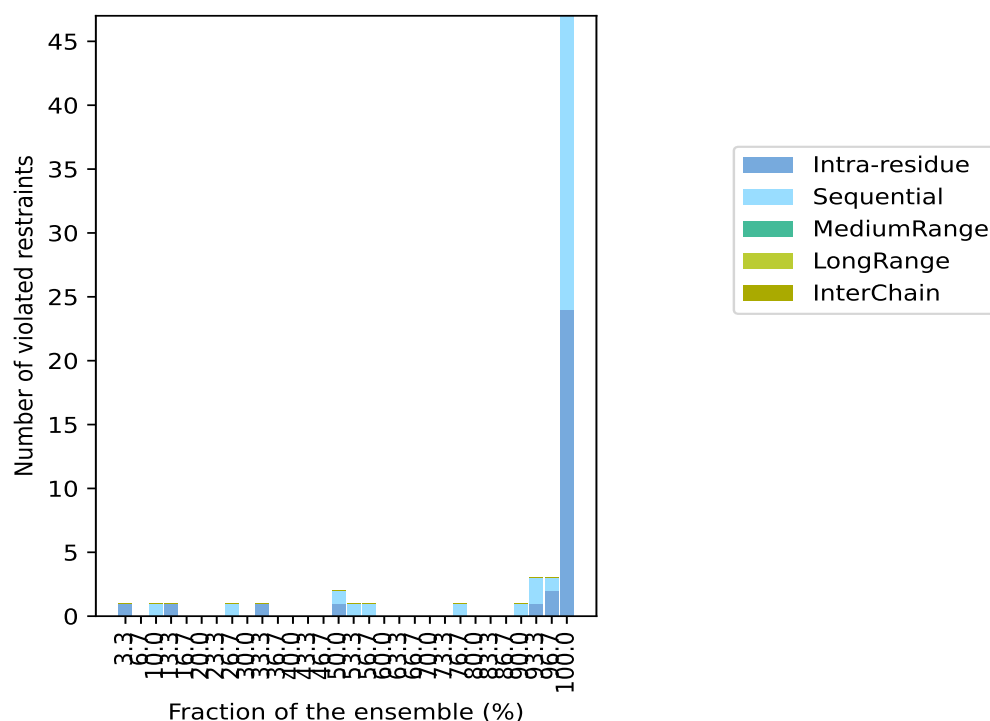
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	7	23.3
0	1	0	0	0	1	8	26.7
0	0	0	0	0	0	9	30.0
1	0	0	0	0	1	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	14	46.7
1	1	0	0	0	2	15	50.0
0	1	0	0	0	1	16	53.3
0	1	0	0	0	1	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	1	0	0	0	1	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	1	0	0	0	1	27	90.0
1	2	0	0	0	3	28	93.3
2	1	0	0	0	3	29	96.7
24	23	0	0	0	47	30	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

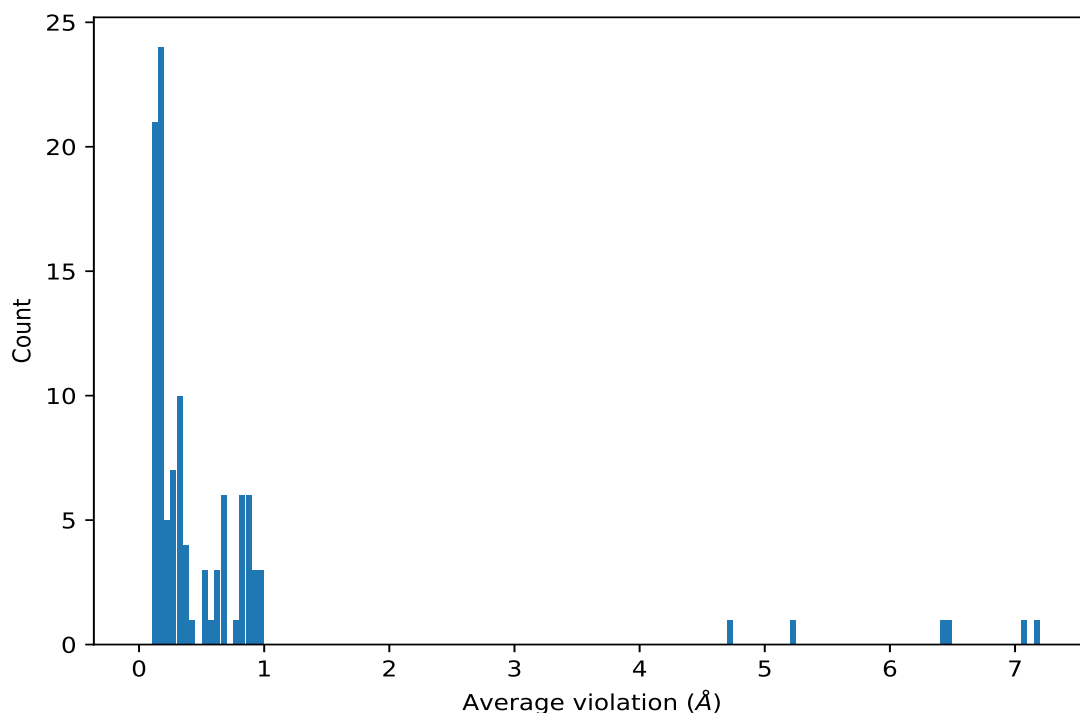
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	30	7.16	0.3	7.08
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	30	7.09	0.34	7.2
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	30	6.45	0.32	6.44
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	30	6.44	0.33	6.53
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	30	5.22	0.49	5.28
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	30	4.72	0.3	4.6
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	30	0.99	0.04	0.99
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	30	0.99	0.04	0.99
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	30	0.99	0.04	0.99
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	30	0.93	0.06	0.93
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	30	0.93	0.06	0.93
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	30	0.93	0.06	0.93
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	30	0.89	0.03	0.88
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	30	0.89	0.03	0.88
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	30	0.89	0.03	0.88
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	30	0.87	0.09	0.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	30	0.87	0.09	0.92
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	30	0.87	0.09	0.92
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	30	0.85	0.04	0.84
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	30	0.85	0.04	0.84
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	30	0.85	0.04	0.84
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	30	0.82	0.06	0.82
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	30	0.82	0.06	0.82
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	30	0.82	0.06	0.82
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	30	0.76	0.09	0.76
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	30	0.67	0.09	0.62
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	30	0.67	0.09	0.62
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	30	0.67	0.09	0.62
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	30	0.65	0.02	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	30	0.65	0.02	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	30	0.65	0.02	0.65
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	30	0.57	0.16	0.6
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	30	0.54	0.07	0.54
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	30	0.54	0.07	0.54
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	30	0.54	0.07	0.54
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	30	0.4	0.0	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	30	0.39	0.01	0.39
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	30	0.39	0.06	0.36
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	30	0.38	0.07	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	30	0.37	0.0	0.37
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	30	0.34	0.0	0.34
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	30	0.34	0.05	0.36
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	30	0.34	0.05	0.36
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	30	0.34	0.05	0.36
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	30	0.32	0.01	0.32
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	30	0.32	0.09	0.32
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	30	0.32	0.09	0.32
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	30	0.32	0.09	0.32
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	30	0.31	0.02	0.31
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	30	0.31	0.03	0.3
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	30	0.29	0.02	0.28
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	30	0.29	0.03	0.28
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	30	0.26	0.04	0.27
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	30	0.26	0.01	0.26
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	30	0.26	0.02	0.26
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	30	0.25	0.01	0.25
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	30	0.23	0.01	0.23
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	30	0.22	0.0	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	30	0.22	0.03	0.22
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	30	0.21	0.02	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	30	0.21	0.0	0.21
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	30	0.19	0.01	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	30	0.19	0.02	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	30	0.19	0.02	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	30	0.19	0.02	0.2
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	30	0.19	0.01	0.19
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	30	0.18	0.06	0.22
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	30	0.18	0.03	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	30	0.17	0.01	0.18
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	30	0.17	0.01	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	30	0.17	0.0	0.17
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	30	0.16	0.01	0.16
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	30	0.15	0.01	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	30	0.15	0.0	0.15
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	30	0.13	0.0	0.13
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	30	0.13	0.01	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	30	0.13	0.0	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	30	0.12	0.01	0.12
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	30	0.12	0.01	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	30	0.12	0.0	0.12
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	29	0.19	0.09	0.15
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	29	0.19	0.09	0.15
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	29	0.19	0.09	0.15
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	29	0.17	0.02	0.17
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	29	0.12	0.01	0.12
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	28	0.61	0.25	0.68
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	28	0.61	0.25	0.68
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	28	0.61	0.25	0.68
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	28	0.17	0.03	0.16
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	28	0.16	0.03	0.16
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	27	0.13	0.02	0.13
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	23	0.17	0.05	0.16
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	23	0.17	0.05	0.16
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	23	0.17	0.05	0.16
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	22	0.27	0.11	0.26
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	17	0.19	0.07	0.21
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	17	0.19	0.07	0.21
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	17	0.19	0.07	0.21
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	16	0.17	0.02	0.17
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	15	0.15	0.01	0.15

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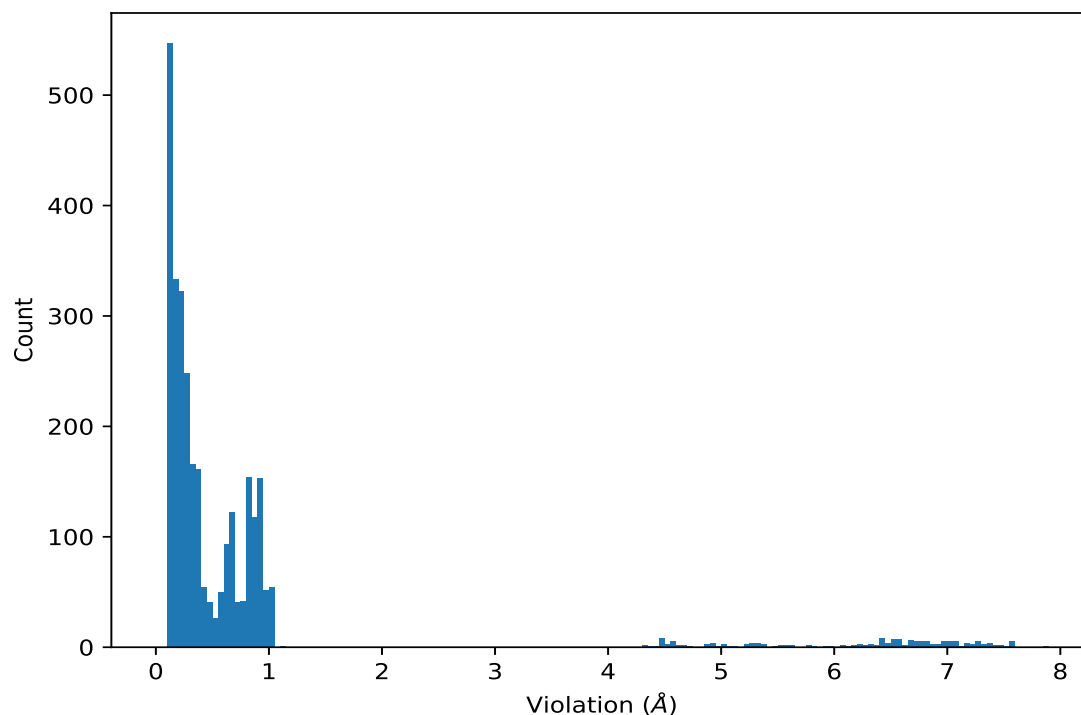
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	15	0.12	0.01	0.12
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	10	0.12	0.01	0.12
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	10	0.12	0.01	0.12
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	10	0.12	0.01	0.12
(1,140)	2:18:B:DG:H8	2:17:B:DG:H2''	8	0.12	0.01	0.11
(2,21)	2:19:B:DT:O4	1:4:A:DA:N6	6	0.11	0.01	0.11
(1,154)	2:19:B:DT:H2''	2:19:B:DT:H6	4	0.12	0.01	0.12
(1,189)	1:2:A:DT:H71	1:1:A:DC:H5	3	0.1	0.0	0.1
(1,189)	1:2:A:DT:H72	1:1:A:DC:H5	3	0.1	0.0	0.1
(1,189)	1:2:A:DT:H73	1:1:A:DC:H5	3	0.1	0.0	0.1

¹Number of violated models, ²Standard 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

