Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 05:31 PM JST

PDB ID	:	5Z8F
BMRB ID	:	36160
Title	:	Solution structure for the unique dimeric 4:2 complex of a platinum(II)-based tripod bound to a hybrid-1 human telomeric G-quadruplex
Authors	:	Liu, W.T.; Zhong, Y.F.; Liu, L.Y.; Zeng, W.J.; Wang, F.Y.; Yang, D.Z.; Mao, Z.W.
Deposited on	:	2018-01-31

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

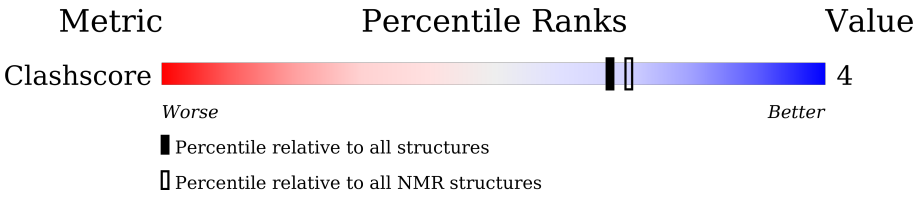
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 23%.

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	26	81% 19%
1	B	26	92% 8%

2 Ensemble composition and analysis (i)

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

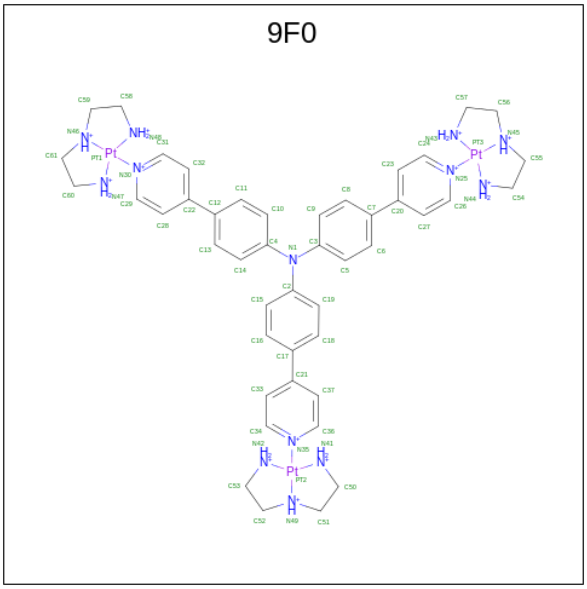
3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2182 atoms, of which 840 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called G-quadruplex DNA (26-MER).

Mol	Chain	Residues	Atoms						Trace
1	A	26	Total	C	H	N	O	P	0
			843	260	294	112	152	25	
1	B	26	Total	C	H	N	O	P	0
			843	260	294	112	152	25	

- Molecule 2 is 4-[1-(2,5,8-triazonia-1$l^4-platinabicyclo[3.3.0]octan-1-yl)pyridin-1-ium-4-yl]-N,N-bis[4-[1-(2,5,8-triazonia-1$l^4-platinabicyclo[3.3.0]octan-1-yl)pyridin-1-ium-4-yl]phenyl]aniline (three-letter code: 9F0) (formula: $C_{45}H_{63}N_{13}Pt_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	N	Pt
			124	45	63	13	3
2	A	1	Total	C	H	N	Pt
			124	45	63	13	3
2	B	1	Total	C	H	N	Pt
			124	45	63	13	3
2	B	1	Total	C	H	N	Pt
			124	45	63	13	3

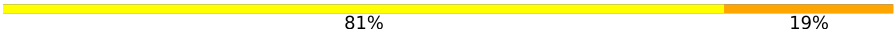
4 Residue-property plots

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.

