Full wwPDB NMR Structure Validation Report (i)

Aug 29, 2023 – 02:11 PM JST

PDB ID	:	7YS5
BMRB ID	:	36505
Title	:	RET G-quadruplex in 10mM Na+
Authors	:	Yin, S.; Cao, C.
Deposited on	:	2022-08-11

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

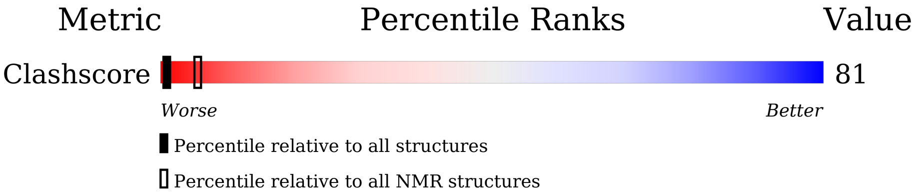
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
SOLUTION NMR

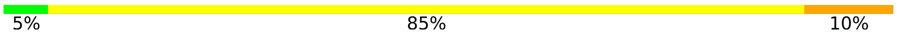
The overall completeness of chemical shifts assignment is 50%.

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	158937	12864

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	20	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 649 atoms, of which 223 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3').

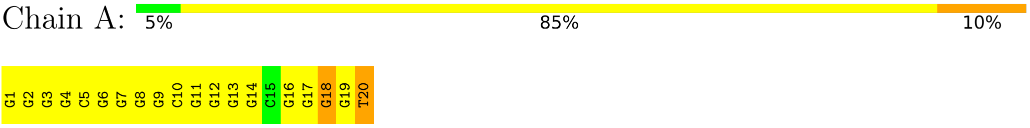
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	20	649	197	223	91	119	19	0

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3')

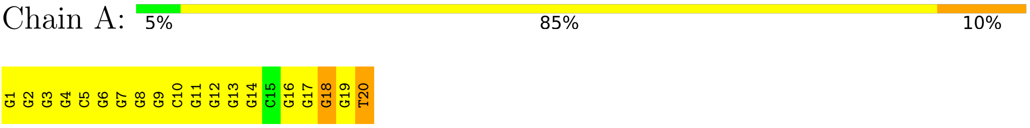


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

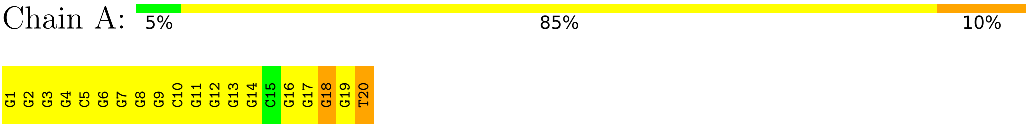
4.2.1 Score per residue for model 1

- Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3')



4.2.2 Score per residue for model 2

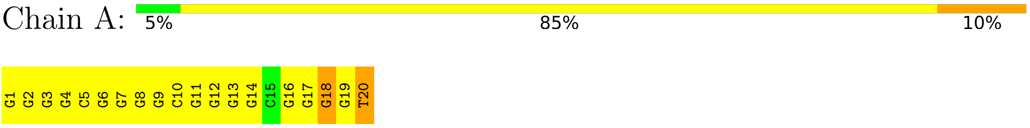
- Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3')



4.2.3 Score per residue for model 3

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)

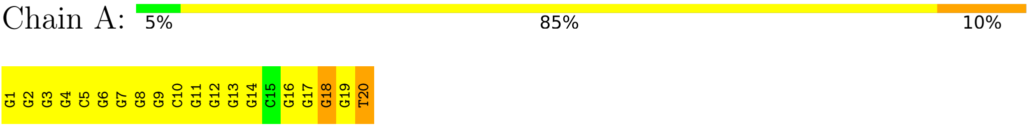
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)

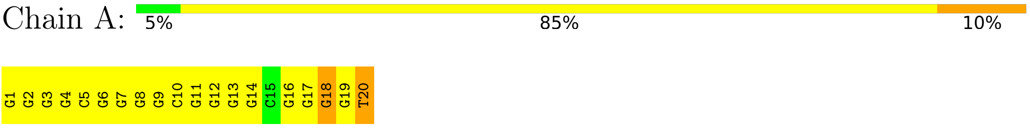
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)

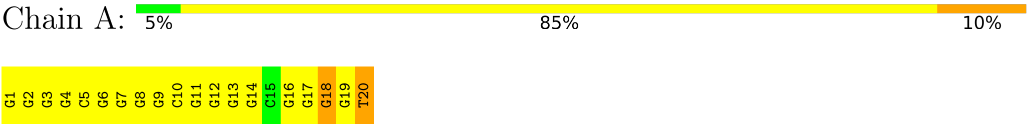
Chain A:



4.2.6 Score per residue for model 6

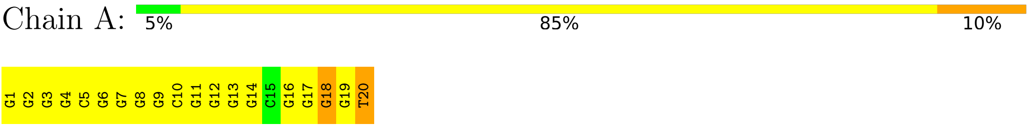
- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)

Chain A:



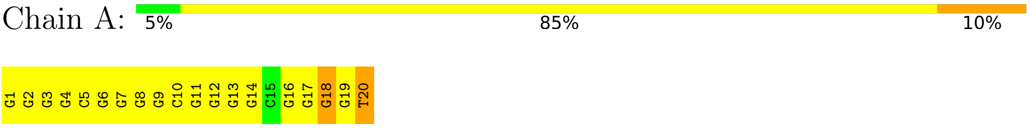
4.2.7 Score per residue for model 7

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)



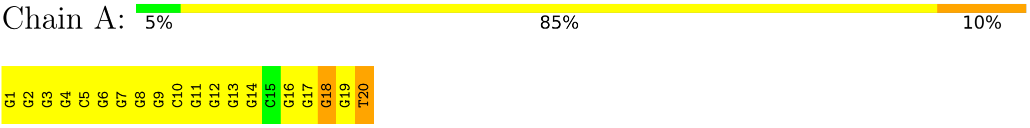
4.2.8 Score per residue for model 8

- Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3')



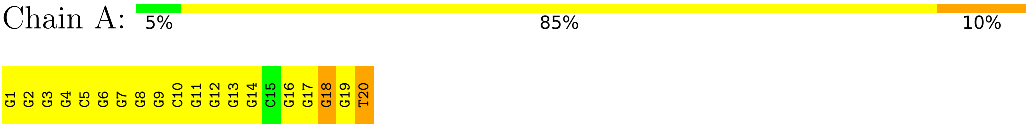
4.2.9 Score per residue for model 9

- Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3')



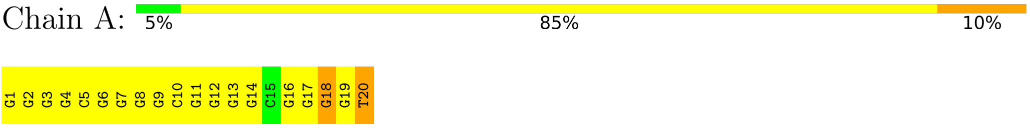
4.2.10 Score per residue for model 10

- Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3')



4.2.11 Score per residue for model 11

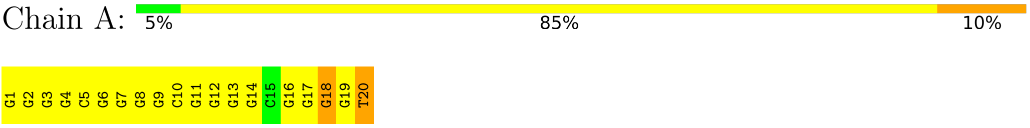
- Molecule 1: DNA (5'-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3')



4.2.12 Score per residue for model 12

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)

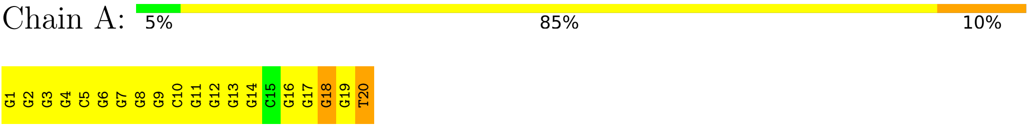
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)

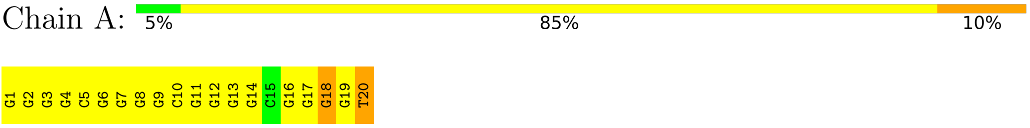
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)

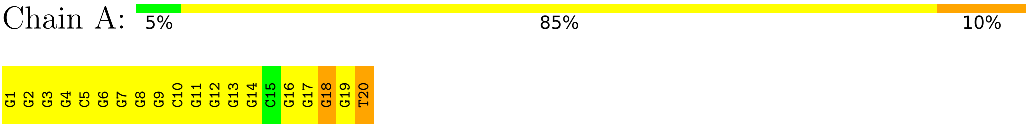
Chain A:



4.2.15 Score per residue for model 15

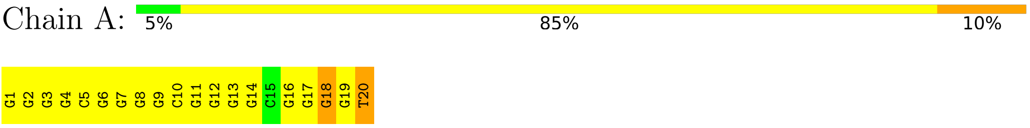
- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)

Chain A:



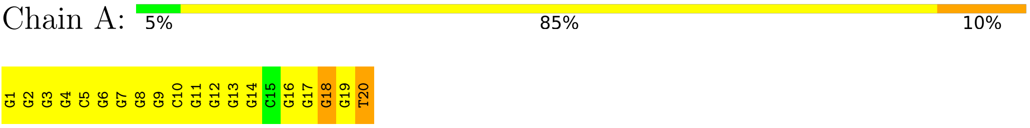
4.2.16 Score per residue for model 16

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)



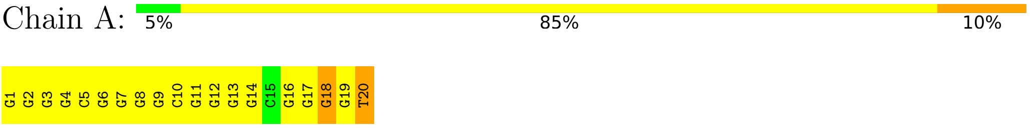
4.2.17 Score per residue for model 17

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)



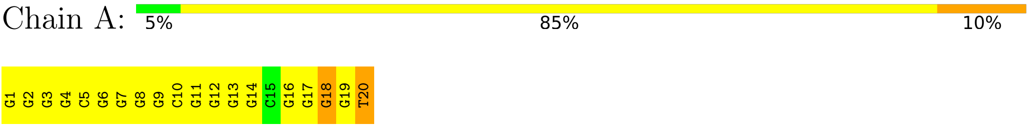
4.2.18 Score per residue for model 18

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)



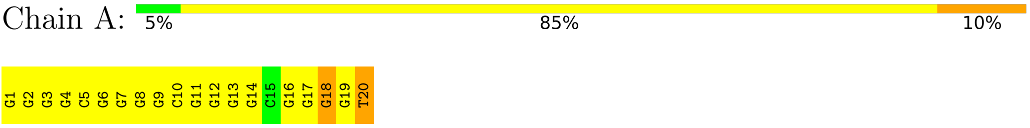
4.2.19 Score per residue for model 19

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)



4.2.20 Score per residue for model 20

- Molecule 1: DNA (5’-D(*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*CP*GP*GP*GP*GP*T)-3’)



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 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**
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	208
Number of shifts mapped to atoms	208
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	50%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.95±0.00	0±0/481 (0.0± 0.0%)	1.34±0.00	4±0/746 (0.5± 0.0%)
All	All	0.95	0/9620 (0.0%)	1.34	80/14920 (0.5%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	DG	C1'-O4'-C4'	-6.85	103.25	110.10	3	20
1	A	20	DT	C1'-O4'-C4'	-6.23	103.87	110.10	10	20
1	A	20	DT	C6-C5-C7	-6.21	119.17	122.90	8	20
1	A	20	DT	C4-C5-C6	5.23	121.14	118.00	19	20

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	426	223	223	53±1
All	All	8520	4460	4460	1051