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)
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	15	7.9
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	30	7.6
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	3	7.59
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	22	7.59
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	29	7.58
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	12	7.56
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	20	7.55
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	27	7.49
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	7	7.46
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	16	7.42
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	17	7.42
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	14	7.38
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	13	7.37
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	22	7.36
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	24	7.36
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	19	7.33
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	20	7.31
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	27	7.31
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	2	7.3
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	18	7.28
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	25	7.27
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	7	7.25
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	8	7.25
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	15	7.22
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	23	7.21
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	28	7.2
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	24	7.19
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	9	7.19
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	16	7.19
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	3	7.15
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	6	7.12
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	17	7.1
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	10	7.09
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	28	7.08
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	14	7.07
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	6	7.06
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	30	7.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	11	7.05
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	19	7.05
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	2	7.02
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	15	7.01
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	5	6.99
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	26	6.98
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	10	6.97
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	23	6.97
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	25	6.95
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	21	6.94
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	30	6.91
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	22	6.9
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	8	6.88
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	7	6.87
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	11	6.86
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	12	6.85
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	4	6.84
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	20	6.83
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	12	6.82
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	3	6.81
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	27	6.79
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	18	6.78
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	29	6.78
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	1	6.77
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	1	6.76
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	13	6.74
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	3	6.73
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	29	6.72
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	21	6.72
(2,27)	3:102:A:B2R:N35	2:17:B:DG:H1	13	6.7
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	8	6.69
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	19	6.69
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	4	6.67
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	7	6.66
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	23	6.65
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	24	6.65
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	5	6.64
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	24	6.61
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	18	6.6
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	27	6.59
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	16	6.58
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	25	6.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	10	6.57
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	17	6.57
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	14	6.56
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	2	6.54
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	2	6.53
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	6	6.53
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	22	6.52
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	16	6.52
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	26	6.51
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	9	6.51
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	5	6.48
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	20	6.47
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	28	6.45
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	14	6.45
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	21	6.44
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	10	6.43
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	17	6.43
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	10	6.43
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	15	6.42
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	30	6.42
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	1	6.41
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	6	6.4
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	28	6.38
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	19	6.37
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	25	6.34
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	11	6.34
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	11	6.31
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	30	6.29
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	26	6.27
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	8	6.24
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	23	6.22
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	13	6.2
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	4	6.16
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	29	6.16
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	5	6.12
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	1	6.1
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	18	6.1
(2,29)	3:101:A:B2R:N35	1:6:A:DG:H1	9	5.99
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	4	5.91
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	12	5.81
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	22	5.79
(2,26)	3:102:A:B2R:N35	2:17:B:DG:N1	21	5.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	14	5.61
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	16	5.61
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	26	5.56
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	20	5.56
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	13	5.51
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	8	5.5
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	18	5.47
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	30	5.37
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	6	5.37
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	3	5.36
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	24	5.34
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	25	5.34
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	3	5.33
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	2	5.32
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	26	5.29
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	29	5.28
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	24	5.27
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	28	5.26
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	15	5.22
(2,28)	3:101:A:B2R:N35	1:6:A:DG:N1	9	5.21
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	27	5.2
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	7	5.11
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	16	5.06
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	19	5.05
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	20	5.04
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	13	5.0
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	8	4.98
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	7	4.94
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	10	4.94
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	18	4.93
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	22	4.91
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	14	4.89
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	12	4.87
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	23	4.86
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	23	4.72
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	11	4.69
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	21	4.65
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	26	4.62
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	25	4.61
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	4	4.59
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	29	4.58
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	9	4.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	15	4.57
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	28	4.55
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	21	4.54
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	27	4.52
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	9	4.5
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	2	4.49
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	17	4.49
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	1	4.48
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	12	4.47
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	6	4.46
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	19	4.46
(2,25)	3:101:A:B2R:N1	2:18:B:DG:N2	5	4.46
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	5	4.45
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	11	4.4
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	4	4.39
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	17	4.33
(2,30)	3:102:A:B2R:N1	1:7:A:DG:N2	1	4.31
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	23	1.15
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	30	1.04
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	30	1.04
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	30	1.04
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	2	1.04
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	2	1.04
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	2	1.04
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	8	1.04
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	8	1.04
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	8	1.04
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	15	1.04
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	15	1.04
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	15	1.04
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	28	1.04
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	28	1.04
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	28	1.04
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	5	1.03
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	5	1.03
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	5	1.03
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	9	1.03
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	9	1.03
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	9	1.03
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	7	1.02
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	7	1.02
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	7	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	12	1.02
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	12	1.02
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	12	1.02
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	29	1.01
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	29	1.01
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	29	1.01
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	23	1.01
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	23	1.01
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	23	1.01
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	24	1.0
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	24	1.0
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	24	1.0
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	4	1.0
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	4	1.0
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	4	1.0
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	10	1.0
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	10	1.0
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	10	1.0
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	13	1.0
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	13	1.0
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	13	1.0
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	17	1.0
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	17	1.0
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	17	1.0
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	25	1.0
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	25	1.0
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	25	1.0
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	27	1.0
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	27	1.0
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	27	1.0
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	20	0.99
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	20	0.99
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	20	0.99
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	28	0.99
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	28	0.99
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	28	0.99
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	30	0.99
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	30	0.99
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	30	0.99
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	11	0.99
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	11	0.99
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	11	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	19	0.99
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	19	0.99
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	19	0.99
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	21	0.99
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	21	0.99
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	21	0.99
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	26	0.99
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	26	0.99
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	26	0.99
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	12	0.98
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	25	0.98
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	25	0.98
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	25	0.98
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	1	0.98
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	1	0.98
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	1	0.98
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	6	0.98
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	6	0.98
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	6	0.98
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	7	0.98
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	7	0.98
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	7	0.98
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	14	0.98
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	14	0.98
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	14	0.98
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	15	0.98
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	15	0.98
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	15	0.98
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	8	0.97
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	8	0.97
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	8	0.97
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	22	0.97
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	22	0.97
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	22	0.97
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	3	0.96
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	3	0.96
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	3	0.96
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	24	0.96
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	24	0.96
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	24	0.96
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	10	0.95
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	10	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	10	0.95
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	13	0.95
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	13	0.95
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	13	0.95
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	16	0.95
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	16	0.95
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	16	0.95
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	18	0.95
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	18	0.95
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	18	0.95
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	7	0.95
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	7	0.95
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	7	0.95
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	16	0.95
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	16	0.95
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	16	0.95
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	20	0.95
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	20	0.95
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	20	0.95
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	29	0.95
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	29	0.95
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	29	0.95
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	3	0.95
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	3	0.95
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	3	0.95
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	18	0.95
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	18	0.95
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	18	0.95
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	26	0.95
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	26	0.95
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	26	0.95
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	1	0.94
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	1	0.94
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	1	0.94
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	15	0.94
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	15	0.94
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	15	0.94
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	18	0.94
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	18	0.94
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	18	0.94
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	6	0.94
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	6	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	6	0.94
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	14	0.94
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	14	0.94
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	14	0.94
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	16	0.94
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	16	0.94
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	16	0.94
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	20	0.94
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	20	0.94
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	20	0.94
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	22	0.94
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	22	0.94
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	22	0.94
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	24	0.94
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	24	0.94
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	24	0.94
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	27	0.94
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	27	0.94
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	27	0.94
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	29	0.94
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	29	0.94
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	29	0.94
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	11	0.94
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	11	0.94
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	11	0.94
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	9	0.93
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	9	0.93
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	9	0.93
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	26	0.93
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	26	0.93
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	26	0.93
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	29	0.93
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	29	0.93
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	29	0.93
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	30	0.93
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	30	0.93
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	30	0.93
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	11	0.93
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	11	0.93
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	11	0.93
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	5	0.92
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	5	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	5	0.92
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	2	0.92
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	2	0.92
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	2	0.92
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	21	0.92
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	21	0.92
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	21	0.92
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	28	0.92
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	28	0.92
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	28	0.92
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	4	0.92
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	4	0.92
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	4	0.92
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	7	0.92
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	7	0.92
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	7	0.92
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	11	0.92
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	11	0.92
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	11	0.92
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	21	0.92
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	21	0.92
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	21	0.92
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	11	0.92
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	11	0.92
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	11	0.92
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	10	0.91
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	10	0.91
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	10	0.91
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	4	0.91
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	4	0.91
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	4	0.91
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	3	0.91
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	3	0.91
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	3	0.91
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	4	0.91
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	4	0.91
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	4	0.91
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	13	0.91
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	13	0.91
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	13	0.91
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	21	0.91
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	21	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	21	0.91
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	10	0.91
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	10	0.91
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	10	0.91
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	5	0.9
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	5	0.9
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	5	0.9
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	1	0.9
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	1	0.9
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	1	0.9
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	9	0.9
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	9	0.9
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	9	0.9
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	24	0.9
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	24	0.9
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	24	0.9
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	25	0.9
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	25	0.9
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	25	0.9
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	26	0.9
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	26	0.9
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	26	0.9
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	9	0.9
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	9	0.9
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	9	0.9
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	11	0.89
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	17	0.89
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	17	0.89
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	17	0.89
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	27	0.89
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	27	0.89
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	27	0.89
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	13	0.89
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	13	0.89
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	13	0.89
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	19	0.88
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	11	0.88
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	11	0.88
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	11	0.88
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	12	0.88
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	12	0.88
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	12	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	22	0.88
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	22	0.88
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	22	0.88
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	6	0.88
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	6	0.88
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	6	0.88
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	11	0.88
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	11	0.88
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	11	0.88
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	12	0.88
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	12	0.88
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	12	0.88
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	14	0.88
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	14	0.88
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	14	0.88
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	19	0.88
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	19	0.88
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	19	0.88
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	23	0.88
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	23	0.88
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	23	0.88
(1,203)	2:14:B:DT:H71	2:13:B:DA:H2''	30	0.88
(1,203)	2:14:B:DT:H72	2:13:B:DA:H2''	30	0.88
(1,203)	2:14:B:DT:H73	2:13:B:DA:H2''	30	0.88
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	2	0.88
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	2	0.88
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	2	0.88
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	5	0.88
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	5	0.88
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	5	0.88
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	25	0.88
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	25	0.88
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	25	0.88
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	1	0.88
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	1	0.88
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	1	0.88
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	24	0.88
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	24	0.88
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	24	0.88
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	4	0.87
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	15	0.87
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	19	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	19	0.87
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	19	0.87
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	23	0.87
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	23	0.87
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	23	0.87
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	8	0.87
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	8	0.87
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	8	0.87
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	10	0.87
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	10	0.87
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	10	0.87
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	15	0.87
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	15	0.87
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	15	0.87
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	16	0.87
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	16	0.87
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	16	0.87
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	20	0.87
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	20	0.87
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	20	0.87
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	28	0.87
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	28	0.87
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	28	0.87
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	23	0.87
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	23	0.87
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	23	0.87
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	8	0.87
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	8	0.87
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	8	0.87
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	9	0.87
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	9	0.87
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	9	0.87
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	28	0.87
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	28	0.87
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	28	0.87
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	1	0.86
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	22	0.86
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	28	0.86
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	14	0.86
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	14	0.86
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	14	0.86
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	17	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	17	0.86
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	17	0.86
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	5	0.86
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	5	0.86
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	5	0.86
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	18	0.86
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	18	0.86
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	18	0.86
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	22	0.86
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	22	0.86
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	22	0.86
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	12	0.86
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	12	0.86
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	12	0.86
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	2	0.86
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	2	0.86
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	2	0.86
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	6	0.85
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	6	0.85
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	6	0.85
(1,210)	2:15:B:DT:H71	2:14:B:DT:H2'	2	0.85
(1,210)	2:15:B:DT:H72	2:14:B:DT:H2'	2	0.85
(1,210)	2:15:B:DT:H73	2:14:B:DT:H2'	2	0.85
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	18	0.85
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	18	0.85
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	18	0.85
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	19	0.85
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	19	0.85
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	19	0.85
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	13	0.85
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	13	0.85
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	13	0.85
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	5	0.85
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	5	0.85
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	5	0.85
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	10	0.85
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	10	0.85
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	10	0.85
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	26	0.85
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	26	0.85
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	26	0.85
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	29	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	29	0.85
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	29	0.85
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	24	0.84
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	27	0.84
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	27	0.84
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	27	0.84
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	4	0.84
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	4	0.84
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	4	0.84
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	8	0.84
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	8	0.84
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	8	0.84
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	14	0.84
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	14	0.84
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	14	0.84
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	19	0.84
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	19	0.84
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	19	0.84
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	22	0.84
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	22	0.84
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	22	0.84
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	25	0.84
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	25	0.84
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	25	0.84
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	5	0.83
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	5	0.83
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	5	0.83
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	16	0.83
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	16	0.83
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	16	0.83
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	22	0.83
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	22	0.83
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	22	0.83
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	24	0.83
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	24	0.83
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	24	0.83
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	7	0.83
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	7	0.83
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	7	0.83
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	12	0.83
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	12	0.83
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	12	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	16	0.83
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	16	0.83
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	16	0.83
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	17	0.83
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	17	0.83
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	17	0.83
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	18	0.83
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	18	0.83
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	18	0.83
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	23	0.83
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	23	0.83
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	23	0.83
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	27	0.83
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	27	0.83
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	27	0.83
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	8	0.82
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	8	0.82
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	8	0.82
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	15	0.82
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	15	0.82
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	15	0.82
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	2	0.82
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	2	0.82
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	2	0.82
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	15	0.82
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	15	0.82
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	15	0.82
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	21	0.82
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	21	0.82
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	21	0.82
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	27	0.82
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	27	0.82
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	27	0.82
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	29	0.82
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	29	0.82
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	29	0.82
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	6	0.82
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	6	0.82
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	6	0.82
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	13	0.82
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	13	0.82
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	13	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	20	0.82
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	20	0.82
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	20	0.82
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	30	0.82
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	30	0.82
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	30	0.82
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	2	0.81
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	28	0.81
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	3	0.81
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	3	0.81
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	3	0.81
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	7	0.81
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	7	0.81
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	7	0.81
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	12	0.81
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	12	0.81
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	12	0.81
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	13	0.81
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	13	0.81
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	13	0.81
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	17	0.81
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	17	0.81
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	17	0.81
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	3	0.81
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	3	0.81
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	3	0.81
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	4	0.81
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	4	0.81
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	4	0.81
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	21	0.8
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	9	0.8
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	9	0.8
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	9	0.8
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	1	0.8
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	1	0.8
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	1	0.8
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	6	0.8
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	6	0.8
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	6	0.8
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	26	0.8
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	26	0.8
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	26	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	30	0.8
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	30	0.8
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	30	0.8
(1,211)	2:15:B:DT:H71	2:14:B:DT:H2''	3	0.79
(1,211)	2:15:B:DT:H72	2:14:B:DT:H2''	3	0.79
(1,211)	2:15:B:DT:H73	2:14:B:DT:H2''	3	0.79
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	14	0.79
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	14	0.79
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	14	0.79
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	21	0.79
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	21	0.79
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	21	0.79
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	20	0.78
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	20	0.78
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	20	0.78
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	4	0.78
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	4	0.78
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	4	0.78
(1,190)	1:2:A:DT:H71	1:1:A:DC:H2'	21	0.78
(1,190)	1:2:A:DT:H72	1:1:A:DC:H2'	21	0.78
(1,190)	1:2:A:DT:H73	1:1:A:DC:H2'	21	0.78
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	7	0.77
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	26	0.77
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	24	0.77
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	24	0.77
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	24	0.77
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	30	0.77
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	30	0.77
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	30	0.77
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	10	0.76
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	16	0.76
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	23	0.76
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	29	0.76
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	3	0.76
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	3	0.76
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	3	0.76
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	19	0.76
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	19	0.76
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	19	0.76
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	23	0.76
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	23	0.76
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	23	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	12	0.75
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	12	0.75
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	12	0.75
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	9	0.74
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	22	0.74
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	22	0.74
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	22	0.74
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	25	0.73
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	8	0.73
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	8	0.73
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	8	0.73
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	10	0.73
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	10	0.73
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	10	0.73
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	25	0.73
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	25	0.73
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	25	0.73
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	28	0.73
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	28	0.73
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	28	0.73
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	5	0.72
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	8	0.72
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	15	0.72
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	15	0.72
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	15	0.72
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	17	0.72
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	17	0.72
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	17	0.72
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	10	0.71
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	13	0.71
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	13	0.71
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	13	0.71
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	17	0.71
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	17	0.71
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	17	0.71
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	19	0.71
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	19	0.71
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	19	0.71
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	6	0.71
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	6	0.71
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	6	0.71
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	18	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	18	0.71
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	18	0.71
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	30	0.7
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	8	0.7
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	8	0.7
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	8	0.7
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	20	0.7
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	20	0.7
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	20	0.7
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	27	0.7
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	27	0.7
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	27	0.7
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	13	0.69
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	13	0.69
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	13	0.69
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	17	0.69
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	17	0.69
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	17	0.69
(1,202)	2:14:B:DT:H71	2:13:B:DA:H2'	1	0.69
(1,202)	2:14:B:DT:H72	2:13:B:DA:H2'	1	0.69
(1,202)	2:14:B:DT:H73	2:13:B:DA:H2'	1	0.69
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	16	0.69
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	16	0.69
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	16	0.69
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	17	0.69
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	17	0.69
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	17	0.69
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	19	0.69
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	19	0.69
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	19	0.69
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	8	0.68
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	13	0.68
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	20	0.68
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	23	0.68
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	1	0.68
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	1	0.68
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	1	0.68
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	16	0.68
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	16	0.68
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	16	0.68
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	24	0.68
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	24	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	24	0.68
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	18	0.68
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	18	0.68
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	18	0.68
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	5	0.68
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	5	0.68
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	5	0.68
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	7	0.68
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	7	0.68
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	7	0.68
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	14	0.68
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	14	0.68
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	14	0.68
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	22	0.68
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	22	0.68
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	22	0.68
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	26	0.68
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	26	0.68
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	26	0.68
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	29	0.68
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	29	0.68
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	29	0.68
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	17	0.67
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	27	0.67
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	6	0.67
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	18	0.67
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	18	0.67
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	18	0.67
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	25	0.67
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	25	0.67
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	25	0.67
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	6	0.67
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	6	0.67
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	6	0.67
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	26	0.67
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	26	0.67
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	26	0.67
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	25	0.66
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	29	0.66
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	4	0.66
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	4	0.66
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	28	0.66
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	28	0.66
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	28	0.66
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	28	0.66
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	28	0.66
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	28	0.66
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	4	0.65
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	6	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	6	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	6	0.65
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	7	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	7	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	7	0.65
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	9	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	9	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	9	0.65
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	11	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	11	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	11	0.65
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	14	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	14	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	14	0.65
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	19	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	19	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	19	0.65
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	24	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	24	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	24	0.65
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	26	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	26	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	26	0.65
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	27	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	27	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	27	0.65
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	29	0.65
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	29	0.65
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	29	0.65
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	8	0.65
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	8	0.65
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	8	0.65
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	6	0.64
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	14	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	8	0.64
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	8	0.64
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	8	0.64
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	10	0.64
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	10	0.64
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	10	0.64
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	15	0.64
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	15	0.64
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	15	0.64
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	20	0.64
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	20	0.64
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	20	0.64
(1,195)	1:10:A:DT:H71	1:9:A:DA:H2'	25	0.64
(1,195)	1:10:A:DT:H72	1:9:A:DA:H2'	25	0.64
(1,195)	1:10:A:DT:H73	1:9:A:DA:H2'	25	0.64
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	18	0.63
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	2	0.63
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	18	0.63
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	2	0.63
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	2	0.63
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	2	0.63
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	3	0.63
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	3	0.63
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	3	0.63
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	5	0.63
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	5	0.63
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	5	0.63
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	12	0.63
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	12	0.63
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	12	0.63
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	21	0.63
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	21	0.63
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	21	0.63
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	23	0.63
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	23	0.63
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	23	0.63
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	5	0.62
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	9	0.62
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	24	0.62
(1,227)	2:20:B:DT:H71	2:19:B:DT:H2''	30	0.62
(1,227)	2:20:B:DT:H72	2:19:B:DT:H2''	30	0.62