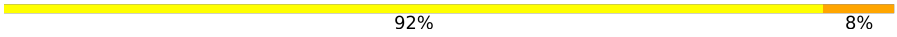
• Molecule 1: G-quadruplex DNA (26-MER)

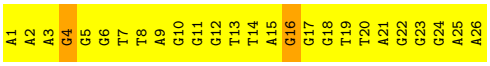
Chain A:



• Molecule 1: G-quadruplex DNA (26-MER)

Chain B:





4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: G-quadruplex DNA (26-MER)

Chain A:

• Molecule 1: G-quadruplex DNA (26-MER)

Chain B:

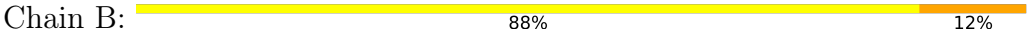
4.2.2 Score per residue for model 2

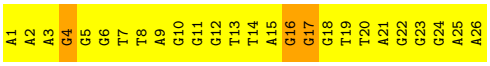
• Molecule 1: G-quadruplex DNA (26-MER)

Chain A:

• Molecule 1: G-quadruplex DNA (26-MER)

Chain B:

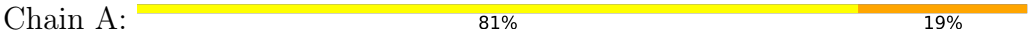




4.2.3 Score per residue for model 3

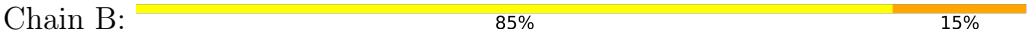
• Molecule 1: G-quadruplex DNA (26-MER)

Chain A:



• Molecule 1: G-quadruplex DNA (26-MER)

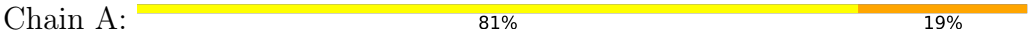
Chain B:

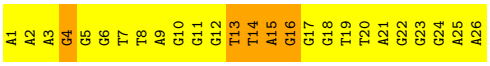


4.2.4 Score per residue for model 4

• Molecule 1: G-quadruplex DNA (26-MER)

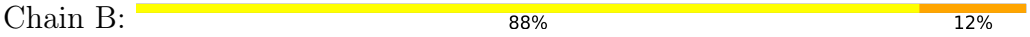
Chain A:

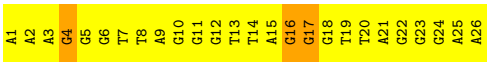




• Molecule 1: G-quadruplex DNA (26-MER)

Chain B:





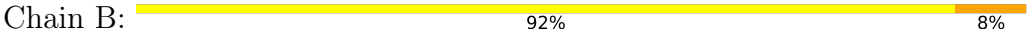
4.2.5 Score per residue for model 5

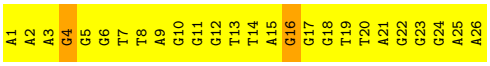
• Molecule 1: G-quadruplex DNA (26-MER)

Chain A:

• Molecule 1: G-quadruplex DNA (26-MER)

Chain B:

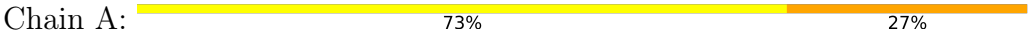




4.2.6 Score per residue for model 6

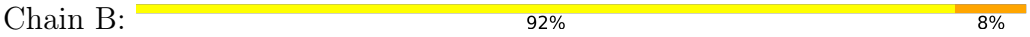
• Molecule 1: G-quadruplex DNA (26-MER)

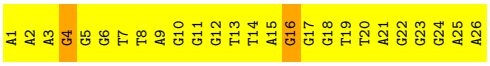
Chain A:



• Molecule 1: G-quadruplex DNA (26-MER)

Chain B:

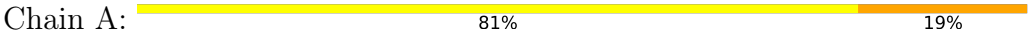




4.2.7 Score per residue for model 7

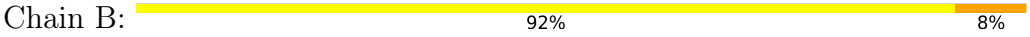
• Molecule 1: G-quadruplex DNA (26-MER)

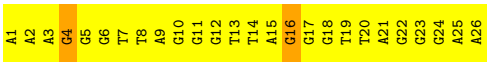
Chain A:



• Molecule 1: G-quadruplex DNA (26-MER)

Chain B:

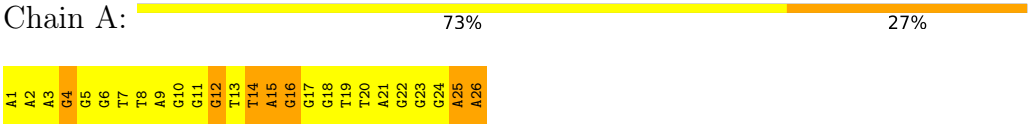




4.2.8 Score per residue for model 8

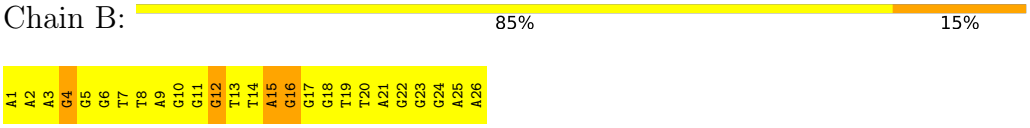
• Molecule 1: G-quadruplex DNA (26-MER)

Chain A:



• Molecule 1: G-quadruplex DNA (26-MER)

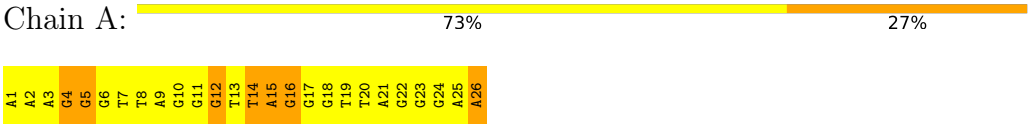
Chain B:



4.2.9 Score per residue for model 9

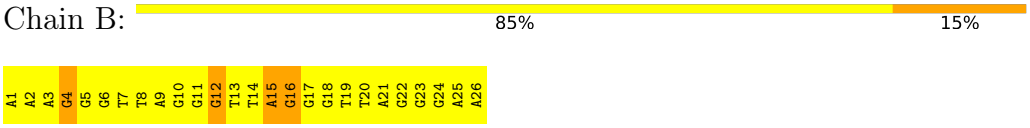
• Molecule 1: G-quadruplex DNA (26-MER)

Chain A:



• Molecule 1: G-quadruplex DNA (26-MER)

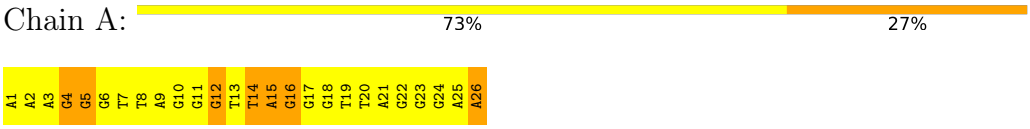
Chain B:



4.2.10 Score per residue for model 10

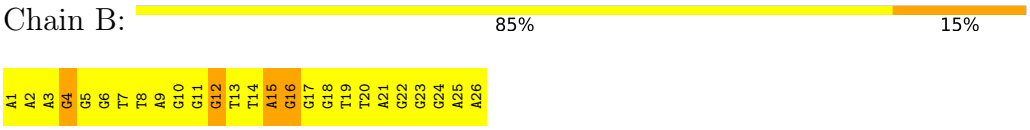
• Molecule 1: G-quadruplex DNA (26-MER)

Chain A:



• Molecule 1: G-quadruplex DNA (26-MER)

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, DGSA-distance geometry simulated annealing, molecular dynamics.*

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

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

Software name	Classification	Version
X-PLOR	refinement	
Discover	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	388
Number of shifts mapped to atoms	388
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	23%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9F0

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	1.74±0.01	6±0/620 (1.0± 0.0%)	2.47±0.01	53±2/960 (5.5± 0.2%)
1	B	1.72±0.01	6±0/620 (1.0± 0.0%)	2.45±0.01	50±1/960 (5.2± 0.1%)
All	All	1.73	120/12400 (1.0%)	2.46	1030/19200 (5.4%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.3
All	All	0	9

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	19	DT	C5-C7	9.03	1.55	1.50	3	10
1	A	19	DT	C5-C7	9.00	1.55	1.50	4	10
1	A	14	DT	C5-C7	8.98	1.55	1.50	6	10
1	A	8	DT	C5-C7	8.96	1.55	1.50	9	10
1	B	14	DT	C5-C7	8.96	1.55	1.50	6	10
1	A	7	DT	C5-C7	8.86	1.55	1.50	3	10
1	A	20	DT	C5-C7	8.86	1.55	1.50	9	10
1	B	8	DT	C5-C7	8.80	1.55	1.50	6	10
1	B	13	DT	C5-C7	8.78	1.55	1.50	7	10
1	B	7	DT	C5-C7	8.75	1.55	1.50	2	10
1	B	20	DT	C5-C7	8.67	1.55	1.50	9	10
1	A	13	DT	C5-C7	8.53	1.55	1.50	9	10