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 81.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:DG:N3	1:A:16:DG:H3'	0.96	1.76	4	20
1:A:13:DG:N3	1:A:14:DG:O4'	0.78	2.16	17	20
1:A:16:DG:N3	1:A:16:DG:C3'	0.77	2.48	4	20
1:A:1:DG:C8	1:A:2:DG:C8	0.67	2.83	5	20
1:A:3:DG:C2	1:A:4:DG:C2	0.65	2.84	8	20
1:A:12:DG:C2	1:A:13:DG:C4	0.65	2.84	16	20
1:A:1:DG:O5'	1:A:16:DG:H1'	0.64	1.92	17	20
1:A:12:DG:C2	1:A:13:DG:C5	0.64	2.86	4	20
1:A:1:DG:C2	1:A:16:DG:C5	0.61	2.89	9	20
1:A:9:DG:N2	1:A:12:DG:N7	0.60	2.49	12	20
1:A:8:DG:C2	1:A:9:DG:C4	0.60	2.89	4	20
1:A:1:DG:N3	1:A:16:DG:C8	0.59	2.70	5	20
1:A:19:DG:C6	1:A:20:DT:H73	0.58	2.33	4	20
1:A:12:DG:N1	1:A:13:DG:C5	0.58	2.72	5	20
1:A:12:DG:N1	1:A:13:DG:C6	0.57	2.72	15	20
1:A:12:DG:C4	1:A:13:DG:C8	0.55	2.94	5	20
1:A:2:DG:C2	1:A:12:DG:N2	0.55	2.75	5	20
1:A:5:DC:O2	1:A:6:DG:C8	0.54	2.60	1	20
1:A:13:DG:C6	1:A:14:DG:N3	0.54	2.75	3	20
1:A:13:DG:C6	1:A:14:DG:C2	0.54	2.95	3	20
1:A:1:DG:C2	1:A:16:DG:C8	0.53	2.96	5	20
1:A:3:DG:H8	1:A:3:DG:O5'	0.53	1.85	20	20
1:A:3:DG:N2	1:A:4:DG:C2	0.53	2.77	15	20
1:A:10:DC:H6	1:A:10:DC:O5'	0.52	1.87	4	20
1:A:5:DC:O2	1:A:5:DC:C2'	0.52	2.55	15	20
1:A:13:DG:O6	1:A:14:DG:C2	0.51	2.64	3	20
1:A:12:DG:C6	1:A:13:DG:C6	0.51	2.99	1	20
1:A:3:DG:O5'	1:A:3:DG:C8	0.49	2.66	20	20
1:A:5:DC:O2	1:A:5:DC:H2'	0.49	2.08	10	20
1:A:1:DG:N1	1:A:16:DG:C5	0.48	2.82	15	20
1:A:6:DG:O4'	1:A:7:DG:C2	0.48	2.67	15	20
1:A:10:DC:O5'	1:A:10:DC:C6	0.48	2.67	4	20
1:A:8:DG:C2	1:A:9:DG:C5	0.47	3.03	4	20
1:A:1:DG:C2	1:A:16:DG:N7	0.46	2.84	5	20
1:A:8:DG:C6	1:A:9:DG:C6	0.46	3.04	4	20
1:A:12:DG:C4	1:A:13:DG:N7	0.45	2.83	5	20
1:A:1:DG:C5	1:A:13:DG:N2	0.45	2.84	4	20
1:A:1:DG:C2	1:A:17:DG:C2	0.45	3.04	9	20
1:A:4:DG:N2	1:A:6:DG:C6	0.45	2.84	15	20
1:A:1:DG:N2	1:A:16:DG:C4	0.45	2.85	8	20
1:A:12:DG:C6	1:A:13:DG:C5	0.44	3.06	5	20
1:A:11:DG:H21	1:A:11:DG:P	0.43	2.37	20	19

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:17:DG:H5”	1:A:18:DG:OP2	0.43	2.14	6	19
1:A:3:DG:C2	1:A:4:DG:N3	0.43	2.87	9	20
1:A:12:DG:C5	1:A:13:DG:N7	0.43	2.87	5	20
1:A:1:DG:HO5’	1:A:16:DG:H1’	0.42	1.74	3	8
1:A:17:DG:H3’	1:A:18:DG:O4’	0.42	2.15	3	20
1:A:12:DG:N3	1:A:13:DG:C8	0.42	2.88	5	20
1:A:4:DG:H4’	1:A:5:DC:C5	0.42	2.50	15	20
1:A:3:DG:N2	1:A:4:DG:N2	0.42	2.68	8	20
1:A:8:DG:N1	1:A:9:DG:C6	0.42	2.88	4	20
1:A:6:DG:H4’	1:A:7:DG:N3	0.41	2.31	9	20
1:A:5:DC:O2	1:A:6:DG:H8	0.41	1.99	1	1
1:A:18:DG:C2	1:A:19:DG:C5	0.41	3.08	15	13
1:A:1:DG:C2	1:A:16:DG:C4	0.41	3.09	15	8
1:A:4:DG:N2	1:A:6:DG:O6	0.40	2.54	15	2
1:A:11:DG:P	1:A:11:DG:H21	0.40	2.40	10	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 monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 50% for the well-defined parts and 50% 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 (i)

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

Total number of shifts	208
Number of shifts mapped to atoms	208
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

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

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 50%, i.e. 205 atoms were assigned a chemical shift out of a possible 414. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Sugar	133/240 (55%)	133/140 (95%)	0/100 (0%)	0/0 (—%)
Base	72/174 (41%)	72/114 (63%)	0/24 (0%)	0/36 (0%)
Overall	205/414 (50%)	205/254 (81%)	0/124 (0%)	0/36 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 205 atoms were assigned a chemical shift out of a possible 414. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Sugar	133/240 (55%)	133/140 (95%)	0/100 (0%)	0/0 (—%)
Base	72/174 (41%)	72/114 (63%)	0/24 (0%)	0/36 (0%)
Overall	205/414 (50%)	205/254 (81%)	0/124 (0%)	0/36 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	6	DG	H5'	2.35	2.99 – 5.28	-7.8
1	A	2	DG	H5'	2.57	2.99 – 5.28	-6.9

7.1.5 Random Coil Index (RCI) plots ⓘ

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

8 NMR restraints analysis ⓘ

8.1 Conformationally restricting restraints ⓘ

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

Description	Value
Total distance restraints	839
Intra-residue (|i-j|=0)	458
Sequential (|i-j|=1)	222
Medium range (|i-j|>1 and |i-j|<5)	68
Long range (|i-j|≥5)	91
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	42.0
Number of long range restraints per residue[1]	4.5

[1] Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations ⓘ

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model ⓘ

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	61.7	0.2
0.2-0.5 (Medium)	40.9	0.4
>0.5 (Large)	9.0	7.02

8.2.2 Average number of dihedral-angle violations per model ⓘ

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis

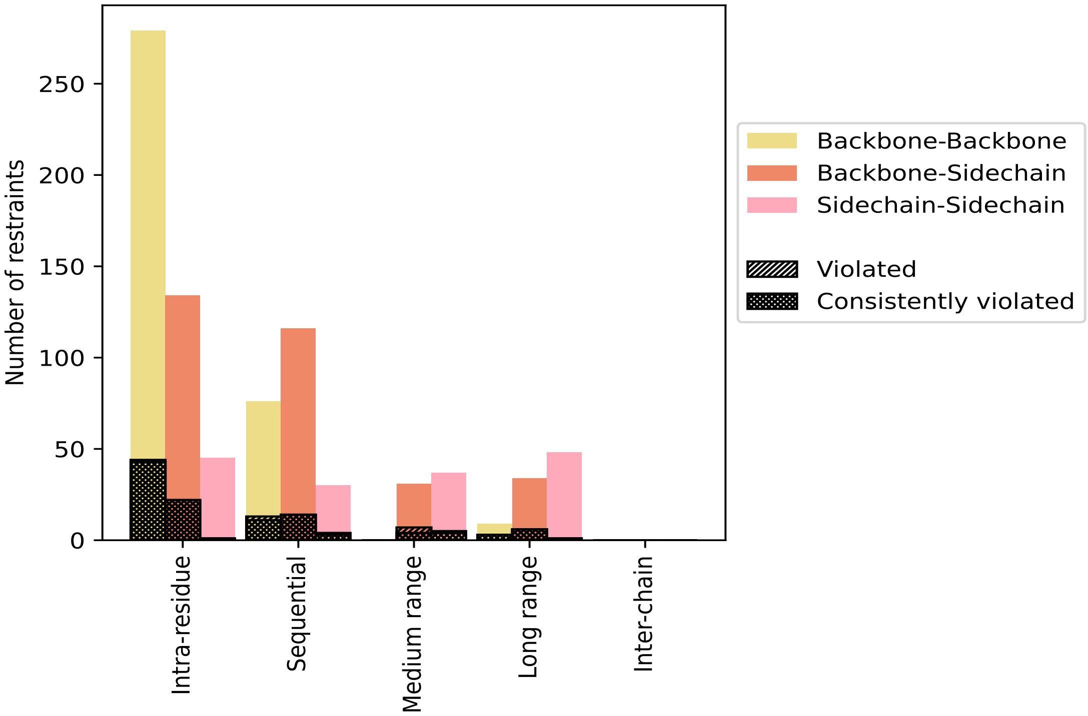
9.1 Summary of distance violations

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

Restraints type	**Count**	%[1]	**Violated**[3]			**Consistently Violated**[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue ($\lvert i-j \rvert=0$)	458	54.6	67	14.6	8.0	66	14.4	7.9
Backbone-Backbone	279	33.3	44	15.8	5.2	43	15.4	5.1
Backbone-Sidechain	134	16.0	22	16.4	2.6	22	16.4	2.6
Sidechain-Sidechain	45	5.4	1	2.2	0.1	1	2.2	0.1
Sequential ($\lvert i-j \rvert=1$)	222	26.5	31	14.0	3.7	28	12.6	3.3
Backbone-Backbone	76	9.1	13	17.1	1.5	11	14.5	1.3
Backbone-Sidechain	116	13.8	14	12.1	1.7	14	12.1	1.7
Sidechain-Sidechain	30	3.6	4	13.3	0.5	3	10.0	0.4
Medium range ($\lvert i-j \rvert>1$ & $\lvert i-j \rvert<5$)	68	8.1	12	17.6	1.4	8	11.8	1.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	31	3.7	7	22.6	0.8	4	12.9	0.5
Sidechain-Sidechain	37	4.4	5	13.5	0.6	4	10.8	0.5
Long range ($\lvert i-j \rvert \geq 5$)	91	10.8	10	11.0	1.2	10	11.0	1.2
Backbone-Backbone	9	1.1	3	33.3	0.4	3	33.3	0.4
Backbone-Sidechain	34	4.1	6	17.6	0.7	6	17.6	0.7
Sidechain-Sidechain	48	5.7	1	2.1	0.1	1	2.1	0.1
Inter-chain	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
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	839	100.0	120	14.3	14.3	112	13.3	13.3
Backbone-Backbone	364	43.4	60	16.5	7.2	57	15.7	6.8
Backbone-Sidechain	315	37.5	49	15.6	5.8	46	14.6	5.5
Sidechain-Sidechain	160	19.1	11	6.9	1.3	9	5.6	1.1

[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 ⓘ



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 ⓘ

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	66	30	10	10	0	116	0.51	6.98	1.2	0.19
2	66	28	11	10	0	115	0.51	6.98	1.21	0.19
3	66	29	12	10	0	117	0.51	7.0	1.2	0.19
4	66	30	9	10	0	115	0.51	7.02	1.21	0.19
5	66	30	10	10	0	116	0.51	6.99	1.21	0.19
6	66	29	12	10	0	117	0.5	6.99	1.2	0.19
7	66	29	12	10	0	117	0.5	6.99	1.2	0.19
8	66	29	12	10	0	117	0.5	7.0	1.2	0.19
9	66	28	11	10	0	115	0.51	6.98	1.21	0.19
10	66	30	10	10	0	116	0.51	7.01	1.2	0.18
11	66	30	12	10	0	118	0.5	6.99	1.19	0.19