(1,227)	2:20:B:DT:H73	2:19:B:DT:H2''	30	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	10	0.62
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	10	0.62
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	10	0.62
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	2	0.62
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	2	0.62
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	2	0.62
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	14	0.62
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	14	0.62
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	14	0.62
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	20	0.62
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	20	0.62
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	20	0.62
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	21	0.62
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	21	0.62
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	21	0.62
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	27	0.62
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	27	0.62
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	27	0.62
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	28	0.62
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	28	0.62
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	28	0.62
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	15	0.62
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	15	0.62
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	15	0.62
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	21	0.61
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	29	0.61
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	29	0.61
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	29	0.61
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	1	0.61
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	1	0.61
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	1	0.61
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	9	0.61
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	9	0.61
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	9	0.61
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	12	0.61
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	12	0.61
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	12	0.61
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	16	0.61
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	16	0.61
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	16	0.61
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	23	0.61
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	23	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	23	0.61
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	25	0.61
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	25	0.61
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	25	0.61
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	29	0.61
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	29	0.61
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	29	0.61
(1,232)	3:102:A:B2R:N29	1:7:A:DG:H1	3	0.6
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	26	0.6
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	18	0.6
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	18	0.6
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	18	0.6
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	22	0.6
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	22	0.6
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	22	0.6
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	12	0.59
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	7	0.59
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	7	0.59
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	7	0.59
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	11	0.59
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	11	0.59
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	11	0.59
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	19	0.58
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	19	0.58
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	19	0.58
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	26	0.58
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	26	0.58
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	26	0.58
(1,219)	2:19:B:DT:H71	2:18:B:DG:H2'	4	0.58
(1,219)	2:19:B:DT:H72	2:18:B:DG:H2'	4	0.58
(1,219)	2:19:B:DT:H73	2:18:B:DG:H2'	4	0.58
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	5	0.57
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	5	0.57
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	5	0.57
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	15	0.57
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	15	0.57
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	15	0.57
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	25	0.57
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	25	0.57
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	25	0.57
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	30	0.57
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	30	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	30	0.57
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	12	0.56
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	2	0.56
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	2	0.56
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	2	0.56
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	28	0.56
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	28	0.56
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	28	0.56
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	13	0.55
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	12	0.55
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	12	0.55
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	12	0.55
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	23	0.55
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	23	0.55
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	23	0.55
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	6	0.54
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	6	0.54
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	6	0.54
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	14	0.54
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	14	0.54
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	14	0.54
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	30	0.53
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	20	0.53
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	20	0.53
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	20	0.53
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	23	0.53
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	23	0.53
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	23	0.53
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	13	0.52
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	13	0.52
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	13	0.52
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	14	0.51
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	15	0.51
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	27	0.51
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	27	0.51
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	27	0.51
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	11	0.5
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	21	0.5
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	21	0.5
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	21	0.5
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	15	0.5
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	3	0.49
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	3	0.49
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	3	0.49
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	7	0.49
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	7	0.49
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	7	0.49
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	12	0.49
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	12	0.49
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	12	0.49
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	12	0.49
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	25	0.49
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	15	0.48
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	19	0.48
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	16	0.48
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	16	0.48
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	16	0.48
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	13	0.48
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	13	0.48
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	13	0.48
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	8	0.48
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	13	0.48
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	22	0.47
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	11	0.47
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	11	0.47
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	11	0.47
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	11	0.47
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	21	0.47
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	1	0.46
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	19	0.46
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	9	0.46
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	9	0.46
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	9	0.46
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	4	0.45
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	28	0.45
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	17	0.45
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	17	0.45
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	17	0.45
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	17	0.45
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	17	0.45
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	17	0.45
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	2	0.44
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	24	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	22	0.44
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	1	0.44
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	1	0.44
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	1	0.44
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	4	0.44
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	4	0.44
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	4	0.44
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	11	0.43
(1,226)	2:20:B:DT:H71	2:19:B:DT:H2'	22	0.43
(1,226)	2:20:B:DT:H72	2:19:B:DT:H2'	22	0.43
(1,226)	2:20:B:DT:H73	2:19:B:DT:H2'	22	0.43
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	4	0.42
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	20	0.41
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	28	0.41
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	21	0.4
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	28	0.4
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	28	0.4
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	28	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	1	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	2	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	3	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	4	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	8	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	9	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	10	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	11	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	12	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	13	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	23	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	24	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	25	0.4
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	30	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	1	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	2	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	4	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	6	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	7	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	11	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	13	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	14	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	15	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	16	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	18	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	19	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	20	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	21	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	22	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	24	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	27	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	28	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	29	0.4
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	30	0.4
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	3	0.39
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	7	0.39
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	7	0.39
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	7	0.39
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	9	0.39
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	9	0.39
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	9	0.39
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	14	0.39
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	14	0.39
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	14	0.39
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	20	0.39
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	20	0.39
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	20	0.39
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	15	0.39
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	17	0.39
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	22	0.39
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	3	0.39
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	5	0.39
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	8	0.39
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	9	0.39
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	10	0.39
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	12	0.39
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	17	0.39
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	23	0.39
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	25	0.39
(1,52)	1:8:A:DA:H8	1:8:A:DA:H1'	26	0.39
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	20	0.39
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	16	0.38
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	26	0.38
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	28	0.38
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	28	0.38
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	28	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	8	0.38
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	8	0.38
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	8	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	5	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	6	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	7	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	14	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	16	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	18	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	19	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	20	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	21	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	26	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	27	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	28	0.38
(1,183)	2:22:B:DG:H2''	2:22:B:DG:H8	29	0.38
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	6	0.38
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	18	0.38
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	19	0.38
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	27	0.38
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	5	0.37
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	10	0.37
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	29	0.37
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	2	0.37
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	2	0.37
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	2	0.37
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	14	0.37
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	14	0.37
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	14	0.37
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	1	0.37
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	1	0.37
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	1	0.37
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	6	0.37
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	6	0.37
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	6	0.37
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	13	0.37
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	13	0.37
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	13	0.37
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	15	0.37
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	15	0.37
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	15	0.37
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	25	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	25	0.37
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	25	0.37
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	26	0.37
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	26	0.37
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	26	0.37
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	27	0.37
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	27	0.37
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	27	0.37
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	30	0.37
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	30	0.37
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	30	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	1	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	2	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	3	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	4	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	5	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	6	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	7	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	9	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	10	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	11	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	12	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	13	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	14	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	15	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	16	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	17	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	19	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	20	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	21	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	22	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	23	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	24	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	25	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	26	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	27	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	29	0.37
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	30	0.37
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	16	0.37
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	22	0.37
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	9	0.36
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	23	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	25	0.36
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	17	0.36
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	27	0.36
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	3	0.36
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	3	0.36
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	3	0.36
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	7	0.36
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	7	0.36
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	7	0.36
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	12	0.36
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	12	0.36
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	12	0.36
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	16	0.36
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	16	0.36
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	16	0.36
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	17	0.36
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	17	0.36
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	17	0.36
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	21	0.36
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	21	0.36
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	21	0.36
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	22	0.36
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	22	0.36
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	22	0.36
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	24	0.36
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	24	0.36
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	24	0.36
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	29	0.36
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	29	0.36
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	29	0.36
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	2	0.36
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	2	0.36
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	2	0.36
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	5	0.36
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	18	0.36
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	28	0.36
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	8	0.36
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	18	0.36
(1,23)	1:3:A:DA:H2'	1:3:A:DA:H1'	28	0.36
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	2	0.36
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	7	0.36
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	14	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	17	0.36
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	26	0.36
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	28	0.36
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	7	0.35
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	7	0.35
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	22	0.35
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	22	0.35
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	22	0.35
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	4	0.35
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	4	0.35
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	4	0.35
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	18	0.35
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	18	0.35
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	18	0.35
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	19	0.35
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	19	0.35
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	19	0.35
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	2	0.35
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	9	0.35
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	11	0.35
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	23	0.35
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	4	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	3	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	4	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	9	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	12	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	13	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	16	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	18	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	20	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	21	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	22	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	24	0.35
(1,105)	2:13:B:DA:H2''	2:13:B:DA:H8	29	0.35
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	26	0.35
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	5	0.35
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	29	0.35
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	30	0.34
(1,230)	3:101:A:B2R:N29	2:18:B:DG:H1	16	0.34
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	15	0.34
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	15	0.34
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	15	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	16	0.34
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	16	0.34
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	16	0.34
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	24	0.34
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	24	0.34
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	24	0.34
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	23	0.34
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	23	0.34
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	23	0.34
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	1	0.34
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	3	0.34
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	10	0.34
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	12	0.34
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	13	0.34
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	15	0.34
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	24	0.34
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	25	0.34
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	30	0.34
(1,142)	2:18:B:DG:H2"	2:18:B:DG:H8	1	0.34
(1,142)	2:18:B:DG:H2"	2:18:B:DG:H8	25	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	1	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	2	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	5	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	6	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	7	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	8	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	10	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	11	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	14	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	15	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	17	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	19	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	23	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	25	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	26	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	27	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	28	0.34
(1,105)	2:13:B:DA:H2"	2:13:B:DA:H8	30	0.34
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	11	0.34
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	20	0.33
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	8	0.33
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	8	0.33
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	8	0.33
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	20	0.33
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	20	0.33
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	20	0.33
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	5	0.33
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	5	0.33
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	5	0.33
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	8	0.33
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	5	0.33
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	11	0.33
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	19	0.33
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	2	0.33
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	9	0.33
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	12	0.33
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	15	0.33
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	17	0.33
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	25	0.33
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	26	0.33
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	27	0.33
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	25	0.33
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	9	0.33
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	24	0.33
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	30	0.33
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	8	0.32
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	13	0.32
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	27	0.32
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	27	0.32
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	27	0.32
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	4	0.32
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	21	0.32
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	22	0.32
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	30	0.32
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	1	0.32
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	3	0.32
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	8	0.32
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	10	0.32
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	13	0.32
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	19	0.32
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	21	0.32
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	23	0.32
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	24	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	28	0.32
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	29	0.32
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	8	0.32
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	11	0.32
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	12	0.32
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	13	0.32
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	15	0.32
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	25	0.32
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	1	0.32
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	3	0.32
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	23	0.32
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	10	0.32
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	17	0.31
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	27	0.31
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	7	0.31
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	9	0.31
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	10	0.31
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	12	0.31
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	15	0.31
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	16	0.31
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	17	0.31
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	20	0.31
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	28	0.31
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	4	0.31
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	6	0.31
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	14	0.31
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	16	0.31
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	18	0.31
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	20	0.31
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	22	0.31
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	30	0.31
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	6	0.31
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	8	0.31
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	14	0.31
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	19	0.31
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	27	0.31
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	29	0.31
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	2	0.31
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	3	0.31
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	9	0.31
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	23	0.31
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	24	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	30	0.31
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	14	0.3
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	6	0.3
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	10	0.3
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	10	0.3
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	10	0.3
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	10	0.3
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	3	0.3
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	3	0.3
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	3	0.3
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	9	0.3
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	9	0.3
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	9	0.3
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	3	0.3
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	9	0.3
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	10	0.3
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	2	0.3
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	3	0.3
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	8	0.3
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	13	0.3
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	14	0.3
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	18	0.3
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	26	0.3
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	27	0.3
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	29	0.3
(1,64)	1:10:A:DT:H6	1:9:A:DA:H8	7	0.3
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	7	0.3
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	11	0.3
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	13	0.3
(1,13)	1:2:A:DT:H6	1:1:A:DC:H3'	10	0.3
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	1	0.3
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	18	0.29
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	29	0.29
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	8	0.29
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	8	0.29
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	8	0.29
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	10	0.29
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	10	0.29
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	10	0.29
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	11	0.29
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	11	0.29
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	2	0.29
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	24	0.29
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	30	0.29
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	21	0.29
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	6	0.29
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	23	0.29
(1,142)	2:18:B:DG:H2''	2:18:B:DG:H8	24	0.29
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	5	0.29
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	20	0.29
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	4	0.29
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	18	0.29
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	19	0.29
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	20	0.29
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	21	0.29
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	27	0.29
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	5	0.29
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	6	0.28
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	4	0.28
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	3	0.28
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	3	0.28
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	3	0.28
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	24	0.28
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	24	0.28
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	24	0.28
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	29	0.28
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	29	0.28
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	29	0.28
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	6	0.28
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	6	0.28
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	6	0.28
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	11	0.28
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	11	0.28
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	11	0.28
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	19	0.28
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	19	0.28
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	19	0.28
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	8	0.28
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	8	0.28
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	8	0.28
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	1	0.28
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	23	0.28
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	18	0.28
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	22	0.28
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	27	0.28
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	2	0.28
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	12	0.28
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	16	0.28
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	1	0.28
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	2	0.28
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	5	0.28
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	6	0.28
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	7	0.28
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	9	0.28
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	23	0.28
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	26	0.28
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	28	0.28
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	29	0.28
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	29	0.28
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	2	0.27
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	24	0.27
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	25	0.27
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	4	0.27
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	4	0.27
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	4	0.27
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	25	0.27
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	25	0.27
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	25	0.27
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	4	0.27
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	11	0.27
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	12	0.27
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	15	0.27
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	25	0.27
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	7	0.27
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	14	0.27
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	16	0.27
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	17	0.27
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	19	0.27
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	20	0.27
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	26	0.27
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	28	0.27
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	29	0.27
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	11	0.27
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	15	0.27
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	17	0.27
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	19	0.27
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	26	0.27
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	27	0.27
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	28	0.27
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	29	0.27
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	3	0.27
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	4	0.27
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	11	0.27
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	18	0.27
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	22	0.27
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	5	0.27
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	9	0.27
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	15	0.27
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	22	0.27
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	30	0.27
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	3	0.27
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	10	0.27
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	14	0.27
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	16	0.27
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	17	0.27
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	22	0.27
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	24	0.27
(1,17)	1:2:A:DT:H2''	1:2:A:DT:H6	30	0.27
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	7	0.27
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	14	0.27
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	16	0.27
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	18	0.27
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	19	0.27
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	26	0.27
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	27	0.27
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	28	0.27
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	18	0.26
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	30	0.26
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	30	0.26
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	30	0.26
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	26	0.26
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	26	0.26
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	26	0.26
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	1	0.26
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	1	0.26
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	10	0.26
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	10	0.26
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	10	0.26
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	30	0.26
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	30	0.26
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	30	0.26
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	8	0.26
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	21	0.26
(1,176)	2:22:B:DG:H8	2:21:B:DA:H8	5	0.26
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	7	0.26
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	11	0.26
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	19	0.26
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	28	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	2	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	3	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	6	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	7	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	8	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	9	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	13	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	14	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	16	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	18	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	20	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	21	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	23	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	24	0.26
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	25	0.26
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	5	0.26
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	9	0.26
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	12	0.26
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	16	0.26
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	20	0.26
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	21	0.26
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	24	0.26
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	29	0.26
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	10	0.26
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	12	0.26
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	15	0.26
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	6	0.26
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	20	0.26
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	22	0.26
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	5	0.25
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	9	0.25
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	21	0.25
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	26	0.25
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	18	0.25
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	18	0.25
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	18	0.25
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	20	0.25
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	20	0.25
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	20	0.25
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	2	0.25
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	2	0.25
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	2	0.25
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	13	0.25
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	16	0.25
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	10	0.25
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	13	0.25
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	17	0.25
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	27	0.25
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	1	0.25
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	4	0.25
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	5	0.25
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	10	0.25
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	22	0.25
(1,134)	2:17:B:DG:H2'	2:17:B:DG:H1'	30	0.25
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	20	0.25
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	29	0.25
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	6	0.25
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	10	0.25
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	13	0.25
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	15	0.25
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	19	0.25
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	25	0.25
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	30	0.25
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	4	0.25
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	21	0.25
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	23	0.25
(1,231)	3:102:A:B2R:N29	1:7:A:DG:N1	3	0.24
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	25	0.24
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	25	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	25	0.24
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	2	0.24
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	2	0.24
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	2	0.24
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	14	0.24
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	14	0.24
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	14	0.24
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	5	0.24
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	6	0.24
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	7	0.24
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	14	0.24
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	17	0.24
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	20	0.24
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	22	0.24
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	16	0.24
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	20	0.24
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	8	0.24
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	12	0.24
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	16	0.24
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	18	0.24
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	19	0.24
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	22	0.24
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	24	0.24
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	1	0.24
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	2	0.24
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	7	0.24
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	8	0.24
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	14	0.24
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	17	0.24
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	27	0.24
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	28	0.24
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	1	0.24
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	17	0.24
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	24	0.24
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	21	0.24
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	1	0.24
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	2	0.24
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	3	0.24
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	8	0.24
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	13	0.24
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	24	0.24
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	30	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	12	0.23
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	2	0.23
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	2	0.23
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	2	0.23
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	15	0.23
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	15	0.23
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	15	0.23
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	18	0.23
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	18	0.23
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	18	0.23
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	5	0.23
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	5	0.23
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	5	0.23
(1,198)	1:10:A:DT:H71	1:10:A:DT:H6	5	0.23
(1,198)	1:10:A:DT:H72	1:10:A:DT:H6	5	0.23
(1,198)	1:10:A:DT:H73	1:10:A:DT:H6	5	0.23
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	18	0.23
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	19	0.23
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	26	0.23
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	27	0.23
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	28	0.23
(1,184)	2:22:B:DG:H3'	2:22:B:DG:H8	29	0.23
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	3	0.23
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	30	0.23
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	1	0.23
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	4	0.23
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	5	0.23
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	15	0.23
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	21	0.23
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	22	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	1	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	2	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	4	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	5	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	6	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	7	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	9	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	10	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	14	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	15	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	25	0.23
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	28	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	30	0.23
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	23	0.23
(1,101)	2:13:B:DA:H8	2:12:B:DC:H3'	26	0.23
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	5	0.23
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	9	0.23
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	10	0.23
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	12	0.23
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	25	0.23
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	26	0.23
(1,33)	1:4:A:DA:H2''	1:4:A:DA:H8	3	0.23
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	9	0.23
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	10	0.23
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	11	0.23
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	21	0.23
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	23	0.23
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	25	0.23
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	4	0.23
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	21	0.23
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	6	0.22
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	6	0.22
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	6	0.22
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	24	0.22
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	24	0.22
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	24	0.22
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	26	0.22
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	26	0.22
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	26	0.22
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	12	0.22
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	14	0.22
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	3	0.22
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	21	0.22
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	27	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	1	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	2	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	3	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	4	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	6	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	8	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	9	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	10	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	11	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	13	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	14	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	15	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	16	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	17	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	18	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	19	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	20	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	21	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	22	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	23	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	24	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	25	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	26	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	27	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	28	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	29	0.22
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	30	0.22
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	2	0.22
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	8	0.22
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	11	0.22
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	15	0.22
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	17	0.22
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	3	0.22
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	24	0.22
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	18	0.22
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	28	0.22
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	12	0.21
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	12	0.21
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	12	0.21
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	23	0.21
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	23	0.21
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	23	0.21
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	28	0.21
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	28	0.21
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	28	0.21
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	17	0.21
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	2	0.21
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	8	0.21
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	15	0.21
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	24	0.21