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	4	DG	N7-C8-N9	10.11	118.15	113.10	3	10
1	B	16	DG	N7-C8-N9	10.10	118.15	113.10	8	10
1	A	16	DG	N7-C8-N9	9.99	118.10	113.10	3	10
1	A	4	DG	N7-C8-N9	9.89	118.05	113.10	8	10
1	A	12	DG	N7-C8-N9	9.72	117.96	113.10	7	10
1	A	11	DG	N7-C8-N9	9.64	117.92	113.10	5	10
1	A	6	DG	N7-C8-N9	9.63	117.92	113.10	2	10
1	A	10	DG	N7-C8-N9	9.63	117.92	113.10	1	10
1	B	17	DG	N7-C8-N9	9.58	117.89	113.10	9	10
1	A	22	DG	N7-C8-N9	9.57	117.89	113.10	6	10
1	A	17	DG	N7-C8-N9	9.57	117.88	113.10	4	10
1	B	11	DG	N7-C8-N9	9.55	117.87	113.10	2	10
1	B	12	DG	N7-C8-N9	9.55	117.87	113.10	10	10
1	B	6	DG	N7-C8-N9	9.54	117.87	113.10	8	10
1	A	5	DG	N7-C8-N9	9.51	117.86	113.10	10	10
1	B	10	DG	N7-C8-N9	9.47	117.83	113.10	1	10
1	B	5	DG	N7-C8-N9	9.46	117.83	113.10	2	10
1	B	18	DG	N7-C8-N9	9.45	117.83	113.10	6	10
1	B	23	DG	N7-C8-N9	9.45	117.83	113.10	9	10
1	A	23	DG	N7-C8-N9	9.42	117.81	113.10	3	10
1	B	22	DG	N7-C8-N9	9.41	117.80	113.10	9	10
1	A	18	DG	N7-C8-N9	9.37	117.79	113.10	2	10
1	B	24	DG	N7-C8-N9	9.17	117.69	113.10	6	10
1	A	24	DG	N7-C8-N9	9.16	117.68	113.10	9	10
1	A	16	DG	C8-N9-C4	-9.02	102.79	106.40	9	10
1	B	16	DG	C8-N9-C4	-8.99	102.80	106.40	5	10
1	A	15	DA	C8-N9-C4	-8.88	102.25	105.80	6	10
1	B	15	DA	C8-N9-C4	-8.77	102.29	105.80	6	10
1	B	4	DG	C8-N9-C4	-8.66	102.93	106.40	3	10
1	A	4	DG	C8-N9-C4	-8.59	102.96	106.40	1	10
1	A	22	DG	C8-N9-C4	-8.34	103.06	106.40	6	10
1	B	22	DG	C8-N9-C4	-8.29	103.08	106.40	9	10
1	A	11	DG	C8-N9-C4	-8.28	103.09	106.40	3	10
1	B	11	DG	C8-N9-C4	-8.24	103.10	106.40	2	10
1	A	10	DG	C8-N9-C4	-8.10	103.16	106.40	1	10
1	A	6	DG	C8-N9-C4	-8.09	103.16	106.40	10	10
1	A	5	DG	C8-N9-C4	-8.06	103.18	106.40	10	10
1	A	12	DG	C8-N9-C4	-8.05	103.18	106.40	7	10
1	B	17	DG	C8-N9-C4	-8.01	103.19	106.40	10	10
1	A	17	DG	C8-N9-C4	-7.98	103.21	106.40	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	6	DG	C8-N9-C4	-7.98	103.21	106.40	7	10
1	A	23	DG	C8-N9-C4	-7.96	103.22	106.40	7	10
1	B	23	DG	C8-N9-C4	-7.96	103.22	106.40	9	10
1	B	26	DA	N7-C8-N9	7.93	117.77	113.80	4	10
1	A	21	DA	N7-C8-N9	7.92	117.76	113.80	4	10
1	B	5	DG	C8-N9-C4	-7.91	103.23	106.40	2	10
1	A	26	DA	N7-C8-N9	7.79	117.69	113.80	1	10
1	A	25	DA	N7-C8-N9	7.76	117.68	113.80	5	10
1	B	3	DA	N7-C8-N9	7.74	117.67	113.80	9	10
1	B	25	DA	N7-C8-N9	7.73	117.67	113.80	9	10
1	B	9	DA	N7-C8-N9	7.70	117.65	113.80	8	10
1	B	10	DG	C8-N9-C4	-7.69	103.32	106.40	5	10
1	A	14	DT	O4'-C1'-N1	7.69	113.38	108.00	4	10
1	A	24	DG	C8-N9-C4	-7.69	103.32	106.40	2	10
1	A	2	DA	N7-C8-N9	7.69	117.64	113.80	4	10
1	B	12	DG	C8-N9-C4	-7.68	103.33	106.40	1	10
1	B	2	DA	N7-C8-N9	7.68	117.64	113.80	8	10
1	B	21	DA	N7-C8-N9	7.67	117.63	113.80	4	10