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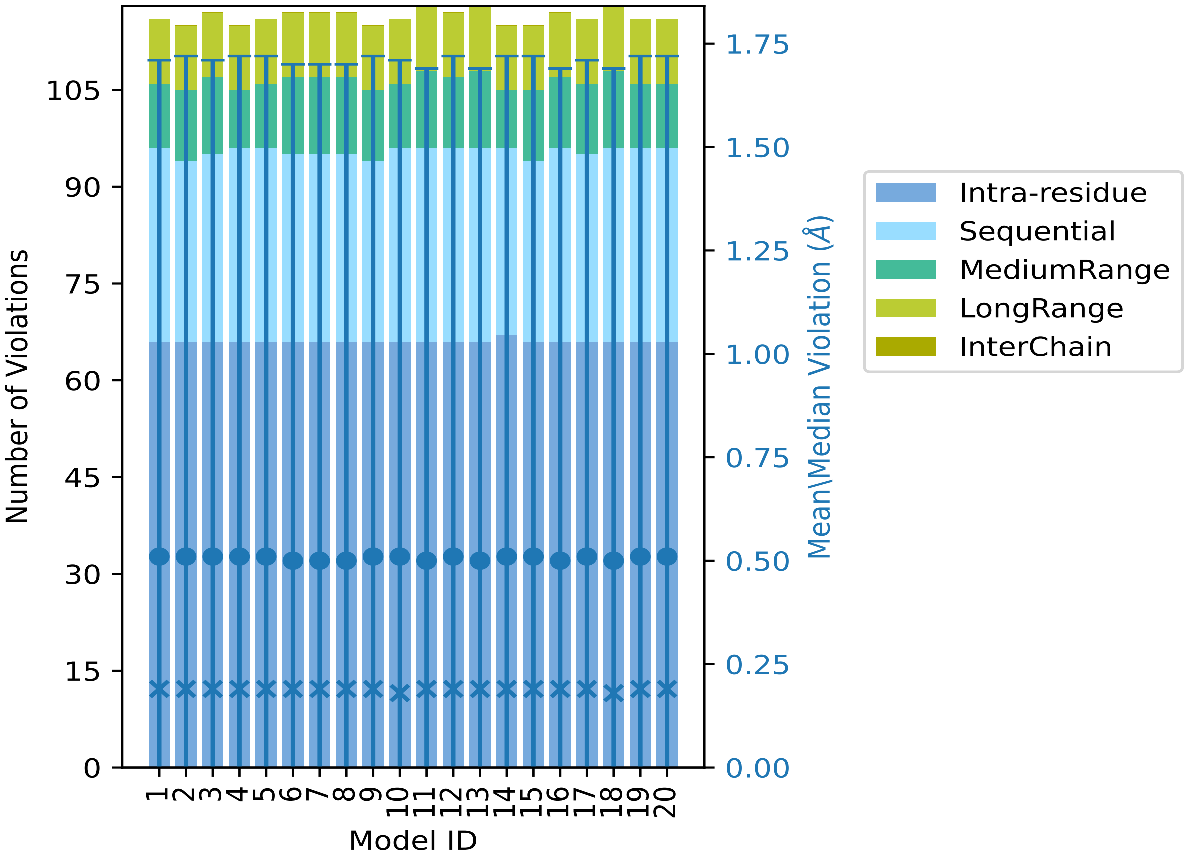
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	66	30	11	10	0	117	0.51	7.02	1.21	0.19
13	66	30	12	10	0	118	0.5	6.98	1.19	0.19
14	67	29	9	10	0	115	0.51	7.0	1.21	0.19
15	66	28	11	10	0	115	0.51	6.98	1.21	0.19
16	66	30	11	10	0	117	0.5	6.98	1.19	0.19
17	66	29	11	10	0	116	0.51	7.0	1.2	0.19
18	66	30	12	10	0	118	0.5	6.98	1.19	0.18
19	66	30	10	10	0	116	0.51	7.01	1.21	0.19
20	66	30	10	10	0	116	0.51	6.99	1.21	0.19

[1] Intra-residue restraints, [2] Sequential restraints, [3] Medium range restraints, [4] Long range restraints, [5] Inter-chain restraints, [6] Standard deviation

9.2.1 Bar graph : Distance 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

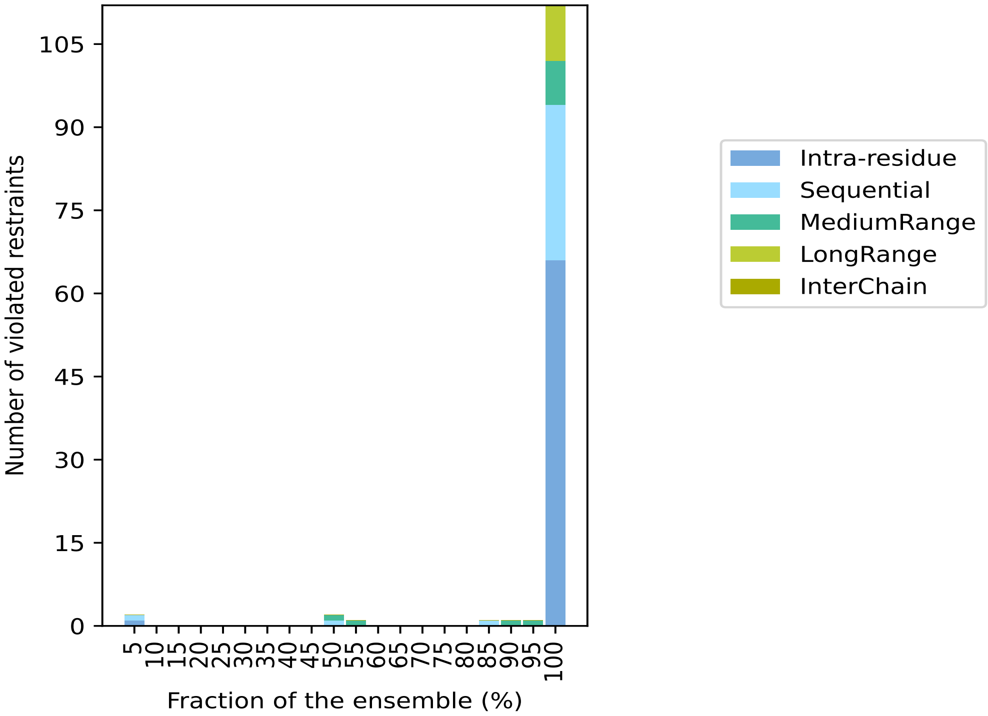
9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 719(IR:391, SQ:191, MR:56, LR:81, IC:0) 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	1	0	0	0	2	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	1	1	0	0	2	10	50.0
0	0	1	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	1	0	0	0	1	17	85.0
0	0	1	0	0	1	18	90.0
0	0	1	0	0	1	19	95.0
66	28	8	10	0	112	20	100.0

[1] Intra-residue restraints, [2] Sequential restraints, [3] Medium range restraints, [4] Long range restraints, [5] Inter-chain restraints, [6] Number of models with violations

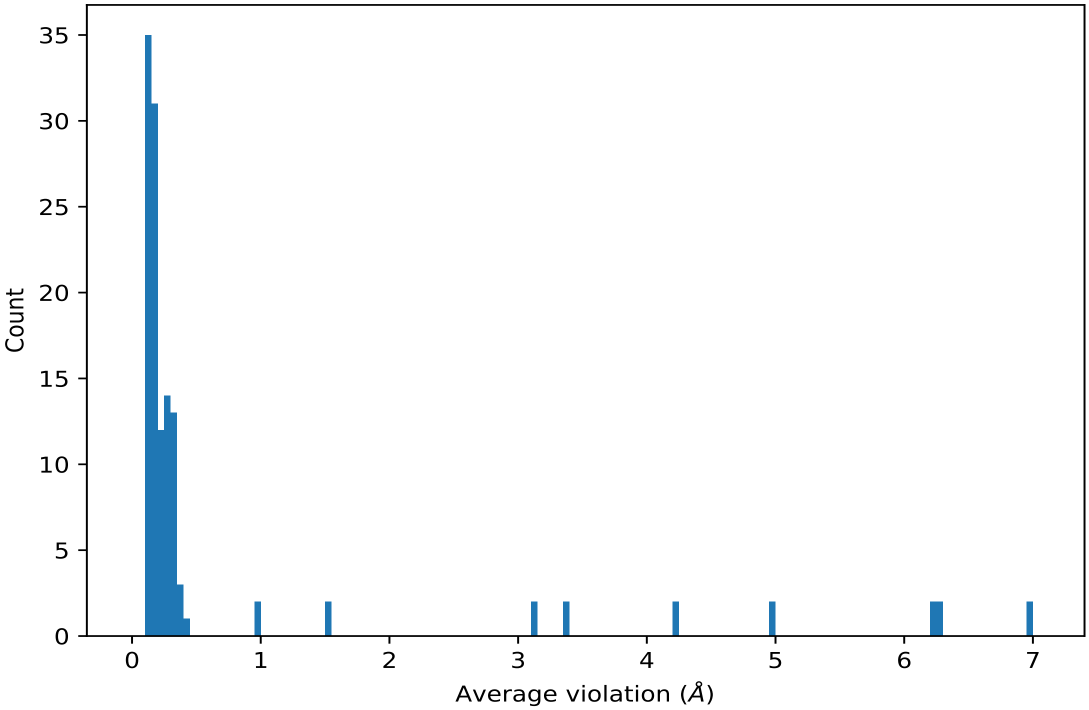
9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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



9.4.2 Table: Most violated distance restraints ⓘ

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)
(1,376)	1:20:A:DT:H5'	1:15:A:DC:H6	20	6.99	0.01	6.99
(1,376)	1:20:A:DT:H5"	1:15:A:DC:H6	20	6.99	0.01	6.99
(1,375)	1:20:A:DT:H5'	1:15:A:DC:H4'	20	6.27	0.01	6.27
(1,375)	1:20:A:DT:H5"	1:15:A:DC:H4'	20	6.27	0.01	6.27
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	20	6.2	0.02	6.19
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	20	6.2	0.02	6.19
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	20	4.95	0.01	4.95
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	20	4.95	0.01	4.95
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	20	4.23	0.01	4.22
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	20	4.23	0.01	4.22
(1,373)	1:20:A:DT:H5'	1:9:A:DG:H8	20	3.38	0.02	3.38
(1,373)	1:20:A:DT:H5"	1:9:A:DG:H8	20	3.38	0.02	3.38
(1,378)	1:20:A:DT:H5'	1:19:A:DG:H1	20	3.11	0.01	3.11
(1,378)	1:20:A:DT:H5"	1:19:A:DG:H1	20	3.11	0.01	3.11
(1,826)	1:20:A:DT:H5'	1:20:A:DT:H6	20	1.53	0.01	1.53
(1,826)	1:20:A:DT:H5"	1:20:A:DT:H6	20	1.53	0.01	1.53

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	20	0.98	0.01	0.98
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	20	0.98	0.01	0.98
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	20	0.4	0.0	0.4
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	20	0.36	0.01	0.36
(1,549)	1:7:A:DG:H4’	1:7:A:DG:H2’	20	0.35	0.0	0.35
(1,786)	1:18:A:DG:H1’	1:18:A:DG:H8	20	0.35	0.0	0.35
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	20	0.34	0.0	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	20	0.34	0.0	0.34
(1,699)	1:14:A:DG:H2’	1:14:A:DG:H4’	20	0.33	0.0	0.33
(1,268)	1:14:A:DG:H5”	1:13:A:DG:H1’	20	0.33	0.0	0.33
(1,360)	1:19:A:DG:H5’	1:18:A:DG:H8	20	0.32	0.0	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	20	0.32	0.0	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	20	0.32	0.0	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	20	0.32	0.0	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	20	0.32	0.0	0.32
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	20	0.31	0.01	0.31
(1,458)	1:4:A:DG:H2’	1:4:A:DG:H4’	20	0.31	0.0	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	20	0.31	0.0	0.31
(1,320)	1:16:A:DG:H1’	1:18:A:DG:H8	20	0.3	0.0	0.3
(1,434)	1:3:A:DG:H2”	1:3:A:DG:H5’	20	0.29	0.0	0.29
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	20	0.28	0.0	0.28
(1,513)	1:6:A:DG:H1’	1:6:A:DG:H8	20	0.28	0.01	0.28
(1,554)	1:7:A:DG:H5’	1:7:A:DG:H1	20	0.27	0.0	0.27
(1,227)	1:11:A:DG:H2’	1:12:A:DG:H1’	20	0.27	0.0	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	20	0.27	0.0	0.27
(1,761)	1:16:A:DG:H3’	1:16:A:DG:H8	20	0.27	0.0	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	20	0.27	0.01	0.27
(1,495)	1:5:A:DC:H5”	1:5:A:DC:H2”	20	0.26	0.0	0.26
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	20	0.25	0.0	0.25
(1,729)	1:15:A:DC:H5’	1:15:A:DC:H6	20	0.25	0.01	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	20	0.25	0.0	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	20	0.25	0.0	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	20	0.25	0.0	0.25
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	20	0.24	0.0	0.24
(1,468)	1:4:A:DG:H2”	1:4:A:DG:H5’	20	0.24	0.0	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	20	0.24	0.0	0.24
(1,245)	1:12:A:DG:H1’	1:13:A:DG:H1’	20	0.24	0.0	0.24
(1,673)	1:13:A:DG:H5’	1:13:A:DG:H2”	20	0.23	0.0	0.23
(1,390)	1:1:A:DG:H5’	1:1:A:DG:H3’	20	0.22	0.0	0.22
(1,461)	1:4:A:DG:H3’	1:4:A:DG:H1’	20	0.22	0.0	0.22
(1,813)	1:20:A:DT:H1’	1:20:A:DT:H6	20	0.22	0.0	0.22
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	20	0.21	0.0	0.21