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	9	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	1	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	2	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	3	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	4	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	5	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	6	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	7	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	8	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	9	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	10	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	11	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	12	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	13	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	14	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	15	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	16	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	17	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	18	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	19	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	20	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	21	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	22	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	23	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	24	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	25	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	26	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	27	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	28	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	29	0.21
(1,110)	2:14:B:DT:H6	2:14:B:DT:H1'	30	0.21
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	11	0.21
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	13	0.21
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	17	0.21
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	23	0.21
(1,107)	2:14:B:DT:H6	2:13:B:DA:H8	26	0.21
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	2	0.21
(1,71)	1:10:A:DT:H2''	1:10:A:DT:H6	7	0.21
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	1	0.21
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	3	0.21
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	19	0.21
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	24	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	27	0.21
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	28	0.21
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	1	0.21
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	4	0.21
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	11	0.21
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	4	0.21
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	3	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	3	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	3	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	5	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	5	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	5	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	6	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	6	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	6	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	7	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	7	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	7	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	10	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	10	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	10	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	14	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	14	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	14	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	16	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	16	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	16	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	17	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	17	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	17	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	18	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	18	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	18	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	19	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	19	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	19	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	20	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	20	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	20	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	22	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	22	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	22	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	23	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	23	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	23	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	26	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	26	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	26	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	27	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	27	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	27	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	29	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	29	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	29	0.2
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	30	0.2
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	30	0.2
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	30	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	1	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	2	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	3	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	4	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	5	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	6	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	7	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	9	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	11	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	12	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	14	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	15	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	16	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	20	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	21	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	22	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	23	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	27	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	28	0.2
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	30	0.2
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	1	0.2
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	9	0.2
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	12	0.2
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	13	0.2
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	23	0.2
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	2	0.2
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	25	0.2
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	30	0.2
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	1	0.2
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	7	0.2
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	8	0.2
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	17	0.2
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	23	0.2
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	26	0.2
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	28	0.2
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	4	0.2
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	13	0.2
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	16	0.2
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	18	0.2
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	23	0.2
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	30	0.2
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	23	0.2
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	17	0.2
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	23	0.2
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	19	0.2
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	25	0.2
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	26	0.2
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	24	0.2
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	11	0.2
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	13	0.2
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	25	0.2
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	13	0.19
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	13	0.19
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	13	0.19
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	13	0.19
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	8	0.19
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	8	0.19
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	8	0.19
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	10	0.19
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	10	0.19
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	10	0.19
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	21	0.19
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	21	0.19
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	21	0.19
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	28	0.19
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	28	0.19
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	28	0.19
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	1	0.19
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	1	0.19
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	2	0.19
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	2	0.19
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	2	0.19
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	4	0.19
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	4	0.19
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	4	0.19
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	9	0.19
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	9	0.19
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	9	0.19
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	21	0.19
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	21	0.19
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	21	0.19
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	24	0.19
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	24	0.19
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	24	0.19
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	10	0.19
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	13	0.19
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	19	0.19
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	4	0.19
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	22	0.19
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	28	0.19
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	6	0.19
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	3	0.19
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	17	0.19
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	21	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	3	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	6	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	10	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	12	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	14	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	15	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	18	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	20	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	24	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	25	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	27	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	29	0.19
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	30	0.19
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	6	0.19
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	20	0.19
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	21	0.19
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	22	0.19
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	29	0.19
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	13	0.19
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	18	0.19
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	21	0.19
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	6	0.19
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	29	0.19
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	8	0.19
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	6	0.18
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	6	0.18
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	6	0.18
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	18	0.18
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	24	0.18
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	26	0.18
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	29	0.18
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	16	0.18
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	25	0.18
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	10	0.18
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	18	0.18
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	23	0.18
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	24	0.18
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	26	0.18
(1,148)	2:19:B:DT:H6	2:18:B:DG:H3'	29	0.18
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	7	0.18
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	18	0.18
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	20	0.18
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	4	0.18
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	6	0.18
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	9	0.18
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	11	0.18
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	13	0.18
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	19	0.18
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	23	0.18
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	30	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	4	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	7	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	8	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	10	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	12	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	18	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	20	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	21	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	22	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	24	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	25	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	28	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	29	0.18
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	30	0.18
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	4	0.18
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	5	0.18
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	9	0.18
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	11	0.18
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	13	0.18
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	16	0.18
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	19	0.18
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	21	0.18
(1,92)	2:12:B:DC:H2''	2:12:B:DC:H6	22	0.18
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	4	0.18
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	8	0.18
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	10	0.18
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	14	0.18
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	9	0.18
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	10	0.18
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	8	0.18
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	13	0.18
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	27	0.18
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	1	0.18
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	9	0.18
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	10	0.18
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	23	0.18
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	30	0.18
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	12	0.18
(1,6)	1:1:A:DC:H2''	1:1:A:DC:H6	15	0.18
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	14	0.17
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	5	0.17
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	5	0.17
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	5	0.17
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	30	0.17
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	30	0.17
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	30	0.17
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	11	0.17
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	11	0.17
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	12	0.17
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	12	0.17
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	12	0.17
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	13	0.17
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	13	0.17
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	13	0.17
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	15	0.17
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	15	0.17
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	15	0.17
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	15	0.17
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	25	0.17
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	8	0.17
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	7	0.17
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	17	0.17
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	18	0.17
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	20	0.17
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	8	0.17
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	10	0.17
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	14	0.17
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	16	0.17
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	24	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	1	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	7	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	12	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	14	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	15	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	22	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	25	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	26	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	27	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	28	0.17
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	29	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	1	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	2	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	3	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	5	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	6	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	9	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	11	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	15	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	17	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	19	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	23	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	26	0.17
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	27	0.17
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	5	0.17
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	25	0.17
(1,56)	1:9:A:DA:H8	1:8:A:DA:H8	7	0.17
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	1	0.17
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	6	0.17
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	7	0.17
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	16	0.17
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	17	0.17
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	19	0.17
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	20	0.17
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	22	0.17
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	25	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	1	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	2	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	3	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	4	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	5	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	6	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	7	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	8	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	9	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	10	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	11	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	12	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	13	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	14	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	15	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	16	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	17	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	18	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	19	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	20	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	21	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	22	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	23	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	24	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	25	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	26	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	27	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	28	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	29	0.17
(1,46)	1:7:A:DG:H2''	1:7:A:DG:H2'	30	0.17
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	2	0.17
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	5	0.17
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	6	0.17
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	13	0.17
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	5	0.17
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	7	0.17
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	2	0.17
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	3	0.17
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	8	0.17
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	15	0.17
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	25	0.17
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	15	0.16
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	3	0.16
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	3	0.16
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	3	0.16
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	20	0.16
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	20	0.16
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	20	0.16
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	21	0.16
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	21	0.16
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	21	0.16
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	29	0.16
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	29	0.16
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	29	0.16
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	7	0.16
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	7	0.16
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	7	0.16
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	26	0.16
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	26	0.16
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	26	0.16
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	27	0.16
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	27	0.16
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	27	0.16
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	30	0.16
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	30	0.16
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	30	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	8	0.16
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	8	0.16
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	8	0.16
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	25	0.16
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	25	0.16
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	25	0.16
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	11	0.16
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	12	0.16
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	25	0.16
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	10	0.16
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	24	0.16
(1,161)	2:20:B:DT:H6	2:19:B:DT:H3'	8	0.16
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	5	0.16
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	11	0.16
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	14	0.16
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	21	0.16
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	2	0.16
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	22	0.16
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	28	0.16
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	29	0.16
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	5	0.16
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	10	0.16
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	16	0.16
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	18	0.16
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	24	0.16
(1,108)	2:14:B:DT:H6	2:13:B:DA:H2'	13	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	3	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	6	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	8	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	9	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	11	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	14	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	15	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	16	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	19	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	21	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	23	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	24	0.16
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	27	0.16
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	24	0.16
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	29	0.16
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	30	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	1	0.16
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	4	0.16
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	5	0.16
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	10	0.16
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	11	0.16
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	12	0.16
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	15	0.16
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	17	0.16
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	21	0.16
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	23	0.16
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	25	0.16
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	12	0.16
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	15	0.16
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	16	0.16
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	20	0.16
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	22	0.16
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	30	0.16
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	14	0.16
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	20	0.16
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	11	0.16
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	12	0.16
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	13	0.16
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	1	0.15
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	30	0.15
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	9	0.15
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	9	0.15
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	9	0.15
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	14	0.15
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	14	0.15
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	14	0.15
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	27	0.15
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	27	0.15
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	27	0.15
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	15	0.15
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	15	0.15
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	15	0.15
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	16	0.15
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	16	0.15
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	16	0.15
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	9	0.15
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	9	0.15
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	1	0.15
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	2	0.15
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	3	0.15
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	8	0.15
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	9	0.15
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	13	0.15
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	30	0.15
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	2	0.15
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	8	0.15
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	30	0.15
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	6	0.15
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	26	0.15
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	27	0.15
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	1	0.15
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	12	0.15
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	13	0.15
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	15	0.15
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	19	0.15
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	23	0.15
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	25	0.15
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	26	0.15
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	30	0.15
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	2	0.15
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	8	0.15
(1,115)	2:14:B:DT:H3'	2:14:B:DT:H6	20	0.15
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	8	0.15
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	20	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	1	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	2	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	4	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	7	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	10	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	12	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	13	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	17	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	18	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	20	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	22	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	26	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	28	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	29	0.15
(1,76)	1:11:A:DG:H8	1:10:A:DT:H6	30	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	2	0.15
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	3	0.15
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	5	0.15
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	9	0.15
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	11	0.15
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	12	0.15
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	15	0.15
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	27	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	2	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	3	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	6	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	7	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	8	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	9	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	13	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	14	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	16	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	18	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	19	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	20	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	22	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	24	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	26	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	27	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	28	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	29	0.15
(1,43)	1:7:A:DG:H8	1:7:A:DG:H1'	30	0.15
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	7	0.15
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	8	0.15
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	19	0.15
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	29	0.15
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	4	0.15
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	2	0.14
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	2	0.14
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	2	0.14
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	1	0.14
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	1	0.14
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	1	0.14
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	3	0.14
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	3	0.14
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	3	0.14
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	13	0.14
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	13	0.14
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	21	0.14
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	21	0.14
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	21	0.14
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	22	0.14
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	22	0.14
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	22	0.14
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	29	0.14
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	29	0.14
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	29	0.14
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	1	0.14
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	1	0.14
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	1	0.14
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	23	0.14
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	24	0.14
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	1	0.14
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	3	0.14
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	9	0.14
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	13	0.14
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	15	0.14
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	23	0.14
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	27	0.14
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	13	0.14
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	18	0.14
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	24	0.14
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	25	0.14
(1,140)	2:18:B:DG:H8	2:17:B:DG:H2''	30	0.14
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	3	0.14
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	4	0.14
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	5	0.14
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	6	0.14
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	9	0.14
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	17	0.14
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	21	0.14
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	27	0.14
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	2	0.14
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	16	0.14
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	18	0.14
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	24	0.14
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	29	0.14
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	20	0.14
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	28	0.14
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	11	0.14
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	14	0.14
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	27	0.14
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	2	0.14
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	9	0.14
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	12	0.14
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	15	0.14
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	16	0.14
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	21	0.14
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	30	0.14
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	17	0.14
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	22	0.14
(1,229)	3:101:A:B2R:N29	2:18:B:DG:N1	19	0.13
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	15	0.13
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	15	0.13
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	15	0.13
(1,218)	2:19:B:DT:H71	2:18:B:DG:H8	25	0.13
(1,218)	2:19:B:DT:H72	2:18:B:DG:H8	25	0.13
(1,218)	2:19:B:DT:H73	2:18:B:DG:H8	25	0.13
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	1	0.13
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	1	0.13
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	1	0.13
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	10	0.13
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	10	0.13
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	10	0.13
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	17	0.13
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	17	0.13
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	17	0.13
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	19	0.13
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	19	0.13
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	19	0.13
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	25	0.13
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	25	0.13
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	25	0.13
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	4	0.13
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	4	0.13
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	4	0.13
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	10	0.13
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	10	0.13
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	17	0.13
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	17	0.13
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	17	0.13
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	18	0.13
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	18	0.13
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	18	0.13
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	19	0.13
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	19	0.13
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	19	0.13
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	23	0.13
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	23	0.13
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	23	0.13
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	24	0.13
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	24	0.13
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	24	0.13
(1,193)	1:2:A:DT:H71	1:2:A:DT:H6	11	0.13
(1,193)	1:2:A:DT:H72	1:2:A:DT:H6	11	0.13
(1,193)	1:2:A:DT:H73	1:2:A:DT:H6	11	0.13
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	23	0.13
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	23	0.13
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	23	0.13
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	24	0.13
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	24	0.13
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	24	0.13
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	10	0.13
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	4	0.13
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	12	0.13
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	25	0.13
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	6	0.13
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	7	0.13
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	19	0.13
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	21	0.13
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	2	0.13
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	10	0.13
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	12	0.13
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	15	0.13
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	23	0.13
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	28	0.13
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	29	0.13
(1,154)	2:19:B:DT:H2''	2:19:B:DT:H6	19	0.13
(1,140)	2:18:B:DG:H8	2:17:B:DG:H2''	1	0.13
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	7	0.13
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	12	0.13
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	14	0.13
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	15	0.13
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	19	0.13
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	22	0.13
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	25	0.13
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	28	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	1	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	2	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	3	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	4	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	5	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	6	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	7	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	8	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	9	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	10	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	11	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	12	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	13	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	14	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	15	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	16	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	17	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	18	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	19	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	20	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	21	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	22	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	23	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	24	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	25	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	26	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	27	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	28	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	29	0.13
(1,79)	1:11:A:DG:H8	1:11:A:DG:H1'	30	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	1	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	2	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	4	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	6	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	7	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	9	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	11	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	12	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	13	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	15	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	16	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	17	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	21	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	22	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	26	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	27	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	28	0.13
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	29	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	1	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	2	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	3	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	8	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	9	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	10	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	12	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	13	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	17	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	25	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	26	0.13
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	28	0.13
(1,53)	1:8:A:DA:H3'	1:8:A:DA:H8	28	0.13
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	5	0.13
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	12	0.13
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	13	0.13
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	16	0.13
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	18	0.13
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	24	0.13
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	27	0.13
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	29	0.13
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	1	0.13
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	10	0.13
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	17	0.13
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	22	0.13
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	6	0.13
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	20	0.13
(2,21)	2:19:B:DT:O4	1:4:A:DA:N6	10	0.12
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	1	0.12
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	1	0.12
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	1	0.12
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	16	0.12
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	16	0.12
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	16	0.12
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	28	0.12
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	28	0.12
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	28	0.12
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	23	0.12
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	23	0.12
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	23	0.12
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	28	0.12
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	28	0.12
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	28	0.12
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	12	0.12
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	12	0.12
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	12	0.12
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	23	0.12
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	23	0.12
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	23	0.12
(1,194)	1:10:A:DT:H71	1:9:A:DA:H8	9	0.12
(1,194)	1:10:A:DT:H72	1:9:A:DA:H8	9	0.12
(1,194)	1:10:A:DT:H73	1:9:A:DA:H8	9	0.12
(1,191)	1:2:A:DT:H71	1:1:A:DC:H2''	30	0.12
(1,191)	1:2:A:DT:H72	1:1:A:DC:H2''	30	0.12
(1,191)	1:2:A:DT:H73	1:1:A:DC:H2''	30	0.12
(1,171)	2:21:B:DA:H8	2:20:B:DT:H3'	4	0.12
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	5	0.12
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	26	0.12
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	28	0.12
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	17	0.12
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	20	0.12
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	22	0.12
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	26	0.12
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	29	0.12
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	1	0.12
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	3	0.12
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	9	0.12
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	14	0.12
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	16	0.12
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	26	0.12
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	29	0.12
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	30	0.12
(1,155)	2:19:B:DT:H3'	2:19:B:DT:H6	19	0.12
(1,154)	2:19:B:DT:H2''	2:19:B:DT:H6	21	0.12
(1,140)	2:18:B:DG:H8	2:17:B:DG:H2''	4	0.12
(1,118)	2:15:B:DT:H6	2:14:B:DT:H2'	11	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	1	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	2	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	3	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	4	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	5	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	6	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	7	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	8	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	9	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	10	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	11	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	12	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	13	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	14	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	15	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	16	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	17	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	18	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	19	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	20	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	21	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	22	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	23	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	24	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	25	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	26	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	27	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	28	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	29	0.12
(1,114)	2:14:B:DT:H2''	2:14:B:DT:H2'	30	0.12
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	1	0.12
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	4	0.12
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	9	0.12
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	10	0.12
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	23	0.12
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	26	0.12
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	27	0.12
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	30	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	3	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	8	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	10	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	14	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	18	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	19	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	20	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	23	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	24	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	25	0.12
(1,72)	1:10:A:DT:H2''	1:10:A:DT:H2'	30	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	4	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	6	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	7	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	11	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	14	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	15	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	16	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	18	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	19	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	20	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	21	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	22	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	23	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	24	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	27	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	29	0.12
(1,60)	1:9:A:DA:H2''	1:9:A:DA:H8	30	0.12
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	2	0.12
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	6	0.12
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	7	0.12
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	8	0.12
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	14	0.12
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	15	0.12
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	19	0.12
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	26	0.12
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	26	0.12
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	4	0.12
(1,20)	1:3:A:DA:H8	1:2:A:DT:H2'	21	0.12
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	7	0.12
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	14	0.12
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	18	0.12
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	19	0.12
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	26	0.12
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	27	0.12
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	28	0.12
(2,21)	2:19:B:DT:O4	1:4:A:DA:N6	3	0.11
(2,21)	2:19:B:DT:O4	1:4:A:DA:N6	4	0.11
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	18	0.11
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	18	0.11
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	18	0.11
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	16	0.11
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	16	0.11
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	16	0.11
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	19	0.11
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	19	0.11
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	19	0.11
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	22	0.11
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	22	0.11
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	22	0.11
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	9	0.11
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	9	0.11
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	9	0.11
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	15	0.11
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	15	0.11
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	15	0.11
(1,189)	1:2:A:DT:H71	1:1:A:DC:H5	10	0.11
(1,189)	1:2:A:DT:H72	1:1:A:DC:H5	10	0.11
(1,189)	1:2:A:DT:H73	1:1:A:DC:H5	10	0.11
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	11	0.11
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	14	0.11
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	16	0.11
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	17	0.11
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	18	0.11
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	20	0.11
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	21	0.11
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	5	0.11
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	14	0.11
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	16	0.11
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	4	0.11
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	5	0.11
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	6	0.11
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	7	0.11
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	17	0.11
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	19	0.11
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	20	0.11
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	22	0.11
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	27	0.11
(1,154)	2:19:B:DT:H2''	2:19:B:DT:H6	29	0.11
(1,143)	2:18:B:DG:H3'	2:18:B:DG:H8	23	0.11
(1,140)	2:18:B:DG:H8	2:17:B:DG:H2''	7	0.11
(1,140)	2:18:B:DG:H8	2:17:B:DG:H2''	10	0.11
(1,140)	2:18:B:DG:H8	2:17:B:DG:H2''	13	0.11
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	3	0.11
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	13	0.11
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	17	0.11
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	21	0.11
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	1	0.11
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	3	0.11
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	4	0.11
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	9	0.11
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	11	0.11
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	17	0.11
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	23	0.11
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	25	0.11
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	30	0.11
(1,30)	1:4:A:DA:H8	1:4:A:DA:H3'	25	0.11
(1,27)	1:4:A:DA:H8	1:3:A:DA:H8	24	0.11
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	29	0.11
(2,21)	2:19:B:DT:O4	1:4:A:DA:N6	1	0.1
(2,21)	2:19:B:DT:O4	1:4:A:DA:N6	9	0.1
(2,21)	2:19:B:DT:O4	1:4:A:DA:N6	30	0.1
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	14	0.1
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	14	0.1
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	14	0.1
(1,225)	2:20:B:DT:H71	2:19:B:DT:H6	25	0.1
(1,225)	2:20:B:DT:H72	2:19:B:DT:H6	25	0.1
(1,225)	2:20:B:DT:H73	2:19:B:DT:H6	25	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	2:19:B:DT:H71	2:18:B:DG:H3'	1	0.1
(1,220)	2:19:B:DT:H72	2:18:B:DG:H3'	1	0.1
(1,220)	2:19:B:DT:H73	2:18:B:DG:H3'	1	0.1
(1,205)	2:14:B:DT:H71	2:14:B:DT:H6	8	0.1
(1,205)	2:14:B:DT:H72	2:14:B:DT:H6	8	0.1
(1,205)	2:14:B:DT:H73	2:14:B:DT:H6	8	0.1
(1,189)	1:2:A:DT:H71	1:1:A:DC:H5	3	0.1
(1,189)	1:2:A:DT:H72	1:1:A:DC:H5	3	0.1
(1,189)	1:2:A:DT:H73	1:1:A:DC:H5	3	0.1
(1,189)	1:2:A:DT:H71	1:1:A:DC:H5	24	0.1
(1,189)	1:2:A:DT:H72	1:1:A:DC:H5	24	0.1
(1,189)	1:2:A:DT:H73	1:1:A:DC:H5	24	0.1
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	6	0.1
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	19	0.1
(1,170)	2:21:B:DA:H8	2:20:B:DT:H2''	29	0.1
(1,167)	2:20:B:DT:H2''	2:20:B:DT:H6	28	0.1
(1,160)	2:20:B:DT:H6	2:19:B:DT:H2''	21	0.1
(1,154)	2:19:B:DT:H2''	2:19:B:DT:H6	5	0.1
(1,140)	2:18:B:DG:H8	2:17:B:DG:H2''	2	0.1
(1,140)	2:18:B:DG:H8	2:17:B:DG:H2''	21	0.1
(1,113)	2:14:B:DT:H2''	2:14:B:DT:H6	11	0.1
(1,45)	1:7:A:DG:H2''	1:7:A:DG:H8	21	0.1
(1,12)	1:2:A:DT:H6	1:1:A:DC:H2''	5	0.1