1	A	9	DA	N7-C8-N9	7.65	117.63	113.80	8	10
1	A	3	DA	N7-C8-N9	7.65	117.63	113.80	10	10
1	B	18	DG	C8-N9-C4	-7.65	103.34	106.40	6	10
1	A	13	DT	O4'-C1'-N1	7.64	113.34	108.00	10	10
1	B	1	DA	N7-C8-N9	7.63	117.62	113.80	4	10
1	A	15	DA	N7-C8-N9	7.62	117.61	113.80	6	10
1	B	14	DT	O4'-C1'-N1	7.61	113.33	108.00	2	10
1	A	17	DG	O4'-C1'-N9	7.60	113.32	108.00	9	10
1	A	1	DA	N7-C8-N9	7.59	117.59	113.80	9	10
1	B	15	DA	N7-C8-N9	7.56	117.58	113.80	6	10
1	A	26	DA	O4'-C1'-N9	7.55	113.29	108.00	8	10
1	A	18	DG	C8-N9-C4	-7.55	103.38	106.40	9	10
1	B	24	DG	C8-N9-C4	-7.51	103.39	106.40	10	10
1	B	10	DG	O4'-C1'-N9	7.41	113.18	108.00	4	10
1	B	17	DG	O4'-C1'-N9	7.32	113.12	108.00	4	10
1	B	26	DA	C8-N9-C4	-7.31	102.87	105.80	4	10
1	A	26	DA	C8-N9-C4	-6.88	103.05	105.80	5	10
1	B	25	DA	C8-N9-C4	-6.88	103.05	105.80	9	10
1	A	21	DA	C8-N9-C4	-6.86	103.06	105.80	7	10
1	A	10	DG	O4'-C1'-N9	6.76	112.73	108.00	4	9
1	B	3	DA	C8-N9-C4	-6.71	103.11	105.80	9	10
1	B	9	DA	C8-N9-C4	-6.66	103.14	105.80	7	10
1	A	3	DA	C8-N9-C4	-6.63	103.15	105.80	5	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	1	DA	C8-N9-C4	-6.61	103.16	105.80	1	10
1	B	1	DA	C8-N9-C4	-6.59	103.17	105.80	6	10
1	B	21	DA	C8-N9-C4	-6.56	103.17	105.80	5	10
1	A	2	DA	C8-N9-C4	-6.52	103.19	105.80	1	10
1	B	2	DA	C8-N9-C4	-6.51	103.19	105.80	8	10
1	A	9	DA	C8-N9-C4	-6.50	103.20	105.80	4	10
1	A	25	DA	C8-N9-C4	-6.44	103.22	105.80	5	10
1	B	13	DT	O4'-C1'-N1	6.24	112.37	108.00	8	10
1	A	12	DG	O4'-C1'-N9	5.74	112.02	108.00	3	10
1	B	26	DA	O4'-C1'-N9	5.73	112.01	108.00	8	9
1	A	20	DT	O4'-C1'-N1	5.49	111.84	108.00	4	8
1	A	24	DG	O4'-C1'-N9	5.36	111.75	108.00	8	5
1	A	18	DG	C5-N7-C8	-5.34	101.63	104.30	2	9
1	B	18	DG	C5-N7-C8	-5.34	101.63	104.30	9	7
1	B	4	DG	O4'-C1'-N9	5.32	111.72	108.00	4	5
1	A	8	DT	C6-C5-C7	-5.29	119.73	122.90	9	10
1	A	7	DT	O4'-C1'-N1	5.22	111.65	108.00	5	6
1	A	25	DA	O4'-C1'-N9	5.21	111.65	108.00	8	2
1	B	20	DT	O4'-C1'-N1	5.20	111.64	108.00	2	5
1	B	13	DT	C6-C5-C7	-5.19	119.79	122.90	3	10
1	A	6	DG	C5-N7-C8	-5.18	101.71	104.30	2	2
1	B	8	DT	C6-C5-C7	-5.15	119.81	122.90	7	9
1	B	7	DT	C6-C5-C7	-5.14	119.82	122.90	6	9
1	B	6	DG	C5-N7-C8	-5.14	101.73	104.30	2	1
1	A	4	DG	O4'-C1'-N9	5.13	111.59	108.00	9	1
1	B	14	DT	C6-C5-C7	-5.12	119.83	122.90	1	2
1	A	19	DT	C6-C5-C7	-5.12	119.83	122.90	9	9
1	A	7	DT	C6-C5-C7	-5.10	119.84	122.90	1	8
1	A	17	DG	C5-N7-C8	-5.09	101.75	104.30	10	4
1	A	16	DG	P-O3'-C3'	5.07	125.78	119.70	2	1
1	A	16	DG	O4'-C1'-N9	5.05	111.54	108.00	9	1
1	A	14	DT	C6-C5-C7	-5.05	119.87	122.90	2	2
1	B	16	DG	O4'-C1'-N9	5.05	111.53	108.00	8	2
1	B	19	DT	C6-C5-C7	-5.03	119.88	122.90	3	2
1	B	4	DG	C5-N7-C8	-5.02	101.79	104.30	3	2