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Key	Atom-1	Atom-2	Models^1	Mean (Å)	SD^1 (Å)	Median (Å)
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	20	0.21	0.0	0.21
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	20	0.2	0.0	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	20	0.2	0.0	0.2
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	20	0.19	0.0	0.19
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	20	0.19	0.0	0.19
(1,763)	1:17:A:DG:H1’	1:17:A:DG:H8	20	0.19	0.0	0.19
(1,102)	1:5:A:DC:H2’	1:11:A:DG:H21	20	0.19	0.0	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	20	0.19	0.0	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	20	0.19	0.0	0.19
(1,703)	1:14:A:DG:H3’	1:14:A:DG:H1’	20	0.19	0.0	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	20	0.19	0.0	0.19
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	20	0.18	0.0	0.18
(1,610)	1:10:A:DC:H1’	1:10:A:DC:H6	20	0.18	0.0	0.18
(1,647)	1:11:A:DG:H5”	1:11:A:DG:H8	20	0.18	0.0	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	20	0.18	0.0	0.18
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	20	0.17	0.0	0.17
(1,411)	1:2:A:DG:H2’	1:2:A:DG:H5’	20	0.17	0.0	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	20	0.17	0.0	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	20	0.17	0.0	0.17
(1,324)	1:16:A:DG:H2’	1:1:A:DG:H5”	20	0.16	0.0	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	20	0.16	0.0	0.16
(1,106)	1:5:A:DC:H3’	1:6:A:DG:H5”	20	0.16	0.0	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	20	0.16	0.0	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	20	0.16	0.0	0.16
(1,746)	1:16:A:DG:H4’	1:16:A:DG:H1’	20	0.16	0.0	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	20	0.16	0.0	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	20	0.16	0.0	0.16
(1,504)	1:6:A:DG:H2’	1:6:A:DG:H1’	20	0.15	0.0	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	20	0.15	0.01	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	20	0.15	0.0	0.15
(1,383)	1:1:A:DG:H1’	1:1:A:DG:H2’	20	0.15	0.0	0.15
(1,578)	1:9:A:DG:H2’	1:9:A:DG:H1’	20	0.15	0.0	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	20	0.15	0.0	0.15
(1,293)	1:14:A:DG:H5’	1:15:A:DC:H6	20	0.15	0.01	0.15
(1,108)	1:5:A:DC:H4’	1:6:A:DG:H8	20	0.14	0.0	0.14
(1,518)	1:6:A:DG:H2”	1:6:A:DG:H5’	20	0.14	0.0	0.14
(1,704)	1:14:A:DG:H4’	1:14:A:DG:H8	20	0.14	0.0	0.14
(1,445)	1:4:A:DG:H2’	1:4:A:DG:H1’	20	0.14	0.0	0.14
(1,453)	1:4:A:DG:H3’	1:4:A:DG:H5’	20	0.14	0.0	0.14
(1,626)	1:11:A:DG:H1’	1:11:A:DG:H2’	20	0.14	0.0	0.14
(1,63)	1:3:A:DG:H4’	1:5:A:DC:H5	20	0.14	0.0	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	20	0.14	0.0	0.14

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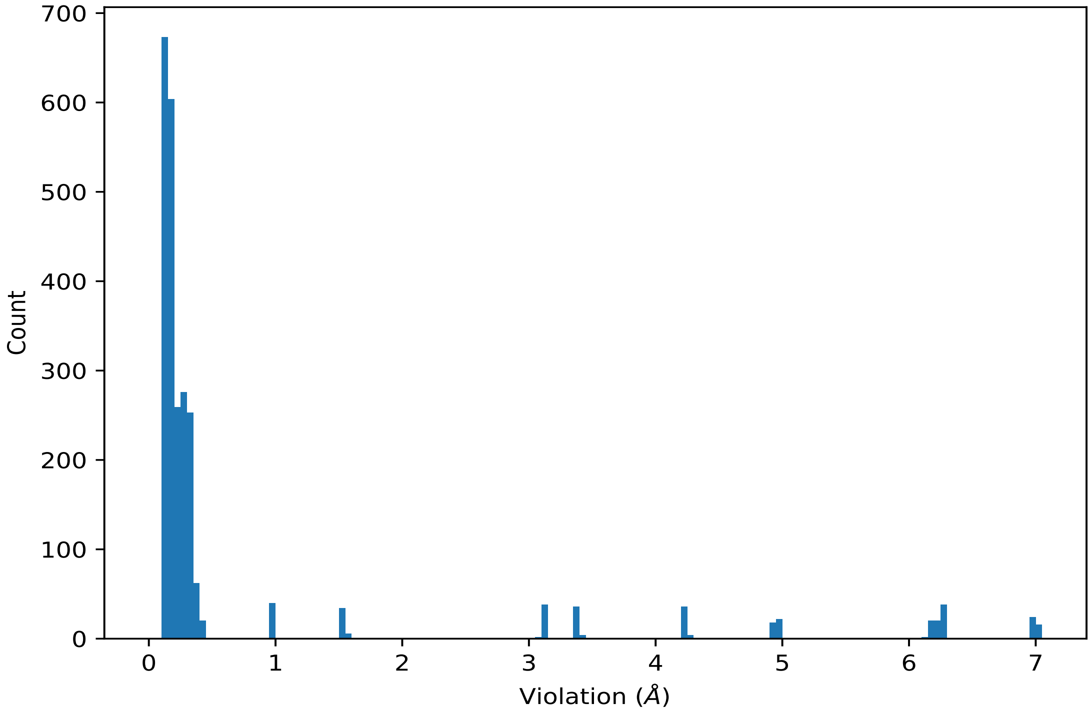
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,275)	1:14:A:DG:H4’	1:13:A:DG:H1’	20	0.13	0.0	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	20	0.13	0.0	0.13
(1,259)	1:17:A:DG:H1’	1:17:A:DG:H1	20	0.13	0.0	0.13
(1,745)	1:16:A:DG:H2”	1:16:A:DG:H3’	20	0.13	0.0	0.13
(1,318)	1:16:A:DG:H3’	1:18:A:DG:H8	20	0.13	0.0	0.13
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	20	0.12	0.0	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	20	0.12	0.0	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	20	0.12	0.0	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	20	0.12	0.0	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	20	0.12	0.0	0.12
(1,634)	1:11:A:DG:H5’	1:11:A:DG:H2”	20	0.12	0.0	0.12
(1,722)	1:15:A:DC:H1’	1:15:A:DC:H6	20	0.12	0.0	0.12
(1,797)	1:19:A:DG:H2”	1:19:A:DG:H3’	20	0.12	0.0	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	20	0.12	0.0	0.12
(1,64)	1:3:A:DG:H5’	1:4:A:DG:H8	20	0.12	0.0	0.12
(1,170)	1:8:A:DG:H1’	1:9:A:DG:H8	20	0.11	0.0	0.11
(1,558)	1:8:A:DG:H2’	1:8:A:DG:H1’	20	0.11	0.0	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	20	0.11	0.0	0.11
(1,78)	1:4:A:DG:H2”	1:5:A:DC:H5’	20	0.11	0.0	0.11
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	20	0.1	0.0	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	20	0.1	0.0	0.1
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	19	0.11	0.0	0.11
(1,210)	1:10:A:DC:H3’	1:8:A:DG:H8	18	0.1	0.0	0.1
(1,304)	1:15:A:DC:H4’	1:16:A:DG:H5’	17	0.1	0.0	0.1
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	11	0.1	0.0	0.1
(1,316)	1:16:A:DG:H2’	1:18:A:DG:H8	10	0.1	0.0	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	10	0.1	0.0	0.1