10 Dihedral-angle violation analysis ⓘ

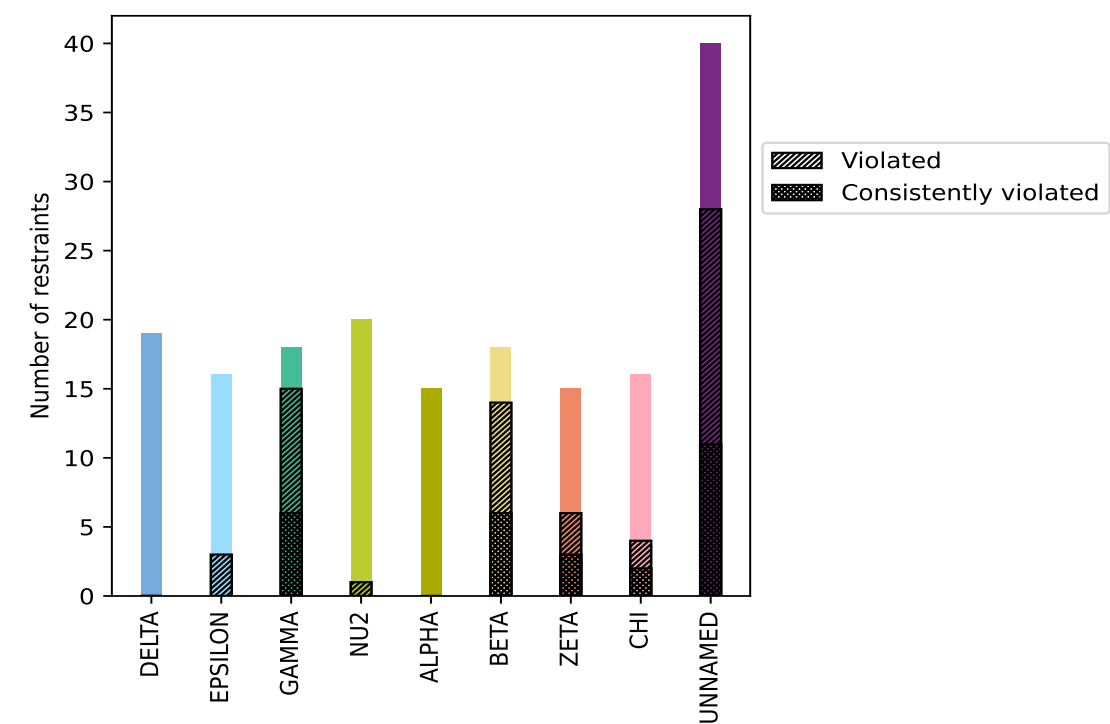
10.1 Summary of dihedral-angle violations ⓘ

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
DELTA	19	10.7	0	0.0	0.0	0	0.0	0.0
EPSILON	16	9.0	3	18.8	1.7	0	0.0	0.0
GAMMA	18	10.2	15	83.3	8.5	6	33.3	3.4
NU2	20	11.3	1	5.0	0.6	0	0.0	0.0
ALPHA	15	8.5	0	0.0	0.0	0	0.0	0.0
BETA	18	10.2	14	77.8	7.9	6	33.3	3.4
ZETA	15	8.5	6	40.0	3.4	3	20.0	1.7
CHI	16	9.0	4	25.0	2.3	2	12.5	1.1
UNNAMED	40	22.6	28	70.0	15.8	11	27.5	6.2
Total	177	100.0	71	40.1	40.1	28	15.8	15.8

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

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



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

10.2 Dihedral-angle violation statistics for each model ⓘ

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

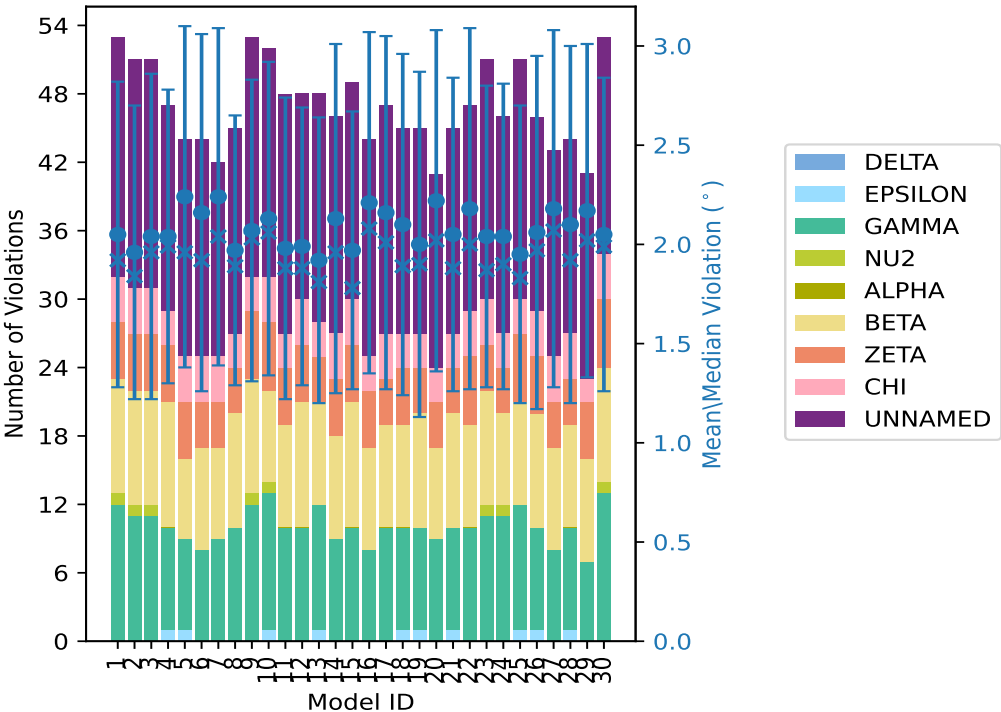
Model ID	Number of violations									Total	Mean (°)	Max (°)	SD (°)	Median (°)
	DELTA	EPSILON	GAMMA	NU2	ALPHA	BETA	ZETA	CHI	UNNAMED					
1	0	0	12	1	0	10	5	4	21	53	2.05	4.08	0.77	1.9
2	0	0	11	1	0	10	5	4	20	51	1.96	3.84	0.74	1.8
3	0	0	11	1	0	10	5	4	20	51	2.04	4.35	0.82	1.9
4	0	1	9	0	0	11	5	3	18	47	2.04	4.1	0.74	1.9
5	0	1	8	0	0	7	5	4	19	44	2.24	5.4	0.86	1.9
6	0	0	8	0	0	9	4	4	19	44	2.16	5.49	0.9	1.9
7	0	0	9	0	0	8	4	4	17	42	2.24	5.74	0.85	2.0
8	0	0	10	0	0	10	4	3	18	45	1.97	3.82	0.68	1.8
9	0	0	12	1	0	10	6	3	21	53	2.07	3.98	0.76	2.0
10	0	1	12	1	0	8	6	4	20	52	2.13	4.41	0.79	2.0
11	0	0	10	0	0	9	5	3	21	48	1.98	4.23	0.76	1.8
12	0	0	10	0	0	11	5	4	18	48	1.99	3.83	0.7	1.8
13	0	1	11	0	0	9	4	3	20	48	1.92	4.04	0.72	1.8
14	0	0	9	0	0	9	5	4	19	46	2.13	5.33	0.88	1.9
15	0	0	10	0	0	11	5	4	19	49	1.97	3.96	0.7	1.7
16	0	0	8	0	0	9	5	3	19	44	2.21	5.44	0.86	2.0
17	0	0	10	0	0	9	4	4	20	47	2.16	5.57	0.89	2.0
18	0	1	9	0	0	9	5	3	18	45	2.1	5.21	0.86	1.8
19	0	1	9	0	0	10	4	3	18	45	2.0	5.2	0.87	1.7
20	0	0	9	0	0	8	4	3	17	41	2.22	5.39	0.86	2.0
21	0	1	9	0	0	10	4	3	18	45	2.05	4.22	0.79	1.8
22	0	0	10	0	0	9	6	4	18	47	2.18	5.63	0.91	2.0
23	0	0	11	1	0	10	4	4	21	51	2.04	3.97	0.76	1.8
24	0	0	11	1	0	8	4	3	19	46	2.04	4.43	0.77	1.7
25	0	1	11	0	0	9	6	3	21	51	1.95	4.04	0.75	1.8
26	0	1	9	0	0	10	5	4	17	46	2.06	5.35	0.89	1.9
27	0	0	8	0	0	9	4	4	18	43	2.18	5.69	0.9	2.0
28	0	1	9	0	0	9	4	4	17	44	2.1	5.18	0.9	1.9

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Model ID	Number of violations										Total	Mean (°)	Max (°)	SD (°)	Median
	DELTA	EPSILON	GAMMA	NU2	ALPHA	BETA	ZETA	CHI	UNNAMED						
29	0	0	7	0	0	9	5	2	18	41	2.17	5.33	0.84	2.0	
30	0	0	13	1	0	10	6	4	19	53	2.05	3.97	0.79	1.9	

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints										Fraction of the ensemble	
DELTA	EPSILON	GAMMA	NU2	ALPHA	BETA	ZETA	CHI	UNNAMED	Total	Count ¹	%
0	0	1	0	0	0	0	0	1	2	1	3.3
0	1	2	0	0	1	0	0	2	6	2	6.7
0	1	0	0	0	0	0	0	1	2	3	10.0
0	0	0	0	0	0	0	0	0	0	4	13.3
0	1	0	0	0	0	0	0	1	2	5	16.7
0	0	0	0	0	0	0	0	1	1	6	20.0
0	0	0	0	0	0	0	0	1	1	7	23.3
0	0	0	1	0	0	1	0	1	3	8	26.7
0	0	1	0	0	1	0	0	1	3	9	30.0

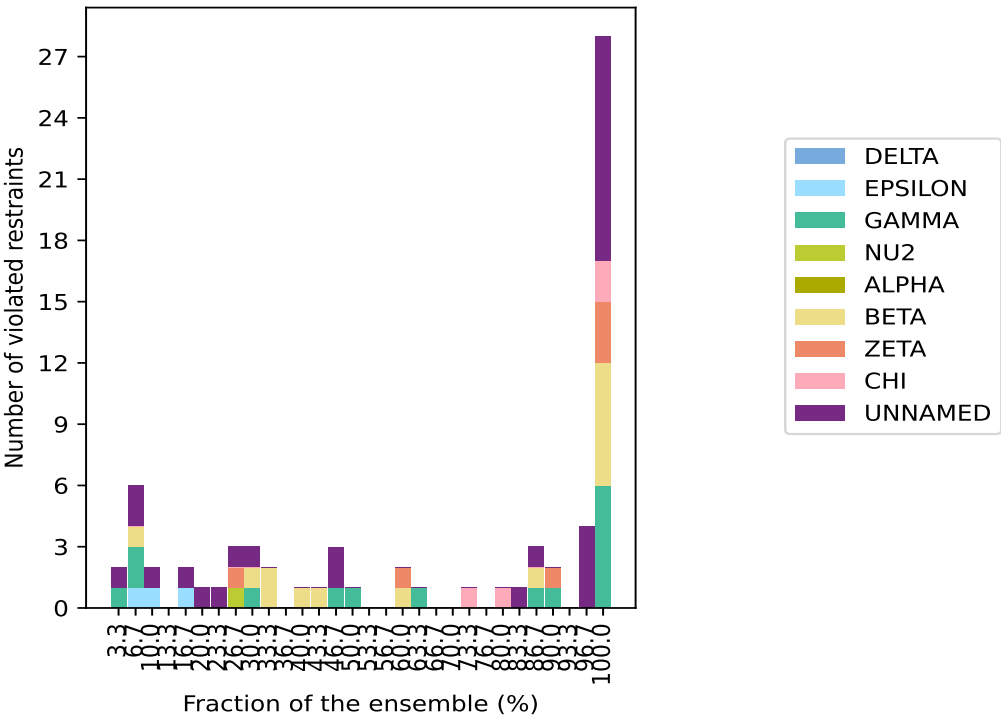
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Number of violated restraints										Fraction of the ensemble	
DELTA	EPSILON	GAMMA	NU2	ALPHA	BETA	ZETA	CHI	UNNAMED	Total	Count ¹	%
0	0	0	0	0	2	0	0	0	2	10	33.3
0	0	0	0	0	0	0	0	0	0	11	36.7
0	0	0	0	0	1	0	0	0	1	12	40.0
0	0	0	0	0	1	0	0	0	1	13	43.3
0	0	1	0	0	0	0	0	2	3	14	46.7
0	0	1	0	0	0	0	0	0	1	15	50.0
0	0	0	0	0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	0	0	0	0	17	56.7
0	0	0	0	0	1	1	0	0	2	18	60.0
0	0	1	0	0	0	0	0	0	1	19	63.3
0	0	0	0	0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	0	1	0	1	22	73.3
0	0	0	0	0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	0	1	0	1	24	80.0
0	0	0	0	0	0	0	0	1	1	25	83.3
0	0	1	0	0	1	0	0	1	3	26	86.7
0	0	1	0	0	0	1	0	0	2	27	90.0
0	0	0	0	0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	0	0	4	4	29	96.7
0	0	6	0	0	6	3	2	11	28	30	100.0