[1] Number of violated models, [2] Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:20:A:DT:H5'	1:15:A:DC:H6	4	7.02
(1,376)	1:20:A:DT:H5"	1:15:A:DC:H6	4	7.02
(1,376)	1:20:A:DT:H5'	1:15:A:DC:H6	12	7.02
(1,376)	1:20:A:DT:H5"	1:15:A:DC:H6	12	7.02
(1,376)	1:20:A:DT:H5'	1:15:A:DC:H6	10	7.01
(1,376)	1:20:A:DT:H5"	1:15:A:DC:H6	10	7.01
(1,376)	1:20:A:DT:H5'	1:15:A:DC:H6	19	7.01
(1,376)	1:20:A:DT:H5"	1:15:A:DC:H6	19	7.01
(1,376)	1:20:A:DT:H5'	1:15:A:DC:H6	3	7.0
(1,376)	1:20:A:DT:H5"	1:15:A:DC:H6	3	7.0
(1,376)	1:20:A:DT:H5'	1:15:A:DC:H6	8	7.0
(1,376)	1:20:A:DT:H5"	1:15:A:DC:H6	8	7.0
(1,376)	1:20:A:DT:H5'	1:15:A:DC:H6	14	7.0
(1,376)	1:20:A:DT:H5"	1:15:A:DC:H6	14	7.0
(1,376)	1:20:A:DT:H5'	1:15:A:DC:H6	17	7.0
(1,376)	1:20:A:DT:H5"	1:15:A:DC:H6	17	7.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	5	6.99
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	5	6.99
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	6	6.99
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	6	6.99
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	7	6.99
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	7	6.99
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	11	6.99
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	11	6.99
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	20	6.99
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	20	6.99
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	1	6.98
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	1	6.98
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	2	6.98
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	2	6.98
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	9	6.98
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	9	6.98
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	13	6.98
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	13	6.98
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	15	6.98
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	15	6.98
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	16	6.98
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	16	6.98
(1,376)	1:20:A:DT:H5’	1:15:A:DC:H6	18	6.98
(1,376)	1:20:A:DT:H5”	1:15:A:DC:H6	18	6.98
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	4	6.29
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	4	6.29
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	12	6.29
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	12	6.29
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	19	6.29
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	19	6.29
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	3	6.28
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	3	6.28
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	5	6.28
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	5	6.28
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	14	6.28
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	14	6.28
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	20	6.28
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	20	6.28
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	1	6.27
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	1	6.27
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	9	6.27
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	9	6.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	10	6.27
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	10	6.27
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	11	6.27
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	11	6.27
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	2	6.26
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	2	6.26
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	6	6.26
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	6	6.26
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	7	6.26
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	7	6.26
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	8	6.26
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	8	6.26
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	15	6.26
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	15	6.26
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	17	6.26
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	17	6.26
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	18	6.26
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	18	6.26
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	13	6.25
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	13	6.25
(1,375)	1:20:A:DT:H5’	1:15:A:DC:H4’	16	6.23
(1,375)	1:20:A:DT:H5”	1:15:A:DC:H4’	16	6.23
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5’	12	6.23
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5”	12	6.23
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5’	4	6.22
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5”	4	6.22
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5’	5	6.22
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5”	5	6.22
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5’	14	6.22
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5”	14	6.22
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5’	3	6.21
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5”	3	6.21
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5’	9	6.21
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5”	9	6.21
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5’	19	6.21
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5”	19	6.21
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5’	20	6.21
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5”	20	6.21
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5’	8	6.2
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5”	8	6.2
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5’	7	6.19
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5”	7	6.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	11	6.19
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	11	6.19
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	15	6.19
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	15	6.19
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	17	6.19
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	17	6.19
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	1	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	1	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	2	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	2	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	6	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	6	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	10	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	10	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	13	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	13	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	18	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	18	6.18
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5'	16	6.14
(1,273)	1:14:A:DG:H21	1:20:A:DT:H5"	16	6.14
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	12	4.98
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	12	4.98
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	4	4.97
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	4	4.97
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	14	4.97
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	14	4.97
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	3	4.96
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	3	4.96
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	5	4.96
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	5	4.96
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	19	4.96
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	19	4.96
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	7	4.95
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	7	4.95
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	8	4.95
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	8	4.95
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	10	4.95
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	10	4.95
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	17	4.95
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	17	4.95
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	20	4.95
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	20	4.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	1	4.94
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	1	4.94
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	2	4.94
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	2	4.94
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	6	4.94
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	6	4.94
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	9	4.94
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	9	4.94
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	11	4.94
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	11	4.94
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	15	4.94
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	15	4.94
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	18	4.94
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	18	4.94
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	13	4.93
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	13	4.93
(1,374)	1:20:A:DT:H5'	1:15:A:DC:H1'	16	4.92
(1,374)	1:20:A:DT:H5"	1:15:A:DC:H1'	16	4.92
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	12	4.25
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	12	4.25
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	14	4.25
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	14	4.25
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	3	4.24
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	3	4.24
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	4	4.24
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	4	4.24
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	5	4.24
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	5	4.24
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	19	4.24
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	19	4.24
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	8	4.23
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	8	4.23
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	9	4.23
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	9	4.23
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	10	4.23
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	10	4.23
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	20	4.23
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	20	4.23
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	1	4.22
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	1	4.22
(1,377)	1:20:A:DT:H5'	1:16:A:DG:H1	6	4.22
(1,377)	1:20:A:DT:H5"	1:16:A:DG:H1	6	4.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:20:A:DT:H5’	1:16:A:DG:H1	7	4.22
(1,377)	1:20:A:DT:H5”	1:16:A:DG:H1	7	4.22
(1,377)	1:20:A:DT:H5’	1:16:A:DG:H1	11	4.22
(1,377)	1:20:A:DT:H5”	1:16:A:DG:H1	11	4.22
(1,377)	1:20:A:DT:H5’	1:16:A:DG:H1	15	4.22
(1,377)	1:20:A:DT:H5”	1:16:A:DG:H1	15	4.22
(1,377)	1:20:A:DT:H5’	1:16:A:DG:H1	17	4.22
(1,377)	1:20:A:DT:H5”	1:16:A:DG:H1	17	4.22
(1,377)	1:20:A:DT:H5’	1:16:A:DG:H1	18	4.22
(1,377)	1:20:A:DT:H5”	1:16:A:DG:H1	18	4.22
(1,377)	1:20:A:DT:H5’	1:16:A:DG:H1	2	4.21
(1,377)	1:20:A:DT:H5”	1:16:A:DG:H1	2	4.21
(1,377)	1:20:A:DT:H5’	1:16:A:DG:H1	13	4.21
(1,377)	1:20:A:DT:H5”	1:16:A:DG:H1	13	4.21
(1,377)	1:20:A:DT:H5’	1:16:A:DG:H1	16	4.2
(1,377)	1:20:A:DT:H5”	1:16:A:DG:H1	16	4.2
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	12	3.41
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	12	3.41
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	14	3.41
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	14	3.41
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	5	3.39
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	5	3.39
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	7	3.39
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	7	3.39
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	9	3.39
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	9	3.39
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	17	3.39
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	17	3.39
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	20	3.39
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	20	3.39
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	4	3.38
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	4	3.38
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	8	3.38
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	8	3.38
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	19	3.38
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	19	3.38
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	2	3.37
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	2	3.37
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	6	3.37
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	6	3.37
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	11	3.37
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	11	3.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	13	3.37
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	13	3.37
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	18	3.37
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	18	3.37
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	1	3.36
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	1	3.36
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	3	3.36
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	3	3.36
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	10	3.36
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	10	3.36
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	15	3.36
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	15	3.36
(1,373)	1:20:A:DT:H5’	1:9:A:DG:H8	16	3.35
(1,373)	1:20:A:DT:H5”	1:9:A:DG:H8	16	3.35
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	12	3.14
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	12	3.14
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	14	3.14
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	14	3.14
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	19	3.13
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	19	3.13
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	4	3.12
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	4	3.12
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	5	3.12
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	5	3.12
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	7	3.12
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	7	3.12
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	8	3.12
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	8	3.12
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	17	3.12
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	17	3.12
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	20	3.12
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	20	3.12
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	3	3.11
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	3	3.11
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	6	3.11
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	6	3.11
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	9	3.11
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	9	3.11
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	10	3.11
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	10	3.11
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	11	3.11
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	11	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	18	3.11
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	18	3.11
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	1	3.1
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	1	3.1
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	2	3.1
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	2	3.1
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	13	3.1
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	13	3.1
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	15	3.1
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	15	3.1
(1,378)	1:20:A:DT:H5’	1:19:A:DG:H1	16	3.08
(1,378)	1:20:A:DT:H5”	1:19:A:DG:H1	16	3.08
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	4	1.55
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	4	1.55
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	12	1.55
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	12	1.55
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	14	1.55
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	14	1.55
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	3	1.54
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	3	1.54
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	8	1.54
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	8	1.54
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	10	1.54
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	10	1.54
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	19	1.54
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	19	1.54
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	20	1.54
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	20	1.54
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	1	1.53
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	1	1.53
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	5	1.53
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	5	1.53
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	6	1.53
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	6	1.53
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	7	1.53
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	7	1.53
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	9	1.53
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	9	1.53
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	11	1.53
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	11	1.53
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	13	1.53
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	13	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	17	1.53
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	17	1.53
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	2	1.52
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	2	1.52
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	15	1.52
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	15	1.52
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	16	1.52
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	16	1.52
(1,826)	1:20:A:DT:H5’	1:20:A:DT:H6	18	1.52
(1,826)	1:20:A:DT:H5”	1:20:A:DT:H6	18	1.52
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	3	0.99
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	3	0.99
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	10	0.99
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	10	0.99
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	12	0.99
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	12	0.99
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	19	0.99
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	19	0.99
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	1	0.98
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	1	0.98
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	4	0.98
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	4	0.98
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	8	0.98
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	8	0.98
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	14	0.98
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	14	0.98
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	15	0.98
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	15	0.98
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	20	0.98
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	20	0.98
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	2	0.97
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	2	0.97
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	5	0.97
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	5	0.97
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	6	0.97
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	6	0.97
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	7	0.97
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	7	0.97
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	9	0.97
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	9	0.97
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	11	0.97
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	11	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	13	0.97
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	13	0.97
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	16	0.97
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	16	0.97
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	17	0.97
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	17	0.97
(1,369)	1:20:A:DT:H5’	1:19:A:DG:H8	18	0.97
(1,369)	1:20:A:DT:H5”	1:19:A:DG:H8	18	0.97
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	1	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	2	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	3	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	4	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	5	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	6	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	7	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	8	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	9	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	10	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	11	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	12	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	13	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	14	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	15	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	16	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	17	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	18	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	19	0.4
(1,474)	1:5:A:DC:H1’	1:5:A:DC:H6	20	0.4
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	1	0.36
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	3	0.36
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	4	0.36
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	5	0.36
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	7	0.36
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	9	0.36
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	16	0.36
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	17	0.36
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	18	0.36
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	20	0.36
(1,786)	1:18:A:DG:H1’	1:18:A:DG:H8	1	0.35
(1,786)	1:18:A:DG:H1’	1:18:A:DG:H8	2	0.35
(1,786)	1:18:A:DG:H1’	1:18:A:DG:H8	3	0.35
(1,786)	1:18:A:DG:H1’	1:18:A:DG:H8	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	5	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	6	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	7	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	8	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	9	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	10	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	11	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	12	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	13	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	14	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	15	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	16	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	17	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	18	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	19	0.35
(1,786)	1:18:A:DG:H1'	1:18:A:DG:H8	20	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	1	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	2	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	3	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	4	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	5	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	6	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	7	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	8	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	9	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	10	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	11	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	12	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	13	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	14	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	15	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	16	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	17	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	18	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	19	0.35
(1,549)	1:7:A:DG:H4'	1:7:A:DG:H2'	20	0.35
(1,392)	1:1:A:DG:H2'	1:1:A:DG:H5'	2	0.35
(1,392)	1:1:A:DG:H2'	1:1:A:DG:H5'	6	0.35
(1,392)	1:1:A:DG:H2'	1:1:A:DG:H5'	8	0.35
(1,392)	1:1:A:DG:H2'	1:1:A:DG:H5'	10	0.35
(1,392)	1:1:A:DG:H2'	1:1:A:DG:H5'	11	0.35
(1,392)	1:1:A:DG:H2'	1:1:A:DG:H5'	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	13	0.35
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	14	0.35
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	15	0.35
(1,392)	1:1:A:DG:H2’	1:1:A:DG:H5’	19	0.35
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	1	0.35
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	4	0.35
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	1	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	3	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	4	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	7	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	8	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	10	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	12	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	13	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	14	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	15	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	16	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	17	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	18	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	19	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	2	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	3	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	5	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	6	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	7	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	8	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	9	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	10	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	11	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	12	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	13	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	14	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	15	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	16	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	17	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	18	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	19	0.34
(1,382)	1:20:A:DT:H6	1:19:A:DG:H8	20	0.34
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	2	0.33
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	5	0.33
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	6	0.33
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2”	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2"	11	0.33
(1,736)	1:15:A:DC:H5	1:15:A:DC:H2"	20	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	1	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	2	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	3	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	4	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	5	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	6	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	7	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	8	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	9	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	10	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	11	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	12	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	13	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	14	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	15	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	16	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	17	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	18	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	19	0.33
(1,699)	1:14:A:DG:H2'	1:14:A:DG:H4'	20	0.33
(1,371)	1:20:A:DT:H3'	1:19:A:DG:H8	14	0.33
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	5	0.33
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	19	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	2	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	3	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	4	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	5	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	6	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	7	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	8	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	11	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	12	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	13	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	14	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	15	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	16	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	17	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	18	0.33
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	20	0.33
(1,702)	1:14:A:DG:H2"	1:14:A:DG:H5'	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	2	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	3	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	4	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	5	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	6	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	7	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	8	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	9	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	10	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	11	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	12	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	13	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	14	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	15	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	16	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	17	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	18	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	19	0.32
(1,702)	1:14:A:DG:H2”	1:14:A:DG:H5’	20	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	1	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	2	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	3	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	4	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	5	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	6	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	7	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	8	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	9	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	10	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	11	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	12	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	13	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	14	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	15	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	16	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	17	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	18	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	19	0.32
(1,643)	1:11:A:DG:H4’	1:11:A:DG:H2’	20	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	1	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	2	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	4	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	5	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	6	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	7	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	8	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	9	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	10	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	11	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	12	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	13	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	14	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	15	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	16	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	17	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	18	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	19	0.32
(1,543)	1:7:A:DG:H1’	1:7:A:DG:H3’	20	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	1	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	2	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	3	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	4	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	5	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	6	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	7	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	8	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	9	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	10	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	11	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	12	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	13	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	14	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	15	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	16	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	17	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	18	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	19	0.32
(1,514)	1:6:A:DG:H2’	1:6:A:DG:H4’	20	0.32
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	4	0.32
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	5	0.32
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	10	0.32
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	12	0.32
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	1	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	2	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	3	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	4	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	6	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	7	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	8	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	9	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	10	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	11	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	12	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	13	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	14	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	15	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	16	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	17	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	18	0.32
(1,360)	1:19:A:DG:H5'	1:18:A:DG:H8	20	0.32
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	1	0.32
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	9	0.32
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	10	0.32
(1,268)	1:14:A:DG:H5"	1:13:A:DG:H1'	19	0.32
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	1	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	2	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	3	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	4	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	5	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	6	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	7	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	8	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	9	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	10	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	11	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	12	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	13	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	14	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	15	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	16	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	17	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	18	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	19	0.31
(1,458)	1:4:A:DG:H2'	1:4:A:DG:H4'	20	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	1	0.31
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	2	0.31
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	3	0.31
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	6	0.31
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	7	0.31
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	8	0.31
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	9	0.31
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	17	0.31
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	18	0.31
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	19	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	1	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	2	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	3	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	4	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	5	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	6	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	7	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	8	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	9	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	10	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	11	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	12	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	13	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	15	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	16	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	17	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	18	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	19	0.31
(1,292)	1:14:A:DG:H5’	1:13:A:DG:H1	20	0.31
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	11	0.3
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	13	0.3
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	15	0.3
(1,371)	1:20:A:DT:H3’	1:19:A:DG:H8	16	0.3
(1,320)	1:16:A:DG:H1’	1:18:A:DG:H8	2	0.3
(1,320)	1:16:A:DG:H1’	1:18:A:DG:H8	3	0.3
(1,320)	1:16:A:DG:H1’	1:18:A:DG:H8	4	0.3
(1,320)	1:16:A:DG:H1’	1:18:A:DG:H8	6	0.3
(1,320)	1:16:A:DG:H1’	1:18:A:DG:H8	7	0.3
(1,320)	1:16:A:DG:H1’	1:18:A:DG:H8	8	0.3
(1,320)	1:16:A:DG:H1’	1:18:A:DG:H8	9	0.3
(1,320)	1:16:A:DG:H1’	1:18:A:DG:H8	11	0.3
(1,320)	1:16:A:DG:H1’	1:18:A:DG:H8	13	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	14	0.3
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	15	0.3
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	16	0.3
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	18	0.3
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	19	0.3
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	20	0.3
(1,292)	1:14:A:DG:H5'	1:13:A:DG:H1	14	0.3
(1,450)	1:4:A:DG:H2"	1:4:A:DG:H8	9	0.29
(1,450)	1:4:A:DG:H2"	1:4:A:DG:H8	13	0.29
(1,450)	1:4:A:DG:H2"	1:4:A:DG:H8	15	0.29
(1,450)	1:4:A:DG:H2"	1:4:A:DG:H8	19	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	1	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	2	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	3	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	4	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	5	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	6	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	7	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	8	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	9	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	10	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	11	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	12	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	13	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	14	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	15	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	16	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	17	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	18	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	19	0.29
(1,434)	1:3:A:DG:H2"	1:3:A:DG:H5'	20	0.29
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	1	0.29
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	5	0.29
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	10	0.29
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	12	0.29
(1,320)	1:16:A:DG:H1'	1:18:A:DG:H8	17	0.29
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	10	0.28
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	15	0.28
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	1	0.28
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	3	0.28
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	7	0.28
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,513)	1:6:A:DG:H1’	1:6:A:DG:H8	9	0.28
(1,513)	1:6:A:DG:H1’	1:6:A:DG:H8	11	0.28
(1,513)	1:6:A:DG:H1’	1:6:A:DG:H8	12	0.28
(1,513)	1:6:A:DG:H1’	1:6:A:DG:H8	14	0.28
(1,513)	1:6:A:DG:H1’	1:6:A:DG:H8	17	0.28
(1,513)	1:6:A:DG:H1’	1:6:A:DG:H8	18	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	1	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	2	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	3	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	4	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	5	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	6	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	7	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	8	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	10	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	11	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	12	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	14	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	16	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	17	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	18	0.28
(1,450)	1:4:A:DG:H2”	1:4:A:DG:H8	20	0.28
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	5	0.28
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	1	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	2	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	3	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	4	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	5	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	6	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	7	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	8	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	9	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	10	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	11	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	12	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	13	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	14	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	15	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	16	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	17	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	18	0.27
(1,772)	1:17:A:DG:H2’	1:17:A:DG:H4’	19	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:17:A:DG:H2'	1:17:A:DG:H4'	20	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	1	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	2	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	3	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	5	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	6	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	7	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	8	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	9	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	10	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	11	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	12	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	13	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	14	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	15	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	16	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	17	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	18	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	20	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	1	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	2	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	3	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	4	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	5	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	6	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	7	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	8	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	9	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	11	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	12	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	13	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	14	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	16	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	17	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	18	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	19	0.27
(1,554)	1:7:A:DG:H5'	1:7:A:DG:H1	20	0.27
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	2	0.27
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	4	0.27
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	5	0.27
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	6	0.27
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	13	0.27
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	15	0.27
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	16	0.27
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	19	0.27
(1,513)	1:6:A:DG:H1'	1:6:A:DG:H8	20	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	2	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	4	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	6	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	7	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	8	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	9	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	12	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	13	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	14	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	15	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	18	0.27
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	20	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	1	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	2	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	3	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	4	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	5	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	6	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	7	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	8	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	9	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	10	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	11	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	12	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	13	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	14	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	15	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	16	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	17	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	18	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	19	0.27
(1,227)	1:11:A:DG:H2'	1:12:A:DG:H1'	20	0.27
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	4	0.26
(1,761)	1:16:A:DG:H3'	1:16:A:DG:H8	19	0.26
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	1	0.26
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	5	0.26
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	20	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	1	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	2	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	4	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	5	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	6	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	7	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	8	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	10	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	12	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	13	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	14	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	15	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	16	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	17	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	18	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	19	0.26
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	20	0.26
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	1	0.26
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	3	0.26
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	10	0.26
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	11	0.26
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	16	0.26
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	17	0.26
(1,249)	1:12:A:DG:H8	1:9:A:DG:H1	19	0.26
(1,827)	1:20:A:DT:H2'	1:20:A:DT:H4'	9	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	2	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	3	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	4	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	6	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	7	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	10	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	11	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	12	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	13	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	15	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	17	0.25
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	18	0.25
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	3	0.25
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	9	0.25
(1,495)	1:5:A:DC:H5"	1:5:A:DC:H2"	11	0.25
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	1	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	2	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	3	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	4	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	5	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	6	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	7	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	8	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	9	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	10	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	11	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	12	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	13	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	14	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	15	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	16	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	17	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	18	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	19	0.25
(1,397)	1:1:A:DG:H4’	1:1:A:DG:H2’	20	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	1	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	2	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	3	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	4	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	5	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	6	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	7	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	8	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	9	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	10	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	11	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	12	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	13	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	15	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	16	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	17	0.25
(1,260)	1:13:A:DG:H2’	1:12:A:DG:H1’	20	0.25
(1,245)	1:12:A:DG:H1’	1:13:A:DG:H1’	4	0.25
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	9	0.25
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	12	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	1	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	3	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	5	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	6	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	7	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	8	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	9	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	10	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	11	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	12	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	13	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	14	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	15	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	16	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	17	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	18	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	19	0.25
(1,199)	1:9:A:DG:H5’	1:10:A:DC:H6	20	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	1	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	2	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	3	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	4	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	6	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	7	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	11	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	13	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	14	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	15	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	16	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	18	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	19	0.25
(1,75)	1:4:A:DG:H2’	1:3:A:DG:H8	20	0.25
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	1	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	2	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	3	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	4	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	5	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	6	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	7	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	8	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	10	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	11	0.24
(1,827)	1:20:A:DT:H2’	1:20:A:DT:H4’	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:20:A:DT:H2'	1:20:A:DT:H4'	13	0.24
(1,827)	1:20:A:DT:H2'	1:20:A:DT:H4'	14	0.24
(1,827)	1:20:A:DT:H2'	1:20:A:DT:H4'	15	0.24
(1,827)	1:20:A:DT:H2'	1:20:A:DT:H4'	16	0.24
(1,827)	1:20:A:DT:H2'	1:20:A:DT:H4'	17	0.24
(1,827)	1:20:A:DT:H2'	1:20:A:DT:H4'	18	0.24
(1,827)	1:20:A:DT:H2'	1:20:A:DT:H4'	19	0.24
(1,827)	1:20:A:DT:H2'	1:20:A:DT:H4'	20	0.24
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	8	0.24
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	14	0.24
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	16	0.24
(1,729)	1:15:A:DC:H5'	1:15:A:DC:H6	19	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	1	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	2	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	3	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	4	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	5	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	6	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	7	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	9	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	10	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	11	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	12	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	13	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	14	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	15	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	16	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	17	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	18	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	19	0.24
(1,468)	1:4:A:DG:H2"	1:4:A:DG:H5'	20	0.24
(1,260)	1:13:A:DG:H2'	1:12:A:DG:H1'	14	0.24
(1,260)	1:13:A:DG:H2'	1:12:A:DG:H1'	18	0.24
(1,260)	1:13:A:DG:H2'	1:12:A:DG:H1'	19	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	1	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	2	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	3	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	5	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	6	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	8	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	9	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	11	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	12	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	13	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	14	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	15	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	16	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	18	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	19	0.24
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	20	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	1	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	2	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	3	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	4	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	5	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	6	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	7	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	8	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	10	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	11	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	13	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	14	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	15	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	16	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	17	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	18	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	19	0.24
(1,222)	1:11:A:DG:H22	1:7:A:DG:H8	20	0.24
(1,199)	1:9:A:DG:H5'	1:10:A:DC:H6	4	0.24
(1,75)	1:4:A:DG:H2'	1:3:A:DG:H8	5	0.24
(1,75)	1:4:A:DG:H2'	1:3:A:DG:H8	8	0.24
(1,75)	1:4:A:DG:H2'	1:3:A:DG:H8	9	0.24
(1,75)	1:4:A:DG:H2'	1:3:A:DG:H8	10	0.24
(1,75)	1:4:A:DG:H2'	1:3:A:DG:H8	12	0.24
(1,75)	1:4:A:DG:H2'	1:3:A:DG:H8	17	0.24
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	1	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	2	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	3	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	4	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	5	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	6	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	7	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	9	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	10	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	11	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	12	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	13	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	14	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	15	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	16	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	17	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	18	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	19	0.23
(1,673)	1:13:A:DG:H5'	1:13:A:DG:H2"	20	0.23
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	7	0.23
(1,245)	1:12:A:DG:H1'	1:13:A:DG:H1'	17	0.23
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	1	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	2	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	3	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	4	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	5	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	6	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	7	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	8	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	9	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	10	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	11	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	12	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	13	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	14	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	15	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	16	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	17	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	18	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	19	0.22
(1,813)	1:20:A:DT:H1'	1:20:A:DT:H6	20	0.22
(1,732)	1:15:A:DC:H2"	1:15:A:DC:H5'	2	0.22
(1,732)	1:15:A:DC:H2"	1:15:A:DC:H5'	6	0.22
(1,732)	1:15:A:DC:H2"	1:15:A:DC:H5'	9	0.22
(1,732)	1:15:A:DC:H2"	1:15:A:DC:H5'	11	0.22
(1,732)	1:15:A:DC:H2"	1:15:A:DC:H5'	18	0.22
(1,732)	1:15:A:DC:H2"	1:15:A:DC:H5'	20	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	1	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	3	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	4	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	5	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	6	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	7	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	8	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	9	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	10	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	11	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	12	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	13	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	14	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	15	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	16	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	17	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	18	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	19	0.22
(1,461)	1:4:A:DG:H3'	1:4:A:DG:H1'	20	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	1	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	2	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	3	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	4	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	5	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	6	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	7	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	8	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	9	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	10	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	11	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	12	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	13	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	14	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	15	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	16	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	17	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	18	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	19	0.22
(1,390)	1:1:A:DG:H5'	1:1:A:DG:H3'	20	0.22
(1,732)	1:15:A:DC:H2"	1:15:A:DC:H5'	1	0.21
(1,732)	1:15:A:DC:H2"	1:15:A:DC:H5'	3	0.21
(1,732)	1:15:A:DC:H2"	1:15:A:DC:H5'	4	0.21
(1,732)	1:15:A:DC:H2"	1:15:A:DC:H5'	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	7	0.21
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	8	0.21
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	10	0.21
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	12	0.21
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	13	0.21
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	14	0.21
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	15	0.21
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	16	0.21
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	17	0.21
(1,732)	1:15:A:DC:H2”	1:15:A:DC:H5’	19	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	1	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	2	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	3	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	4	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	5	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	6	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	8	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	9	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	11	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	12	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	14	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	15	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	16	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	18	0.21
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	20	0.21
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	9	0.21
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	17	0.21
(1,763)	1:17:A:DG:H1’	1:17:A:DG:H8	11	0.2
(1,763)	1:17:A:DG:H1’	1:17:A:DG:H8	12	0.2
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	7	0.2
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	10	0.2
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	13	0.2
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	17	0.2
(1,654)	1:12:A:DG:H2’	1:12:A:DG:H8	19	0.2
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	7	0.2
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	9	0.2
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	16	0.2
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	20	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	2	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	3	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	4	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	6	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	7	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	8	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	10	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	11	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	12	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	13	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	14	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	16	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	17	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	18	0.2
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	20	0.2
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	1	0.2
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	3	0.2
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	4	0.2
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	10	0.2
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	13	0.2
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	16	0.2
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	17	0.2
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	19	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	1	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	2	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	3	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	4	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	5	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	6	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	7	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	8	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	10	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	11	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	12	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	13	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	14	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	15	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	16	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	18	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	19	0.2
(1,107)	1:5:A:DC:H3’	1:11:A:DG:H1	20	0.2
(1,763)	1:17:A:DG:H1’	1:17:A:DG:H8	1	0.19
(1,763)	1:17:A:DG:H1’	1:17:A:DG:H8	2	0.19