¹ Number of models with violations

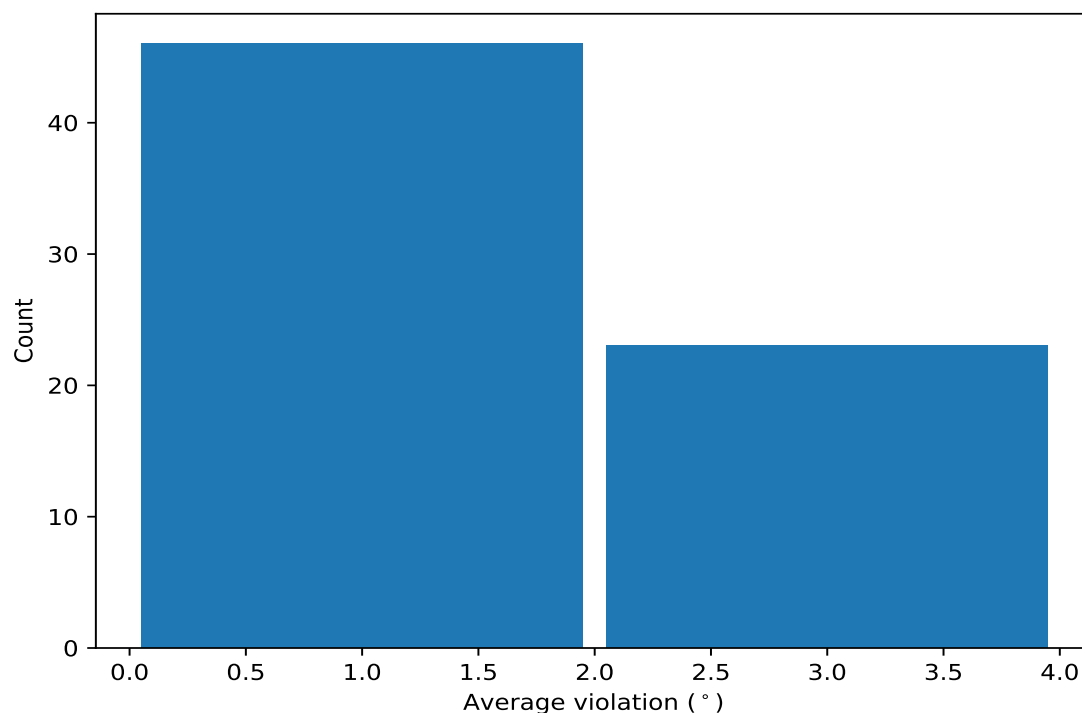
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	30	3.95	1.45	3.89
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	30	3.89	0.09	3.88
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	30	3.63	0.42	3.72
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	30	3.31	0.14	3.33
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	30	3.21	0.6	2.91
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	30	2.94	0.14	2.92
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	30	2.92	0.17	2.92
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	30	2.66	0.31	2.7
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	30	2.61	0.19	2.62
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	30	2.52	0.48	2.55
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	30	2.4	0.16	2.42
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	30	2.35	0.07	2.34
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	30	2.32	0.49	2.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	30	2.26	0.26	2.3
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	30	2.24	0.39	2.3
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	30	2.21	0.28	2.16
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	30	2.19	0.66	2.12
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	30	2.17	0.27	2.17
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	30	2.12	0.1	2.11
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	30	2.1	0.26	2.14
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	30	2.09	0.25	2.13
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	30	1.99	0.39	1.96
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	30	1.96	0.12	1.92
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	30	1.95	0.11	1.98
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	30	1.76	0.11	1.77
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	30	1.73	0.22	1.72
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	30	1.67	0.14	1.66
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	30	1.61	0.3	1.52
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	29	2.45	0.51	2.53
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	29	1.81	0.52	1.46
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	29	1.69	0.29	1.81
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	29	1.65	0.22	1.68
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	27	1.8	0.26	1.87
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	27	1.66	0.35	1.72
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	26	1.46	0.23	1.47
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	26	1.26	0.16	1.27
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	26	1.16	0.16	1.12
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	25	1.93	0.37	2.0
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	24	1.17	0.12	1.15
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	22	1.12	0.09	1.1
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	19	1.32	0.23	1.36
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	18	1.35	0.24	1.31
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	18	1.08	0.06	1.06
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	15	1.15	0.14	1.08
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	14	2.92	1.34	3.64
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	14	1.4	0.18	1.33
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	14	1.19	0.14	1.16
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	13	1.32	0.1	1.34
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	12	1.05	0.04	1.04
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	10	1.52	0.22	1.54
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	10	1.34	0.23	1.34
(1,84)	1:2:A:DT:O5'	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	9	1.71	0.17	1.72
(1,109)	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:C2'	9	1.19	0.15	1.13
(1,51)	1:7:A:DG:P	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	9	1.18	0.18	1.07
(1,102)	1:1:A:DC:C1'	1:1:A:DC:C2'	1:1:A:DC:C3'	1:1:A:DC:C4'	8	1.64	0.21	1.7
(1,27)	2:17:B:DG:C3'	2:17:B:DG:O3'	2:18:B:DG:P	2:18:B:DG:O5'	8	1.45	0.31	1.42
(1,158)	2:21:B:DA:C1'	2:21:B:DA:O4'	2:21:B:DA:C4'	2:21:B:DA:C5'	8	1.09	0.05	1.09
(1,119)	1:7:A:DG:C1'	1:7:A:DG:O4'	1:7:A:DG:C4'	1:7:A:DG:C5'	7	1.81	0.28	1.83
(1,116)	1:6:A:DG:C1'	1:6:A:DG:O4'	1:6:A:DG:C4'	1:6:A:DG:C5'	6	1.38	0.22	1.34
(1,106)	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	1:2:A:DT:C2'	5	1.17	0.19	1.1
(1,3)	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	5	1.08	0.04	1.08
(1,146)	2:17:B:DG:C1'	2:17:B:DG:O4'	2:17:B:DG:C4'	2:17:B:DG:C5'	3	1.62	0.28	1.67
(1,5)	1:7:A:DG:C4'	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	3	1.34	0.3	1.27
(1,16)	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:O3'	2:22:B:DG:P	2	1.37	0.23	1.37

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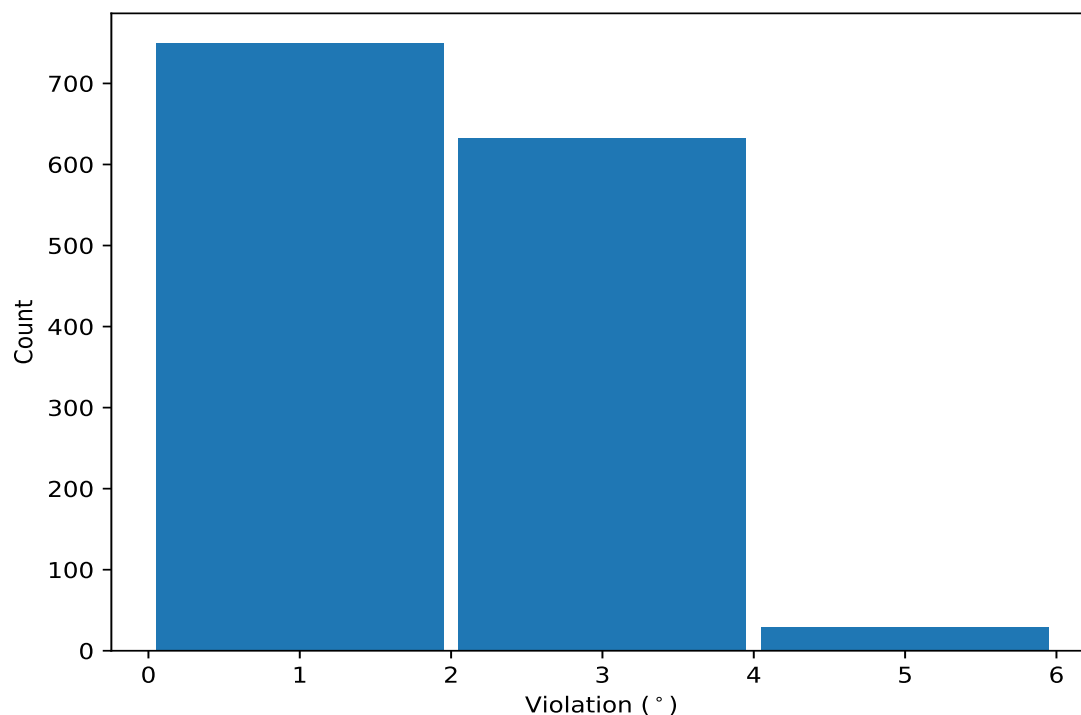
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,87)	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	1:6:A:DG:C3'	2	1.3	0.09	1.3
(1,48)	1:3:A:DA:P	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	2	1.14	0.03	1.14
(1,113)	1:4:A:DA:C1'	1:4:A:DA:O4'	1:4:A:DA:C4'	1:4:A:DA:C5'	2	1.12	0.08	1.12
(1,99)	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2	1.08	0.05	1.08
(1,131)	1:11:A:DG:C1'	1:11:A:DG:O4'	1:11:A:DG:C4'	1:11:A:DG:C5'	2	1.04	0.02	1.04

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	7	5.74
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	27	5.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	22	5.63
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	17	5.57
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	6	5.49
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	16	5.44
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	5	5.4
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	20	5.39
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	26	5.35
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	14	5.33
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	29	5.33
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	18	5.21
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	19	5.2
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	28	5.18
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	24	4.43
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	10	4.41
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	3	4.35
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	11	4.23
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	21	4.22
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	3	4.19
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	21	4.14
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	4	4.1
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	17	4.1
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	1	4.08
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	27	4.06
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	1	4.05
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	6	4.05
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	13	4.04
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	25	4.04
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	4	3.99
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	9	3.98
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	11	3.98
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	26	3.97
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	21	3.97
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	23	3.97
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	30	3.97
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	30	3.97
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	20	3.97
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	15	3.96
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	9	3.96
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	3	3.95
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	22	3.95
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	19	3.94
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	10	3.94
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	6	3.93
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	23	3.93
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	7	3.92
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	23	3.9
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	14	3.9
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	18	3.9
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	1	3.88
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	17	3.88
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	28	3.88

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	27	3.87
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	5	3.87
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	28	3.87
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	7	3.86
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	16	3.86
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	14	3.86
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	6	3.85
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	30	3.84
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	2	3.84
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	17	3.84
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	12	3.83
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	27	3.83
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	8	3.82
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	5	3.81
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	20	3.8
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	22	3.8
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	18	3.8
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	26	3.8
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	29	3.8
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	9	3.79
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	24	3.79
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	16	3.79
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	12	3.78
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	29	3.78
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	19	3.77
(1,128)	1:10:A:DT:C1'	1:10:A:DT:O4'	1:10:A:DT:C4'	1:10:A:DT:C5'	26	3.76
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	25	3.74
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	28	3.69
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	15	3.66
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	5	3.59
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	10	3.58
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	4	3.56
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	14	3.51
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	22	3.49
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	11	3.48
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	15	3.48
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	24	3.47
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	5	3.46
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	19	3.46
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	22	3.45
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	13	3.44
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	23	3.44
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	5	3.44
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	29	3.43
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	16	3.43
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	18	3.43
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	3	3.42
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	5	3.42
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	10	3.41
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	20	3.41
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	30	3.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	21	3.4
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	14	3.39
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	13	3.38
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	30	3.36
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	2	3.36
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	24	3.35
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	2	3.33
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	25	3.33
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	26	3.32
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	28	3.32
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	17	3.27
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	29	3.25
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	7	3.25
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	25	3.25
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	7	3.23
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	7	3.23
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	25	3.23
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	19	3.22
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	6	3.21
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	27	3.21
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	20	3.19
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	5	3.18
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	15	3.18
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	8	3.18
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	2	3.16
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	9	3.16
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	16	3.15
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	1	3.15
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	16	3.14
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	13	3.14
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	1	3.14
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	20	3.13
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	3	3.12
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	14	3.11
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	28	3.11
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	10	3.11
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	24	3.1
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	17	3.1
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	4	3.09
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	16	3.09
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	22	3.09
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	12	3.08
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	9	3.08
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	3	3.08
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	29	3.07
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	1	3.06
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	6	3.05
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	30	3.04
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	12	3.03
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	21	3.03
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	10	3.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	6	3.03
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	8	3.02
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	20	3.01
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	20	3.01
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	8	3.01
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	13	3.0
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	6	2.99
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	19	2.99
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	10	2.99
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	10	2.98
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	23	2.98
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	7	2.98
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	21	2.98
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	14	2.97
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	10	2.97
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	25	2.96
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	12	2.95
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	3	2.95
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	30	2.95
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	10	2.94
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	19	2.94
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	15	2.94
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	8	2.94
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	18	2.94
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	2	2.93
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	22	2.93
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	28	2.93
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	11	2.92
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	17	2.92
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	27	2.92
(1,140)	2:14:B:DT:C1'	2:14:B:DT:O4'	2:14:B:DT:C4'	2:14:B:DT:C5'	30	2.92
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	2	2.92
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	1	2.92
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	22	2.91
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	9	2.9
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	4	2.9
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	18	2.9
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	26	2.9
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	10	2.9
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	24	2.9
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	24	2.89
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	11	2.89
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	7	2.89
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	1	2.89
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	13	2.88
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	28	2.87
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	27	2.87
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	3	2.86
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	30	2.86
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	16	2.86
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	8	2.85

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	1	2.85
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	30	2.84
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	26	2.84
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	23	2.84
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	3	2.84
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	18	2.83
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	29	2.83
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	14	2.83
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	4	2.83
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	13	2.83
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2	2.82
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	11	2.82
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	8	2.81
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	12	2.81
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	17	2.81
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	24	2.81
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	9	2.81
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	23	2.8
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	10	2.8
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	30	2.8
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	10	2.79
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	22	2.79
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	18	2.79
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	22	2.79
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	15	2.79
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	3	2.78
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	13	2.78
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	23	2.78
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	2	2.78
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	12	2.78
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	9	2.77
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	10	2.77
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	24	2.76
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	15	2.76
(1,143)	2:15:B:DT:C1'	2:15:B:DT:O4'	2:15:B:DT:C4'	2:15:B:DT:C5'	18	2.76
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	30	2.76
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1	2.76
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	14	2.76
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	9	2.75
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	14	2.75
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	22	2.75
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	11	2.75
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	21	2.75
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	22	2.74
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	26	2.74
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	28	2.74
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	25	2.74
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	25	2.73
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	16	2.73
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	7	2.73
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	4	2.73

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	20	2.72
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	9	2.72
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	25	2.72
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	2	2.72
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	16	2.72
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	17	2.71
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	17	2.71
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	30	2.71
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	17	2.71
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	8	2.71
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	8	2.71
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	2	2.7
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	11	2.69
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	9	2.69
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	18	2.68
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	25	2.68
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	13	2.68
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	23	2.68
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	9	2.68
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	15	2.67
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	15	2.67
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	9	2.67
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	16	2.66
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	10	2.66
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	12	2.66
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	4	2.65
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	2	2.65
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	6	2.65
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	16	2.64
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	23	2.64
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	9	2.64
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	25	2.63
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2	2.63
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	8	2.63
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	1	2.62
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	29	2.62
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	21	2.62
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	23	2.62
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	29	2.61
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	26	2.61
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	4	2.61
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	5	2.61
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	13	2.61
(1,161)	2:22:B:DG:C1'	2:22:B:DG:O4'	2:22:B:DG:C4'	2:22:B:DG:C5'	4	2.6
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	24	2.6
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	6	2.6
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	19	2.6
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	18	2.6
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	28	2.59
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	3	2.59
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	11	2.58