(1,763)	1:17:A:DG:H1’	1:17:A:DG:H8	3	0.19
(1,763)	1:17:A:DG:H1’	1:17:A:DG:H8	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	5	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	6	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	7	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	8	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	9	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	10	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	13	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	14	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	15	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	16	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	17	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	18	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	19	0.19
(1,763)	1:17:A:DG:H1'	1:17:A:DG:H8	20	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	1	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	2	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	3	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	4	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	5	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	6	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	7	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	8	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	9	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	10	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	11	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	12	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	13	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	14	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	15	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	17	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	18	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	19	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	20	0.19
(1,618)	1:10:A:DC:H5"	1:10:A:DC:H2'	1	0.19
(1,618)	1:10:A:DC:H5"	1:10:A:DC:H2'	2	0.19
(1,618)	1:10:A:DC:H5"	1:10:A:DC:H2'	3	0.19
(1,618)	1:10:A:DC:H5"	1:10:A:DC:H2'	4	0.19
(1,618)	1:10:A:DC:H5"	1:10:A:DC:H2'	5	0.19
(1,618)	1:10:A:DC:H5"	1:10:A:DC:H2'	6	0.19
(1,618)	1:10:A:DC:H5"	1:10:A:DC:H2'	8	0.19
(1,618)	1:10:A:DC:H5"	1:10:A:DC:H2'	11	0.19
(1,618)	1:10:A:DC:H5"	1:10:A:DC:H2'	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	13	0.19
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	14	0.19
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	15	0.19
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	17	0.19
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	18	0.19
(1,618)	1:10:A:DC:H5”	1:10:A:DC:H2’	19	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	1	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	2	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	3	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	4	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	5	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	6	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	7	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	8	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	9	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	11	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	12	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	13	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	14	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	15	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	16	0.19
(1,615)	1:10:A:DC:H5’	1:10:A:DC:H2”	17	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	1	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	2	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	3	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	4	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	5	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	6	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	7	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	8	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	9	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	10	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	11	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	12	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	13	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	14	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	15	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	16	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	17	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	18	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	19	0.19
(1,522)	1:6:A:DG:H5’	1:6:A:DG:H8	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	1	0.19
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	9	0.19
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	15	0.19
(1,302)	1:15:A:DC:H4’	1:16:A:DG:H3’	19	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	1	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	2	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	3	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	4	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	5	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	6	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	8	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	9	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	10	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	11	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	12	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	13	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	14	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	15	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	16	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	17	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	18	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	19	0.19
(1,189)	1:8:A:DG:H3’	1:7:A:DG:H8	20	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	2	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	5	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	6	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	7	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	8	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	9	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	11	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	12	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	14	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	15	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	18	0.19
(1,181)	1:8:A:DG:H2”	1:9:A:DG:H1’	20	0.19
(1,102)	1:5:A:DC:H2’	1:11:A:DG:H21	1	0.19
(1,102)	1:5:A:DC:H2’	1:11:A:DG:H21	2	0.19
(1,102)	1:5:A:DC:H2’	1:11:A:DG:H21	3	0.19
(1,102)	1:5:A:DC:H2’	1:11:A:DG:H21	4	0.19
(1,102)	1:5:A:DC:H2’	1:11:A:DG:H21	5	0.19
(1,102)	1:5:A:DC:H2’	1:11:A:DG:H21	6	0.19
(1,102)	1:5:A:DC:H2’	1:11:A:DG:H21	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	8	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	9	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	10	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	11	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	12	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	13	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	14	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	15	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	16	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	17	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	18	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	19	0.19
(1,102)	1:5:A:DC:H2'	1:11:A:DG:H21	20	0.19
(1,703)	1:14:A:DG:H3'	1:14:A:DG:H1'	16	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	1	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	2	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	3	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	4	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	5	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	6	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	7	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	8	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	9	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	10	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	11	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	12	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	13	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	14	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	15	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	16	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	17	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	18	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	19	0.18
(1,647)	1:11:A:DG:H5"	1:11:A:DG:H8	20	0.18
(1,618)	1:10:A:DC:H5"	1:10:A:DC:H2'	10	0.18
(1,615)	1:10:A:DC:H5'	1:10:A:DC:H2"	10	0.18
(1,615)	1:10:A:DC:H5'	1:10:A:DC:H2"	18	0.18
(1,615)	1:10:A:DC:H5'	1:10:A:DC:H2"	19	0.18
(1,615)	1:10:A:DC:H5'	1:10:A:DC:H2"	20	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	1	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	2	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	4	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	5	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	6	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	7	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	8	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	9	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	10	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	11	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	12	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	13	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	14	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	15	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	16	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	17	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	18	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	19	0.18
(1,610)	1:10:A:DC:H1'	1:10:A:DC:H6	20	0.18
(1,497)	1:5:A:DC:H1'	1:5:A:DC:H5	3	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	1	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	2	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	3	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	4	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	5	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	6	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	7	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	8	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	9	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	10	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	11	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	12	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	13	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	14	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	15	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	16	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	17	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	18	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	19	0.18
(1,492)	1:5:A:DC:H5	1:5:A:DC:H41	20	0.18
(1,189)	1:8:A:DG:H3'	1:7:A:DG:H8	7	0.18
(1,125)	1:5:A:DC:H5"	1:6:A:DG:H8	1	0.18
(1,125)	1:5:A:DC:H5"	1:6:A:DG:H8	2	0.18
(1,125)	1:5:A:DC:H5"	1:6:A:DG:H8	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	4	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	5	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	6	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	7	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	8	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	10	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	11	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	12	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	13	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	14	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	15	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	16	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	17	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	18	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	19	0.18
(1,125)	1:5:A:DC:H5”	1:6:A:DG:H8	20	0.18
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	1	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	2	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	3	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	4	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	5	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	6	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	7	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	8	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	9	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	10	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	11	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	12	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	13	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	14	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	15	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	16	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	17	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	18	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	19	0.17
(1,728)	1:15:A:DC:H5’	1:15:A:DC:H3’	20	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	1	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	2	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	3	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	4	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	5	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	7	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	8	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	9	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	10	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	11	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	12	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	13	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	14	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	15	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	16	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	17	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	18	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	19	0.17
(1,601)	1:9:A:DG:H5”	1:9:A:DG:H8	20	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	1	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	2	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	4	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	5	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	6	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	7	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	8	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	9	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	10	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	11	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	12	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	13	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	14	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	15	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	16	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	17	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	18	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	19	0.17
(1,497)	1:5:A:DC:H1’	1:5:A:DC:H5	20	0.17
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	1	0.17
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	2	0.17
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	7	0.17
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	8	0.17
(1,411)	1:2:A:DG:H2’	1:2:A:DG:H5’	1	0.17
(1,411)	1:2:A:DG:H2’	1:2:A:DG:H5’	2	0.17
(1,411)	1:2:A:DG:H2’	1:2:A:DG:H5’	3	0.17
(1,411)	1:2:A:DG:H2’	1:2:A:DG:H5’	4	0.17
(1,411)	1:2:A:DG:H2’	1:2:A:DG:H5’	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	6	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	7	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	8	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	9	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	10	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	11	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	12	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	13	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	14	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	15	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	16	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	17	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	18	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	19	0.17
(1,411)	1:2:A:DG:H2'	1:2:A:DG:H5'	20	0.17
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	1	0.17
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	9	0.17
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	10	0.17
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	11	0.17
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	13	0.17
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	15	0.17
(1,125)	1:5:A:DC:H5"	1:6:A:DG:H8	9	0.17
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	1	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	2	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	3	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	4	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	5	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	6	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	7	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	8	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	9	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	10	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	11	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	12	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	13	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	14	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	15	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	16	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	17	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	18	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	19	0.16
(1,746)	1:16:A:DG:H4'	1:16:A:DG:H1'	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	3	0.16
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	8	0.16
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	10	0.16
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	14	0.16
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	16	0.16
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	19	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	1	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	2	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	3	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	4	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	5	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	6	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	7	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	8	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	9	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	10	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	11	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	12	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	13	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	14	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	15	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	16	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	17	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	18	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	19	0.16
(1,694)	1:14:A:DG:H5’	1:14:A:DG:H3’	20	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	1	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	2	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	3	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	5	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	7	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	9	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	10	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	11	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	12	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	13	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	14	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	15	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	16	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	17	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	18	0.16
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	20	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	1	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	2	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	3	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	4	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	7	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	8	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	9	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	10	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	11	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	13	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	15	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	19	0.16
(1,586)	1:9:A:DG:H3’	1:9:A:DG:H1’	20	0.16
(1,504)	1:6:A:DG:H2’	1:6:A:DG:H1’	1	0.16
(1,504)	1:6:A:DG:H2’	1:6:A:DG:H1’	5	0.16
(1,504)	1:6:A:DG:H2’	1:6:A:DG:H1’	7	0.16
(1,504)	1:6:A:DG:H2’	1:6:A:DG:H1’	9	0.16
(1,504)	1:6:A:DG:H2’	1:6:A:DG:H1’	11	0.16
(1,504)	1:6:A:DG:H2’	1:6:A:DG:H1’	13	0.16
(1,504)	1:6:A:DG:H2’	1:6:A:DG:H1’	14	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	3	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	4	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	5	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	6	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	9	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	10	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	11	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	12	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	13	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	14	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	15	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	16	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	17	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	18	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	19	0.16
(1,413)	1:2:A:DG:H2”	1:2:A:DG:H5’	20	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	1	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	2	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	3	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	4	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	6	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	7	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	8	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	9	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	10	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	11	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	12	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	13	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	14	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	15	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	16	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	17	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	18	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	19	0.16
(1,357)	1:18:A:DG:H8	1:16:A:DG:H1	20	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	2	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	3	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	4	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	5	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	6	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	7	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	8	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	12	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	14	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	16	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	17	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	18	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	19	0.16
(1,324)	1:16:A:DG:H2'	1:1:A:DG:H5"	20	0.16
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	10	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	1	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	2	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	3	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	4	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	5	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	6	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	7	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	8	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	9	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	10	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	11	0.16
(1,106)	1:5:A:DC:H3'	1:6:A:DG:H5"	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:5:A:DC:H3’	1:6:A:DG:H5”	13	0.16
(1,106)	1:5:A:DC:H3’	1:6:A:DG:H5”	14	0.16
(1,106)	1:5:A:DC:H3’	1:6:A:DG:H5”	15	0.16
(1,106)	1:5:A:DC:H3’	1:6:A:DG:H5”	16	0.16
(1,106)	1:5:A:DC:H3’	1:6:A:DG:H5”	17	0.16
(1,106)	1:5:A:DC:H3’	1:6:A:DG:H5”	18	0.16
(1,106)	1:5:A:DC:H3’	1:6:A:DG:H5”	19	0.16
(1,106)	1:5:A:DC:H3’	1:6:A:DG:H5”	20	0.16
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	1	0.16
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	4	0.16
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	10	0.16
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	1	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	2	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	4	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	5	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	7	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	11	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	12	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	13	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	15	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	17	0.15
(1,730)	1:15:A:DC:H2’	1:15:A:DC:H5’	18	0.15
(1,704)	1:14:A:DG:H4’	1:14:A:DG:H8	4	0.15
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	4	0.15
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	6	0.15
(1,688)	1:14:A:DG:H2”	1:14:A:DG:H8	8	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	1	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	2	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	3	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	4	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	5	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	6	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	7	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	8	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	9	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	10	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	11	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	12	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	13	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	14	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	15	0.15
(1,667)	1:13:A:DG:H1’	1:13:A:DG:H2’	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:13:A:DG:H1'	1:13:A:DG:H2'	17	0.15
(1,667)	1:13:A:DG:H1'	1:13:A:DG:H2'	18	0.15
(1,667)	1:13:A:DG:H1'	1:13:A:DG:H2'	19	0.15
(1,667)	1:13:A:DG:H1'	1:13:A:DG:H2'	20	0.15
(1,586)	1:9:A:DG:H3'	1:9:A:DG:H1'	5	0.15
(1,586)	1:9:A:DG:H3'	1:9:A:DG:H1'	6	0.15
(1,586)	1:9:A:DG:H3'	1:9:A:DG:H1'	12	0.15
(1,586)	1:9:A:DG:H3'	1:9:A:DG:H1'	14	0.15
(1,586)	1:9:A:DG:H3'	1:9:A:DG:H1'	16	0.15
(1,586)	1:9:A:DG:H3'	1:9:A:DG:H1'	17	0.15
(1,586)	1:9:A:DG:H3'	1:9:A:DG:H1'	18	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	1	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	2	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	3	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	4	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	5	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	6	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	7	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	8	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	9	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	10	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	11	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	12	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	13	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	14	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	15	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	16	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	17	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	18	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	19	0.15
(1,578)	1:9:A:DG:H2'	1:9:A:DG:H1'	20	0.15
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	13	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	2	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	3	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	4	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	6	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	8	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	10	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	12	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	15	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	16	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	18	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	19	0.15
(1,504)	1:6:A:DG:H2'	1:6:A:DG:H1'	20	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	1	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	2	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	3	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	4	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	5	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	6	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	7	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	8	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	9	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	10	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	11	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	12	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	13	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	14	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	15	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	16	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	17	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	18	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	19	0.15
(1,383)	1:1:A:DG:H1'	1:1:A:DG:H2'	20	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	1	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	3	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	4	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	7	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	8	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	11	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	13	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	14	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	16	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	17	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	18	0.15
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	19	0.15
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	3	0.15
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	9	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	2	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	3	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	5	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	6	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	8	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	9	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	11	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	12	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	13	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	14	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	15	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	16	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	17	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	18	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	19	0.15
(1,18)	1:1:A:DG:H8	1:12:A:DG:H1	20	0.15
(1,730)	1:15:A:DC:H2'	1:15:A:DC:H5'	6	0.14
(1,730)	1:15:A:DC:H2'	1:15:A:DC:H5'	9	0.14
(1,730)	1:15:A:DC:H2'	1:15:A:DC:H5'	20	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	1	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	2	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	3	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	5	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	6	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	7	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	8	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	9	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	10	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	11	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	12	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	13	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	14	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	15	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	16	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	17	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	18	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	19	0.14
(1,704)	1:14:A:DG:H4'	1:14:A:DG:H8	20	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	1	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	2	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	3	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	4	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	5	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	6	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	7	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	9	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	10	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	11	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	12	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	13	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	14	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	15	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	16	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	17	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	18	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	19	0.14