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	17	2.57
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	1	2.56
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	2	2.56
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	9	2.56
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	30	2.56
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	5	2.56
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	14	2.56
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	14	2.55
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	23	2.55
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	12	2.55
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	27	2.55
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	9	2.55
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	18	2.54
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	4	2.54
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	5	2.54
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	21	2.54
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	18	2.54
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	27	2.54
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	8	2.53
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	12	2.53
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	27	2.53
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	13	2.53
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	25	2.53
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	27	2.53
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	16	2.53
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	22	2.53
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	26	2.52
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	28	2.52
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	21	2.52
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	2	2.52
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	22	2.51
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	2	2.51
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	4	2.51
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	11	2.51
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	11	2.51
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	12	2.51
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	23	2.51
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	5	2.5
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	8	2.5
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	11	2.5
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	27	2.49
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	26	2.49
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	30	2.49
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	12	2.49
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	18	2.49
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	24	2.49
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	29	2.49
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	24	2.48
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	5	2.48
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	16	2.48
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1	2.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	20	2.48
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	24	2.48
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	4	2.48
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	22	2.48
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	28	2.47
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	9	2.47
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	4	2.47
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	12	2.47
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	7	2.46
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	26	2.46
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	11	2.46
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	9	2.46
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	4	2.46
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	15	2.46
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	25	2.46
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	14	2.45
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	28	2.45
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	2	2.45
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	6	2.45
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	8	2.45
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	26	2.45
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	13	2.45
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	11	2.45
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	15	2.45
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	5	2.44
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	22	2.44
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	3	2.44
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	24	2.44
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1	2.44
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	12	2.44
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	15	2.43
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	21	2.43
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	21	2.43
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	8	2.43
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	9	2.43
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	12	2.43
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	11	2.43
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	5	2.42
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	1	2.42
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	12	2.42
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	15	2.42
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	1	2.42
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	3	2.42
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	7	2.42
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	23	2.42
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	6	2.41
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	20	2.41
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	23	2.41
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	19	2.41
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	17	2.41
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	20	2.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	17	2.41
(1,125)	1:9:A:DA:C1'	1:9:A:DA:O4'	1:9:A:DA:C4'	1:9:A:DA:C5'	5	2.4
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	1	2.4
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	23	2.4
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	3	2.4
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	1	2.39
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	20	2.39
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	6	2.39
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	18	2.38
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	30	2.38
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	11	2.38
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	3	2.38
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	27	2.38
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	22	2.38
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	29	2.37
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	4	2.37
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	23	2.37
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	25	2.37
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	11	2.37
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	27	2.37
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	30	2.37
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	23	2.37
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	30	2.36
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	2	2.36
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	20	2.35
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	7	2.35
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	23	2.35
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	25	2.35
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	9	2.35
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	29	2.35
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	29	2.34
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	4	2.34
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	14	2.34
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	3	2.34
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	19	2.34
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	28	2.34
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	6	2.34
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	10	2.34
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	27	2.33
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	18	2.33
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	22	2.33
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	25	2.33
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	2	2.33
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	18	2.33
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	21	2.33
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	19	2.32
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	7	2.32
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	20	2.32
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	5	2.32
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	9	2.32
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	29	2.32

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	14	2.32
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	23	2.32
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	14	2.32
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	19	2.32
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	6	2.31
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	16	2.31
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	22	2.31
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	10	2.31
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	14	2.31
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	15	2.31
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	20	2.31
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	22	2.31
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	24	2.31
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	21	2.31
(1,63)	2:21:B:DA:P	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	15	2.31
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	21	2.31
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	3	2.3
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	10	2.3
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	23	2.3
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	29	2.3
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	12	2.3
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	10	2.3
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	3	2.3
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1	2.3
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	25	2.3
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	10	2.29
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	15	2.29
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	11	2.29
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	6	2.29
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	11	2.29
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	28	2.29
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	20	2.29
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	17	2.28
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	27	2.28
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	24	2.28
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	10	2.28
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	5	2.28
(1,94)	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	17	2.28
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	16	2.28
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	26	2.28
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	7	2.28
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	17	2.27
(1,91)	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	1:10:A:DT:C3'	10	2.27
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	13	2.27
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	21	2.27
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	3	2.27
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	10	2.26
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1	2.26
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	7	2.25
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	1	2.25
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	4	2.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	26	2.25
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	2	2.24
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	26	2.24
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	14	2.24
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	20	2.24
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	16	2.24
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	16	2.23
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	9	2.23
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	18	2.23
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	15	2.23
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	2	2.22
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	1	2.21
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	3	2.21
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	4	2.21
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	19	2.2
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	7	2.2
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	21	2.2
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	5	2.2
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	22	2.2
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	28	2.2
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	2	2.19
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	6	2.19
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	7	2.19
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	7	2.18
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	12	2.18
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	27	2.18
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	3	2.18
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	16	2.18
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	19	2.18
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	30	2.18
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	9	2.17
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	17	2.17
(1,119)	1:7:A:DG:C1'	1:7:A:DG:O4'	1:7:A:DG:C4'	1:7:A:DG:C5'	1	2.17
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	9	2.17
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	8	2.17
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	17	2.17
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	24	2.17
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	11	2.16
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	2	2.16
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	7	2.16
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	28	2.16
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	27	2.16
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	7	2.16
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	19	2.16
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	17	2.15
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	13	2.15
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	12	2.15
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	29	2.14
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	8	2.14
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	24	2.14
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	30	2.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	22	2.14
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	21	2.13
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	4	2.13
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	9	2.13
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	13	2.13
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	19	2.13
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	25	2.13
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	18	2.13
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	30	2.13
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	12	2.12
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	14	2.12
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	4	2.12
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	15	2.12
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	25	2.12
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	28	2.12
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	16	2.12
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	8	2.11
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	30	2.11
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	30	2.11
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	21	2.1
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	27	2.1
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	3	2.1
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	3	2.1
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	23	2.1
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	17	2.1
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	27	2.1
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	10	2.09
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	16	2.09
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	29	2.09
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	27	2.09
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	14	2.09
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	10	2.09
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	30	2.08
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	1	2.08
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	6	2.08
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	16	2.08
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	4	2.07
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	16	2.07
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	29	2.07
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	27	2.07
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	30	2.07
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	26	2.06
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	20	2.06
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	1	2.06
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	10	2.06
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	10	2.06
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	22	2.06
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	9	2.06
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	27	2.06
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	28	2.05
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	21	2.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	28	2.05
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	2	2.05
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	25	2.05
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	8	2.05
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	27	2.04
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	29	2.04
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	4	2.04
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	16	2.04
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	20	2.04
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	28	2.04
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	7	2.04
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	8	2.04
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	13	2.03
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	18	2.03
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	24	2.03
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	15	2.03
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	13	2.03
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	7	2.03
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	12	2.03
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	9	2.03
(1,52)	1:8:A:DA:P	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	26	2.03
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	17	2.03
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	13	2.02
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	15	2.02
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	14	2.02
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	29	2.02
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	29	2.02
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	20	2.02
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	29	2.02
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	17	2.01
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	23	2.01
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	6	2.01
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	16	2.01
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	17	2.01
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	29	2.01
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	8	2.01
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	11	2.0
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	14	2.0
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	7	2.0
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	26	2.0
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	20	2.0
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	9	2.0
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	10	2.0
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	22	2.0
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	19	2.0
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	12	2.0
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	7	2.0
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	7	1.99
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	29	1.99
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	25	1.99
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	7	1.99

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	19	1.99
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	20	1.99
(1,137)	2:13:B:DA:C1'	2:13:B:DA:O4'	2:13:B:DA:C4'	2:13:B:DA:C5'	22	1.99
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	8	1.99
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	30	1.99
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	3	1.99
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	30	1.99
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	4	1.99
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	26	1.99
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	7	1.99
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	12	1.99
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	22	1.99
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	26	1.99
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	29	1.99
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	26	1.98
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	5	1.98
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	14	1.98
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	26	1.98
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	6	1.98
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	7	1.98
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	20	1.98
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	24	1.98
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	3	1.98
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	27	1.97
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	21	1.97
(1,119)	1:7:A:DG:C1'	1:7:A:DG:O4'	1:7:A:DG:C4'	1:7:A:DG:C5'	4	1.97
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	19	1.97
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	15	1.97
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	5	1.97
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	23	1.97
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	20	1.96
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	19	1.96
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	5	1.96
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	13	1.96
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	19	1.96
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	23	1.96
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	3	1.96
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	5	1.96
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	13	1.96
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	26	1.96
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	6	1.95
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	8	1.95
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	7	1.95
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	22	1.95
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	18	1.95
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	19	1.95
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	24	1.95
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	25	1.95
(1,27)	2:17:B:DG:C3'	2:17:B:DG:O3'	2:18:B:DG:P	2:18:B:DG:O5'	5	1.95
(1,146)	2:17:B:DG:C1'	2:17:B:DG:O4'	2:17:B:DG:C4'	2:17:B:DG:C5'	25	1.94
(1,119)	1:7:A:DG:C1'	1:7:A:DG:O4'	1:7:A:DG:C4'	1:7:A:DG:C5'	11	1.94

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	14	1.94
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	11	1.93
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	10	1.93
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	5	1.93
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	22	1.93
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	18	1.93
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	29	1.93
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	15	1.93
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	6	1.93
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	20	1.93
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	25	1.93
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	22	1.92
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	22	1.92
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	14	1.92
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	3	1.92
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	12	1.92
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	24	1.92
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	10	1.92
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	1	1.92
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	24	1.92
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	1	1.92
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	2	1.92
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	28	1.92
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	14	1.91
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	14	1.91
(1,101)	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2:22:B:DG:C3'	28	1.91
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	5	1.91
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	15	1.91
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	21	1.91
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	17	1.9
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	19	1.9
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	6	1.9
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	22	1.9
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	17	1.9
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	28	1.9
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	4	1.9
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	13	1.9
(1,84)	1:2:A:DT:O5'	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	9	1.9
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	22	1.9
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	11	1.9
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	20	1.9
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	6	1.89
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	18	1.89
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	5	1.89
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	18	1.89
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	25	1.89
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	28	1.89
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	30	1.89
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	8	1.89
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	2	1.89
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	15	1.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	17	1.89
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	18	1.89
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	6	1.89
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	16	1.89
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	14	1.88
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	29	1.88
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	30	1.88
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	17	1.88
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	1	1.88
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	30	1.88
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	21	1.88
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	23	1.87
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	26	1.87
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	17	1.87
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	18	1.87
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	16	1.87
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	14	1.87
(1,84)	1:2:A:DT:O5'	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	24	1.87
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	16	1.87
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	23	1.87
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	11	1.87
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	8	1.86
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	13	1.86
(1,27)	2:17:B:DG:C3'	2:17:B:DG:O3'	2:18:B:DG:P	2:18:B:DG:O5'	30	1.86
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	23	1.85
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	18	1.85
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	21	1.85
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	9	1.85
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	12	1.85
(1,90)	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	13	1.85
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	29	1.84
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	2	1.84
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	3	1.84
(1,102)	1:1:A:DC:C1'	1:1:A:DC:C2'	1:1:A:DC:C3'	1:1:A:DC:C4'	23	1.84
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	26	1.84
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	27	1.84
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	12	1.84
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	16	1.84
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	28	1.84
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	6	1.84
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	7	1.84
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	16	1.83
(1,119)	1:7:A:DG:C1'	1:7:A:DG:O4'	1:7:A:DG:C4'	1:7:A:DG:C5'	17	1.83
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	1	1.83
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	22	1.83
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	27	1.83
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	25	1.83
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	9	1.82
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	16	1.82
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	4	1.82
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	12	1.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	24	1.82
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	12	1.82
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	13	1.82
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	12	1.81
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	18	1.81
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	6	1.81
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	8	1.81
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	10	1.81
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	23	1.81
(1,84)	1:2:A:DT:O5'	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	10	1.81
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	27	1.81
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	8	1.8
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	20	1.8
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	12	1.8
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	14	1.8
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	20	1.8
(1,102)	1:1:A:DC:C1'	1:1:A:DC:C2'	1:1:A:DC:C3'	1:1:A:DC:C4'	24	1.8
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	7	1.8
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	5	1.8
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	6	1.8
(1,30)	2:20:B:DT:C3'	2:20:B:DT:O3'	2:21:B:DA:P	2:21:B:DA:O5'	13	1.8
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	26	1.8
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	27	1.79
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	19	1.79
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	21	1.79
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	16	1.79
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	10	1.79
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	14	1.79
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	9	1.79
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	23	1.79
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	28	1.78
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	17	1.78
(1,116)	1:6:A:DG:C1'	1:6:A:DG:O4'	1:6:A:DG:C4'	1:6:A:DG:C5'	21	1.78
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	15	1.78
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	1	1.78
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	6	1.78
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	26	1.78
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	5	1.78
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	15	1.78
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	5	1.77
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	16	1.77
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	2	1.77
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	4	1.77
(1,119)	1:7:A:DG:C1'	1:7:A:DG:O4'	1:7:A:DG:C4'	1:7:A:DG:C5'	21	1.77
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	3	1.77
(1,84)	1:2:A:DT:O5'	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	30	1.77
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	9	1.77
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	3	1.77
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	22	1.77
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	15	1.76
(1,119)	1:7:A:DG:C1'	1:7:A:DG:O4'	1:7:A:DG:C4'	1:7:A:DG:C5'	9	1.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,102)	1:1:A:DC:C1'	1:1:A:DC:C2'	1:1:A:DC:C3'	1:1:A:DC:C4'	1	1.76
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	11	1.76
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	5	1.76
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	14	1.76
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	24	1.75
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	16	1.75
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	15	1.75
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	23	1.75
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	26	1.75
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	14	1.75
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	1	1.74
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	6	1.74
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	9	1.74
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	19	1.74
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	1	1.73
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	23	1.73
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	24	1.73
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	27	1.73
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	17	1.73
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	10	1.73
(1,5)	1:7:A:DG:C4'	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	5	1.73
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	1	1.72
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	25	1.72
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	5	1.72
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	6	1.72
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	16	1.72
(1,84)	1:2:A:DT:O5'	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	3	1.72
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	28	1.72
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	15	1.71
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	20	1.71
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	6	1.71
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	21	1.71
(1,102)	1:1:A:DC:C1'	1:1:A:DC:C2'	1:1:A:DC:C3'	1:1:A:DC:C4'	9	1.71
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	8	1.71
(1,84)	1:2:A:DT:O5'	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	1	1.71
(1,84)	1:2:A:DT:O5'	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	23	1.71
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	2	1.71
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	18	1.71
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	11	1.71
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	16	1.71
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	3	1.71
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	5	1.7
(1,124)	1:9:A:DA:C5'	1:9:A:DA:C4'	1:9:A:DA:C3'	1:9:A:DA:C2'	20	1.7
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	20	1.7
(1,93)	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2:13:B:DA:C3'	17	1.7
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	14	1.7
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	5	1.69
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	26	1.69
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	19	1.69
(1,102)	1:1:A:DC:C1'	1:1:A:DC:C2'	1:1:A:DC:C3'	1:1:A:DC:C4'	3	1.69
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	27	1.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	28	1.68
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	16	1.68
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	19	1.68
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	25	1.68
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	19	1.68
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	30	1.68
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	8	1.68
(1,146)	2:17:B:DG:C1'	2:17:B:DG:O4'	2:17:B:DG:C4'	2:17:B:DG:C5'	5	1.67
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	23	1.67
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	11	1.67
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	21	1.67
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	17	1.67
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	18	1.67
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	7	1.66
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	27	1.66
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	13	1.66
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	25	1.66
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	4	1.66
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	25	1.65
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	6	1.65
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	29	1.65
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	17	1.65
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	19	1.65
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	2	1.65
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	4	1.65
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	5	1.65
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	4	1.65
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	22	1.64
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	13	1.64
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	21	1.64
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	27	1.64
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	29	1.64
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	15	1.64
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	28	1.64
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	19	1.63
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	30	1.63
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	18	1.63
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	12	1.63
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	12	1.62
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	20	1.62
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	15	1.62
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	25	1.62
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	19	1.62
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	17	1.61
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	11	1.61
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	17	1.61
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	23	1.61
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	4	1.61
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	13	1.61
(1,102)	1:1:A:DC:C1'	1:1:A:DC:C2'	1:1:A:DC:C3'	1:1:A:DC:C4'	30	1.6
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	6	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	26	1.6
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	1	1.6
(1,16)	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:O3'	2:22:B:DG:P	21	1.6
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	21	1.59
(1,102)	1:1:A:DC:C1'	1:1:A:DC:C2'	1:1:A:DC:C3'	1:1:A:DC:C4'	10	1.59
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	15	1.59
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	13	1.58
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	24	1.58
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	17	1.58
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	4	1.58
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	7	1.58
(1,84)	1:2:A:DT:O5'	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	2	1.58
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	29	1.58
(1,27)	2:17:B:DG:C3'	2:17:B:DG:O3'	2:18:B:DG:P	2:18:B:DG:O5'	10	1.58
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	6	1.57
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	3	1.57
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	20	1.57
(1,53)	1:9:A:DA:P	1:9:A:DA:O5'	1:9:A:DA:C5'	1:9:A:DA:C4'	29	1.57
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	3	1.57
(1,20)	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	1:8:A:DA:O5'	30	1.57
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	21	1.56
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	12	1.56
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	28	1.56
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	15	1.55
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	25	1.55
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	14	1.55
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	12	1.55
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	22	1.55
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	13	1.55
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	7	1.55
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	29	1.55
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	7	1.54
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	3	1.54
(1,116)	1:6:A:DG:C1'	1:6:A:DG:O4'	1:6:A:DG:C4'	1:6:A:DG:C5'	4	1.54
(1,110)	1:3:A:DA:C1'	1:3:A:DA:O4'	1:3:A:DA:C4'	1:3:A:DA:C5'	24	1.54
(1,106)	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	1:2:A:DT:C2'	24	1.54
(1,57)	2:14:B:DT:P	2:14:B:DT:O5'	2:14:B:DT:C5'	2:14:B:DT:C4'	15	1.54
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	11	1.53
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	10	1.53
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	4	1.52
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	29	1.52
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	7	1.52
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	5	1.52
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	8	1.52
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	8	1.52
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	28	1.51
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	29	1.51
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	26	1.51
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	13	1.51
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	15	1.5
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	8	1.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	27	1.5
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	4	1.5
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	21	1.5
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	2	1.5
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	7	1.5
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	18	1.5
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	13	1.49
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	30	1.49
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	19	1.49
(1,60)	2:18:B:DG:P	2:18:B:DG:O5'	2:18:B:DG:C5'	2:18:B:DG:C4'	7	1.49
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	20	1.49
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	21	1.48
(1,109)	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:C2'	8	1.48
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	5	1.48
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	2	1.48
(1,51)	1:7:A:DG:P	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	7	1.48
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	18	1.48
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	2	1.48
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	9	1.47
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	27	1.47
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	1	1.47
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2	1.47
(1,86)	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	24	1.47
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	1	1.47
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	18	1.47
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	27	1.47
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	9	1.47
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	11	1.46
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	10	1.46
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	24	1.46
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	10	1.45
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	12	1.45
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	18	1.45
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	1	1.45
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	13	1.45
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	14	1.45
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	21	1.45
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	24	1.45
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	22	1.45
(1,23)	1:10:A:DT:C3'	1:10:A:DT:O3'	1:11:A:DG:P	1:11:A:DG:O5'	24	1.45
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	12	1.44
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	25	1.44
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	26	1.44
(1,27)	2:17:B:DG:C3'	2:17:B:DG:O3'	2:18:B:DG:P	2:18:B:DG:O5'	4	1.44
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	15	1.44
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	1	1.43
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	24	1.43
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	10	1.43
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	13	1.43
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	11	1.43
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	25	1.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	21	1.42
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	27	1.41
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	9	1.41
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	10	1.41
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	29	1.41
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	10	1.41
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	12	1.41
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	10	1.41
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	23	1.4
(1,109)	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:C2'	28	1.4
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	23	1.4
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	28	1.4
(1,87)	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	1:6:A:DG:C3'	30	1.4
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1	1.4
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	12	1.4
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	23	1.4
(1,51)	1:7:A:DG:P	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	6	1.4
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	15	1.39
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	20	1.39
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	30	1.39
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	24	1.39
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	4	1.39
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	21	1.39
(1,27)	2:17:B:DG:C3'	2:17:B:DG:O3'	2:18:B:DG:P	2:18:B:DG:O5'	25	1.39
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	11	1.38
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	19	1.38
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	30	1.38
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	3	1.37
(1,116)	1:6:A:DG:C1'	1:6:A:DG:O4'	1:6:A:DG:C4'	1:6:A:DG:C5'	1	1.37
(1,112)	1:4:A:DA:C5'	1:4:A:DA:C4'	1:4:A:DA:C3'	1:4:A:DA:C2'	13	1.37
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	30	1.37
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	2	1.37
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	26	1.36
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	10	1.36
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	9	1.36
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	9	1.36
(1,51)	1:7:A:DG:P	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	26	1.36
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	3	1.35
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	11	1.35
(1,139)	2:14:B:DT:C5'	2:14:B:DT:C4'	2:14:B:DT:C3'	2:14:B:DT:C2'	17	1.35
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	2	1.35
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	2	1.35
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	24	1.34
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	19	1.34
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	25	1.34
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	30	1.34
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	8	1.34
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	8	1.33
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	15	1.33
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	6	1.33
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	20	1.33

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	15	1.33
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	17	1.33
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	24	1.32
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	8	1.32
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	6	1.32
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	15	1.32
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	25	1.32
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	2	1.32
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	23	1.31
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	25	1.31
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	18	1.31
(1,116)	1:6:A:DG:C1'	1:6:A:DG:O4'	1:6:A:DG:C4'	1:6:A:DG:C5'	11	1.31
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	25	1.31
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	24	1.31
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	3	1.31
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	9	1.31
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	23	1.31
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	2	1.3
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	4	1.3
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	2	1.3
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	5	1.3
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	15	1.3
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	23	1.3
(1,84)	1:2:A:DT:O5'	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	13	1.3
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	15	1.3
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	7	1.29
(1,163)	1:2:A:DT:O4'	1:2:A:DT:C1'	1:2:A:DT:N1	1:2:A:DT:C2	12	1.29
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	29	1.29
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	11	1.29
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	6	1.29
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	9	1.28
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	25	1.28
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	8	1.28
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	25	1.28
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	8	1.28
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	13	1.28
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	5	1.28
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	13	1.28
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	14	1.28
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	3	1.28
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	2	1.28
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	19	1.27
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	26	1.27
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	28	1.27
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	13	1.27
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	1	1.27
(1,51)	1:7:A:DG:P	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	11	1.27
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	11	1.27
(1,5)	1:7:A:DG:C4'	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	10	1.27
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	18	1.26
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	1	1.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,109)	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:C2'	13	1.26
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	26	1.26
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	8	1.25
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	4	1.25
(1,155)	2:20:B:DT:C1'	2:20:B:DT:O4'	2:20:B:DT:C4'	2:20:B:DT:C5'	11	1.25
(1,146)	2:17:B:DG:C1'	2:17:B:DG:O4'	2:17:B:DG:C4'	2:17:B:DG:C5'	23	1.25
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	11	1.25
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	30	1.25
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	8	1.24
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	19	1.24
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	18	1.24
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	15	1.24
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	13	1.23
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	24	1.23
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	19	1.23
(1,151)	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	2:19:B:DT:C2'	24	1.23
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	12	1.23
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	2	1.23
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	11	1.22
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	14	1.22
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	3	1.22
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	26	1.22
(1,152)	2:19:B:DT:C1'	2:19:B:DT:O4'	2:19:B:DT:C4'	2:19:B:DT:C5'	19	1.22
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	25	1.22
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	25	1.22
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	26	1.22
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	21	1.21
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	5	1.21
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	23	1.21
(1,119)	1:7:A:DG:C1'	1:7:A:DG:O4'	1:7:A:DG:C4'	1:7:A:DG:C5'	25	1.21
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	12	1.21
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	24	1.21
(1,87)	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	1:6:A:DG:C3'	28	1.21
(1,49)	1:4:A:DA:P	1:4:A:DA:O5'	1:4:A:DA:C5'	1:4:A:DA:C4'	21	1.21
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	30	1.2
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	3	1.2
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	9	1.2
(1,113)	1:4:A:DA:C1'	1:4:A:DA:O4'	1:4:A:DA:C4'	1:4:A:DA:C5'	3	1.2
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	13	1.2
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	14	1.2
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	8	1.2
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	10	1.19
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	3	1.19
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	2	1.18
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	9	1.18
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	18	1.18
(1,109)	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:C2'	25	1.18
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	1	1.18
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	1	1.18
(1,48)	1:3:A:DA:P	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	13	1.18
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	26	1.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,177)	2:22:B:DG:O4'	2:22:B:DG:C1'	2:22:B:DG:N9	2:22:B:DG:C4	30	1.17
(1,122)	1:8:A:DA:C1'	1:8:A:DA:O4'	1:8:A:DA:C4'	1:8:A:DA:C5'	28	1.17
(1,116)	1:6:A:DG:C1'	1:6:A:DG:O4'	1:6:A:DG:C4'	1:6:A:DG:C5'	17	1.17
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	25	1.17
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	26	1.17
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	27	1.17
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	12	1.17
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	11	1.17
(1,50)	1:6:A:DG:P	1:6:A:DG:O5'	1:6:A:DG:C5'	1:6:A:DG:C4'	17	1.17
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	14	1.17
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	22	1.16
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	27	1.16
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	27	1.16
(1,158)	2:21:B:DA:C1'	2:21:B:DA:O4'	2:21:B:DA:C4'	2:21:B:DA:C5'	15	1.16
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	10	1.16
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	11	1.16
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	11	1.16
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	9	1.16
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	18	1.16
(1,27)	2:17:B:DG:C3'	2:17:B:DG:O3'	2:18:B:DG:P	2:18:B:DG:O5'	22	1.16
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	6	1.15
(1,158)	2:21:B:DA:C1'	2:21:B:DA:O4'	2:21:B:DA:C4'	2:21:B:DA:C5'	24	1.15
(1,107)	1:2:A:DT:C1'	1:2:A:DT:O4'	1:2:A:DT:C4'	1:2:A:DT:C5'	11	1.15
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	20	1.15
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	11	1.15
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	16	1.15
(1,29)	2:19:B:DT:C3'	2:19:B:DT:O3'	2:20:B:DT:P	2:20:B:DT:O5'	25	1.15
(1,27)	2:17:B:DG:C3'	2:17:B:DG:O3'	2:18:B:DG:P	2:18:B:DG:O5'	1	1.15
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	5	1.14
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	6	1.14
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	3	1.14
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	22	1.14
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	10	1.14
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	28	1.14
(1,16)	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:O3'	2:22:B:DG:P	4	1.14
(1,157)	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2:21:B:DA:C2'	30	1.13
(1,154)	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	2:20:B:DT:C2'	28	1.13
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	15	1.13
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	26	1.13
(1,116)	1:6:A:DG:C1'	1:6:A:DG:O4'	1:6:A:DG:C4'	1:6:A:DG:C5'	9	1.13
(1,109)	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:C2'	18	1.13
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	30	1.13
(1,64)	2:22:B:DG:P	2:22:B:DG:O5'	2:22:B:DG:C5'	2:22:B:DG:C4'	25	1.13
(1,3)	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	19	1.13
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	3	1.12
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	15	1.12
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	17	1.12
(1,109)	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:C2'	16	1.12
(1,106)	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	1:2:A:DT:C2'	10	1.12
(1,102)	1:1:A:DC:C1'	1:1:A:DC:C2'	1:1:A:DC:C3'	1:1:A:DC:C4'	2	1.12
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	8	1.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,99)	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	22	1.12
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	8	1.12
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	20	1.12
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	3	1.12
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	22	1.11
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	23	1.11
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	30	1.11
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	13	1.11
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	18	1.11
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1	1.11
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	1	1.11
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	23	1.11
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	29	1.11
(1,48)	1:3:A:DA:P	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	8	1.11
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	16	1.11
(1,3)	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	28	1.11
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	5	1.1
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	13	1.1
(1,158)	2:21:B:DA:C1'	2:21:B:DA:O4'	2:21:B:DA:C4'	2:21:B:DA:C5'	30	1.1
(1,106)	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	1:2:A:DT:C2'	23	1.1
(1,98)	2:19:B:DT:O5'	2:19:B:DT:C5'	2:19:B:DT:C4'	2:19:B:DT:C3'	19	1.1
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	18	1.1
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	1	1.09
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	17	1.09
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	28	1.09
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	6	1.09
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	17	1.09
(1,158)	2:21:B:DA:C1'	2:21:B:DA:O4'	2:21:B:DA:C4'	2:21:B:DA:C5'	2	1.09
(1,158)	2:21:B:DA:C1'	2:21:B:DA:O4'	2:21:B:DA:C4'	2:21:B:DA:C5'	10	1.09
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	27	1.09
(1,106)	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	1:2:A:DT:C2'	9	1.09
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	14	1.09
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	22	1.09
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	28	1.09
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	21	1.09
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	4	1.09
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	23	1.08
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	9	1.08
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	10	1.08
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	21	1.08
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	24	1.08
(1,109)	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:C2'	11	1.08
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	2	1.08
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	19	1.08
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	30	1.08
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	26	1.08
(1,3)	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	18	1.08
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	4	1.07
(1,158)	2:21:B:DA:C1'	2:21:B:DA:O4'	2:21:B:DA:C4'	2:21:B:DA:C5'	13	1.07
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	2	1.07
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	15	1.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	8	1.07
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	28	1.07
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	15	1.07
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	21	1.07
(1,51)	1:7:A:DG:P	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	29	1.07
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	22	1.07
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	26	1.06
(1,158)	2:21:B:DA:C1'	2:21:B:DA:O4'	2:21:B:DA:C4'	2:21:B:DA:C5'	25	1.06
(1,131)	1:11:A:DG:C1'	1:11:A:DG:O4'	1:11:A:DG:C4'	1:11:A:DG:C5'	23	1.06
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	4	1.06
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	19	1.06
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	9	1.06
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	4	1.06
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	21	1.06
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	16	1.06
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	27	1.06
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	12	1.06
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	9	1.06
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	2	1.05
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	10	1.05
(1,100)	2:21:B:DA:O5'	2:21:B:DA:C5'	2:21:B:DA:C4'	2:21:B:DA:C3'	23	1.05
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	12	1.05
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	18	1.05
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	19	1.05
(1,27)	2:17:B:DG:C3'	2:17:B:DG:O3'	2:18:B:DG:P	2:18:B:DG:O5'	9	1.05
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	16	1.04
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	7	1.04
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	3	1.04
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	12	1.04
(1,109)	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:C2'	2	1.04
(1,109)	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:C2'	14	1.04
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	8	1.04
(1,88)	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	1:7:A:DG:C3'	11	1.04
(1,59)	2:17:B:DG:P	2:17:B:DG:O5'	2:17:B:DG:C5'	2:17:B:DG:C4'	16	1.04
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	4	1.04
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	30	1.04
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	25	1.04
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	30	1.04
(1,51)	1:7:A:DG:P	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	19	1.04
(1,3)	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	13	1.04
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	2	1.03
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	12	1.03
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	12	1.03
(1,131)	1:11:A:DG:C1'	1:11:A:DG:O4'	1:11:A:DG:C4'	1:11:A:DG:C5'	13	1.03
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	16	1.03
(1,118)	1:7:A:DG:C5'	1:7:A:DG:C4'	1:7:A:DG:C3'	1:7:A:DG:C2'	6	1.03
(1,113)	1:4:A:DA:C1'	1:4:A:DA:O4'	1:4:A:DA:C4'	1:4:A:DA:C5'	30	1.03
(1,103)	1:1:A:DC:C5'	1:1:A:DC:C4'	1:1:A:DC:C3'	1:1:A:DC:C2'	12	1.03
(1,99)	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	2:20:B:DT:C3'	7	1.03
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	9	1.03
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	24	1.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	19	1.03
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	22	1.03
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	23	1.03
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	27	1.03
(1,18)	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	1:4:A:DA:O5'	29	1.03
(1,3)	1:3:A:DA:C4'	1:3:A:DA:C3'	1:3:A:DA:O3'	1:4:A:DA:P	26	1.03
(1,176)	2:21:B:DA:O4'	2:21:B:DA:C1'	2:21:B:DA:N9	2:21:B:DA:C4	20	1.02
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	2	1.02
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	14	1.02
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	29	1.02
(1,106)	1:2:A:DT:C5'	1:2:A:DT:C4'	1:2:A:DT:C3'	1:2:A:DT:C2'	3	1.02
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	3	1.02
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	6	1.02
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	21	1.02
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	3	1.02
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	26	1.02
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	1	1.01
(1,168)	1:10:A:DT:O4'	1:10:A:DT:C1'	1:10:A:DT:N1	1:10:A:DT:C2	14	1.01
(1,121)	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	1:8:A:DA:C2'	22	1.01
(1,95)	2:15:B:DT:O5'	2:15:B:DT:C5'	2:15:B:DT:C4'	2:15:B:DT:C3'	20	1.01
(1,89)	1:8:A:DA:O5'	1:8:A:DA:C5'	1:8:A:DA:C4'	1:8:A:DA:C3'	17	1.01
(1,85)	1:3:A:DA:O5'	1:3:A:DA:C5'	1:3:A:DA:C4'	1:3:A:DA:C3'	17	1.01
(1,62)	2:20:B:DT:P	2:20:B:DT:O5'	2:20:B:DT:C5'	2:20:B:DT:C4'	4	1.01
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	22	1.01
(1,51)	1:7:A:DG:P	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	1	1.01
(1,51)	1:7:A:DG:P	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	15	1.01
(1,51)	1:7:A:DG:P	1:7:A:DG:O5'	1:7:A:DG:C5'	1:7:A:DG:C4'	28	1.01
(1,5)	1:7:A:DG:C4'	1:7:A:DG:C3'	1:7:A:DG:O3'	1:8:A:DA:P	25	1.01
(1,158)	2:21:B:DA:C1'	2:21:B:DA:O4'	2:21:B:DA:C4'	2:21:B:DA:C5'	1	1.0
(1,56)	2:13:B:DA:P	2:13:B:DA:O5'	2:13:B:DA:C5'	2:13:B:DA:C4'	14	1.0
(1,54)	1:10:A:DT:P	1:10:A:DT:O5'	1:10:A:DT:C5'	1:10:A:DT:C4'	14	1.0