(1,626)	1:11:A:DG:H1'	1:11:A:DG:H2'	20	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	1	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	2	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	3	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	4	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	5	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	6	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	7	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	8	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	9	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	10	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	11	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	12	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	14	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	15	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	16	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	17	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	18	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	19	0.14
(1,518)	1:6:A:DG:H2"	1:6:A:DG:H5'	20	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	1	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	2	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	3	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	4	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	5	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	6	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	7	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	8	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	9	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	10	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	12	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	13	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	14	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	15	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	16	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	17	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	18	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	19	0.14
(1,453)	1:4:A:DG:H3'	1:4:A:DG:H5'	20	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	1	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	2	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	3	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	4	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	5	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	6	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	7	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	8	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	9	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	10	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	11	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	12	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	13	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	14	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	15	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	16	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	17	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	18	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	19	0.14
(1,445)	1:4:A:DG:H2'	1:4:A:DG:H1'	20	0.14
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	2	0.14
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	5	0.14
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	6	0.14
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	9	0.14
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	12	0.14
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	15	0.14
(1,293)	1:14:A:DG:H5'	1:15:A:DC:H6	20	0.14
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	5	0.14
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	6	0.14
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	7	0.14
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	8	0.14
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	14	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	2	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	3	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	5	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	6	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	7	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	8	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	9	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	10	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	11	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	12	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	14	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	15	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	16	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	17	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	18	0.14
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	20	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	1	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	2	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	4	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	5	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	6	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	7	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	8	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	10	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	11	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	12	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	13	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	14	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	15	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	16	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	17	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	18	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	19	0.14
(1,108)	1:5:A:DC:H4'	1:6:A:DG:H8	20	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	1	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	2	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	3	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	4	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	5	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	6	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	7	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	10	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	11	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	12	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	13	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	14	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	16	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	17	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	18	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	19	0.14
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	20	0.14
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	1	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	2	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	3	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	4	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	5	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	6	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	7	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	8	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	9	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	10	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	11	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	12	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	13	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	14	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	15	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	16	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	17	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	18	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	19	0.13
(1,745)	1:16:A:DG:H2"	1:16:A:DG:H3'	20	0.13
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	1	0.13
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	3	0.13
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	14	0.13
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	16	0.13
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	19	0.13
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	1	0.13
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	3	0.13
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	7	0.13
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	8	0.13
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	9	0.13
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	10	0.13
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	15	0.13
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	16	0.13
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	17	0.13
(1,318)	1:16:A:DG:H3'	1:18:A:DG:H8	19	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	1	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	2	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	3	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	4	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	9	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	10	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	11	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	12	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	13	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	15	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	16	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	17	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	18	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	19	0.13
(1,275)	1:14:A:DG:H4'	1:13:A:DG:H1'	20	0.13
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	4	0.13
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	13	0.13
(1,267)	1:14:A:DG:H21	1:16:A:DG:H1	19	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	1	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	2	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	3	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	4	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	5	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	6	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	7	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	8	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	9	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	10	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	11	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	12	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	13	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	14	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	15	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	16	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	17	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	18	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	19	0.13
(1,259)	1:17:A:DG:H1'	1:17:A:DG:H1	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:10:A:DC:H2'	1:9:A:DG:H1'	10	0.13
(1,182)	1:8:A:DG:H2"	1:19:A:DG:H1	6	0.13
(1,182)	1:8:A:DG:H2"	1:19:A:DG:H1	14	0.13
(1,182)	1:8:A:DG:H2"	1:19:A:DG:H1	16	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	1	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	2	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	3	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	4	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	5	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	6	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	7	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	8	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	9	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	10	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	11	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	12	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	13	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	14	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	15	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	16	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	17	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	18	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	19	0.13
(1,113)	1:5:A:DC:H41	1:4:A:DG:H8	20	0.13
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	9	0.13
(1,63)	1:3:A:DG:H4'	1:5:A:DC:H5	15	0.13
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	1	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	2	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	3	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	4	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	5	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	6	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	7	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	8	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	9	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	10	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	11	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	12	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	13	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	14	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	15	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	17	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	18	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	19	0.12
(1,797)	1:19:A:DG:H2"	1:19:A:DG:H3'	20	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	1	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	2	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	3	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	4	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	5	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	6	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	7	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	8	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	9	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	10	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	11	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	12	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	13	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	14	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	15	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	16	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	17	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	18	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	19	0.12
(1,722)	1:15:A:DC:H1'	1:15:A:DC:H6	20	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	1	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	2	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	3	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	4	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	5	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	6	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	7	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	8	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	9	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	10	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	11	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	12	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	13	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	14	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	15	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	16	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	17	0.12
(1,634)	1:11:A:DG:H5'	1:11:A:DG:H2"	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,634)	1:11:A:DG:H5’	1:11:A:DG:H2”	19	0.12
(1,634)	1:11:A:DG:H5’	1:11:A:DG:H2”	20	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	1	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	2	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	3	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	4	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	5	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	6	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	7	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	8	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	9	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	10	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	11	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	12	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	13	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	14	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	15	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	16	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	17	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	18	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	19	0.12
(1,532)	1:6:A:DG:H3’	1:6:A:DG:H8	20	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	1	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	2	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	3	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	4	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	5	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	6	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	7	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	8	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	9	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	10	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	11	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	12	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	13	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	14	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	15	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	16	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	17	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	18	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	19	0.12
(1,393)	1:1:A:DG:H2’	1:1:A:DG:H5”	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	2	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	4	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	5	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	6	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	7	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	8	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	9	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	10	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	11	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	12	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	13	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	15	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	17	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	18	0.12
(1,333)	1:17:A:DG:H8	1:18:A:DG:H8	20	0.12
(1,318)	1:16:A:DG:H3’	1:18:A:DG:H8	2	0.12
(1,318)	1:16:A:DG:H3’	1:18:A:DG:H8	4	0.12
(1,318)	1:16:A:DG:H3’	1:18:A:DG:H8	5	0.12
(1,318)	1:16:A:DG:H3’	1:18:A:DG:H8	6	0.12
(1,318)	1:16:A:DG:H3’	1:18:A:DG:H8	11	0.12
(1,318)	1:16:A:DG:H3’	1:18:A:DG:H8	12	0.12
(1,318)	1:16:A:DG:H3’	1:18:A:DG:H8	14	0.12
(1,318)	1:16:A:DG:H3’	1:18:A:DG:H8	18	0.12
(1,318)	1:16:A:DG:H3’	1:18:A:DG:H8	20	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	1	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	2	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	3	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	4	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	5	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	6	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	7	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	8	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	9	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	11	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	12	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	13	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	14	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	15	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	16	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	17	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	18	0.12
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:10:A:DC:H2’	1:9:A:DG:H1’	20	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	1	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	2	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	3	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	4	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	5	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	7	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	8	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	9	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	10	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	11	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	12	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	13	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	15	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	17	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	18	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	19	0.12
(1,182)	1:8:A:DG:H2”	1:19:A:DG:H1	20	0.12
(1,170)	1:8:A:DG:H1’	1:9:A:DG:H8	5	0.12
(1,170)	1:8:A:DG:H1’	1:9:A:DG:H8	14	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	1	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	2	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	3	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	4	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	5	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	6	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	8	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	12	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	14	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	16	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	17	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	18	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	19	0.12
(1,123)	1:5:A:DC:H5’	1:6:A:DG:H8	20	0.12
(1,64)	1:3:A:DG:H5’	1:4:A:DG:H8	1	0.12
(1,64)	1:3:A:DG:H5’	1:4:A:DG:H8	2	0.12
(1,64)	1:3:A:DG:H5’	1:4:A:DG:H8	5	0.12
(1,64)	1:3:A:DG:H5’	1:4:A:DG:H8	6	0.12
(1,64)	1:3:A:DG:H5’	1:4:A:DG:H8	7	0.12
(1,64)	1:3:A:DG:H5’	1:4:A:DG:H8	8	0.12
(1,64)	1:3:A:DG:H5’	1:4:A:DG:H8	10	0.12
(1,64)	1:3:A:DG:H5’	1:4:A:DG:H8	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	12	0.12
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	13	0.12
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	14	0.12
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	15	0.12
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	16	0.12
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	18	0.12
(1,832)	1:20:A:DT:H2"	1:20:A:DT:H5'	3	0.11
(1,832)	1:20:A:DT:H2"	1:20:A:DT:H5'	7	0.11
(1,832)	1:20:A:DT:H2"	1:20:A:DT:H5'	9	0.11
(1,832)	1:20:A:DT:H2"	1:20:A:DT:H5'	10	0.11
(1,832)	1:20:A:DT:H2"	1:20:A:DT:H5'	11	0.11
(1,832)	1:20:A:DT:H2"	1:20:A:DT:H5'	12	0.11
(1,832)	1:20:A:DT:H2"	1:20:A:DT:H5'	13	0.11
(1,832)	1:20:A:DT:H2"	1:20:A:DT:H5'	14	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	1	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	2	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	3	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	4	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	5	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	6	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	7	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	8	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	9	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	10	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	11	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	12	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	13	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	14	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	15	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	16	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	17	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	18	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	19	0.11
(1,558)	1:8:A:DG:H2'	1:8:A:DG:H1'	20	0.11
(1,316)	1:16:A:DG:H2'	1:18:A:DG:H8	16	0.11
(1,310)	1:15:A:DC:H5"	1:13:A:DG:H1	1	0.11
(1,310)	1:15:A:DC:H5"	1:13:A:DG:H1	2	0.11
(1,310)	1:15:A:DC:H5"	1:13:A:DG:H1	3	0.11
(1,310)	1:15:A:DC:H5"	1:13:A:DG:H1	5	0.11
(1,310)	1:15:A:DC:H5"	1:13:A:DG:H1	6	0.11
(1,310)	1:15:A:DC:H5"	1:13:A:DG:H1	7	0.11
(1,310)	1:15:A:DC:H5"	1:13:A:DG:H1	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	9	0.11
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	10	0.11
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	11	0.11
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	13	0.11
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	14	0.11
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	15	0.11
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	16	0.11
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	17	0.11
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	18	0.11
(1,310)	1:15:A:DC:H5”	1:13:A:DG:H1	20	0.11
(1,304)	1:15:A:DC:H4’	1:16:A:DG:H5’	5	0.11
(1,304)	1:15:A:DC:H4’	1:16:A:DG:H5’	14	0.11
(1,304)	1:15:A:DC:H4’	1:16:A:DG:H5’	18	0.11
(1,304)	1:15:A:DC:H4’	1:16:A:DG:H5’	19	0.11
(1,210)	1:10:A:DC:H3’	1:8:A:DG:H8	3	0.11
(1,210)	1:10:A:DC:H3’	1:8:A:DG:H8	4	0.11
(1,210)	1:10:A:DC:H3’	1:8:A:DG:H8	6	0.11
(1,210)	1:10:A:DC:H3’	1:8:A:DG:H8	9	0.11
(1,210)	1:10:A:DC:H3’	1:8:A:DG:H8	10	0.11
(1,210)	1:10:A:DC:H3’	1:8:A:DG:H8	16	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	1	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	2	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	3	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	5	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	7	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	8	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	9	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	10	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	11	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	12	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	13	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	15	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	16	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	17	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	18	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	19	0.11
(1,192)	1:9:A:DG:H5’	1:8:A:DG:H1’	20	0.11
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	6	0.11
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	9	0.11
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	12	0.11
(1,170)	1:8:A:DG:H1’	1:9:A:DG:H8	1	0.11
(1,170)	1:8:A:DG:H1’	1:9:A:DG:H8	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	3	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	6	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	7	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	8	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	9	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	10	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	11	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	12	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	13	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	15	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	16	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	17	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	18	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	19	0.11
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	20	0.11
(1,123)	1:5:A:DC:H5'	1:6:A:DG:H8	7	0.11
(1,123)	1:5:A:DC:H5'	1:6:A:DG:H8	9	0.11
(1,123)	1:5:A:DC:H5'	1:6:A:DG:H8	10	0.11
(1,123)	1:5:A:DC:H5'	1:6:A:DG:H8	11	0.11
(1,123)	1:5:A:DC:H5'	1:6:A:DG:H8	13	0.11
(1,123)	1:5:A:DC:H5'	1:6:A:DG:H8	15	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	1	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	3	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	4	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	5	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	6	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	8	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	9	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	10	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	11	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	12	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	14	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	16	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	17	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	18	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	19	0.11
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	20	0.11
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	3	0.11
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	4	0.11
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	9	0.11
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	17	0.11
(1,64)	1:3:A:DG:H5'	1:4:A:DG:H8	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:3:A:DG:H5’	1:4:A:DG:H8	20	0.11
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	1	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	2	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	4	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	5	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	6	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	8	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	15	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	16	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	17	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	18	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	19	0.1
(1,832)	1:20:A:DT:H2”	1:20:A:DT:H5’	20	0.1
(1,806)	1:19:A:DG:H5”	1:19:A:DG:H1’	14	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	1	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	2	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	3	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	4	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	5	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	6	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	7	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	8	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	9	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	10	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	11	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	12	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	13	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	14	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	15	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	16	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	17	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	18	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	19	0.1
(1,652)	1:12:A:DG:H2’	1:12:A:DG:H1’	20	0.1
(1,316)	1:16:A:DG:H2’	1:18:A:DG:H8	3	0.1
(1,316)	1:16:A:DG:H2’	1:18:A:DG:H8	6	0.1
(1,316)	1:16:A:DG:H2’	1:18:A:DG:H8	7	0.1
(1,316)	1:16:A:DG:H2’	1:18:A:DG:H8	8	0.1
(1,316)	1:16:A:DG:H2’	1:18:A:DG:H8	11	0.1
(1,316)	1:16:A:DG:H2’	1:18:A:DG:H8	13	0.1
(1,316)	1:16:A:DG:H2’	1:18:A:DG:H8	15	0.1
(1,316)	1:16:A:DG:H2’	1:18:A:DG:H8	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:16:A:DG:H2'	1:18:A:DG:H8	20	0.1
(1,310)	1:15:A:DC:H5"	1:13:A:DG:H1	12	0.1
(1,310)	1:15:A:DC:H5"	1:13:A:DG:H1	19	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	1	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	3	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	4	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	6	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	7	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	8	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	10	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	11	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	12	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	13	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	16	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	17	0.1
(1,304)	1:15:A:DC:H4'	1:16:A:DG:H5'	20	0.1
(1,303)	1:15:A:DC:H4'	1:16:A:DG:H4'	16	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	1	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	2	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	5	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	7	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	8	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	11	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	12	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	13	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	15	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	17	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	18	0.1
(1,210)	1:10:A:DC:H3'	1:8:A:DG:H8	19	0.1
(1,192)	1:9:A:DG:H5'	1:8:A:DG:H1'	4	0.1
(1,192)	1:9:A:DG:H5'	1:8:A:DG:H1'	6	0.1
(1,192)	1:9:A:DG:H5'	1:8:A:DG:H1'	14	0.1
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	2	0.1
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	3	0.1
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	7	0.1
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	8	0.1
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	11	0.1
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	13	0.1
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	17	0.1
(1,185)	1:8:A:DG:H21	1:11:A:DG:H8	18	0.1
(1,170)	1:8:A:DG:H1'	1:9:A:DG:H8	4	0.1
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	7	0.1
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	13	0.1
(1,78)	1:4:A:DG:H2"	1:5:A:DC:H5'	15	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	1	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	4	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	5	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	10	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	11	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	12	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	13	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	18	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	19	0.1
(1,32)	1:2:A:DG:H22	1:3:A:DG:H1	20	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found