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	12	DG	Sidechain	9

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	549	294	294	4±1
1	B	549	294	294	3±1
All	All	13420	8400	5880	75

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:DG:H2"	1:A:5:DG:O5'	0.60	1.95	9	3
1:A:16:DG:N3	1:A:16:DG:H2'	0.60	2.11	6	10
1:A:14:DT:H4'	1:A:15:DA:OP1	0.60	1.97	8	10
1:A:4:DG:N3	1:A:4:DG:H2'	0.58	2.14	7	10
1:B:4:DG:N3	1:B:4:DG:H2'	0.58	2.13	7	10
1:B:16:DG:N3	1:B:16:DG:H2'	0.57	2.15	5	10
1:B:12:DG:H2'	1:B:15:DA:N1	0.53	2.18	8	4
1:A:13:DT:H2"	1:A:14:DT:OP2	0.46	2.10	4	1
1:A:16:DG:H2"	1:A:17:DG:OP2	0.45	2.12	2	2
1:B:14:DT:H2"	1:B:15:DA:OP2	0.44	2.13	3	1
1:A:25:DA:H2"	1:A:26:DA:O5'	0.44	2.13	8	1
1:A:16:DG:H1'	1:A:17:DG:O5'	0.43	2.12	6	1
1:B:16:DG:H2"	1:B:17:DG:OP2	0.42	2.13	4	2
1:B:16:DG:N3	1:B:16:DG:C2'	0.41	2.83	2	3
1:A:4:DG:N3	1:A:4:DG:C2'	0.41	2.84	1	2
1:A:16:DG:N3	1:A:16:DG:C2'	0.41	2.83	4	3
1:A:26:DA:H3'	1:B:15:DA:OP1	0.40	2.17	9	2

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

There are no protein molecules in this entry.

6.3.2 Protein sidechains

There are no protein molecules in this entry.

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	9F0	B	101	-	48,72,72	0.61±0.02	0±0 (0±0%)
2	9F0	B	102	-	48,72,72	0.56±0.01	0±0 (0±0%)
2	9F0	A	102	-	48,72,72	0.56±0.01	0±0 (0±0%)
2	9F0	A	101	-	48,72,72	0.61±0.00	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	9F0	B	101	-	57,108,108	0.65±0.01	0±0 (0±0%)
2	9F0	B	102	-	57,108,108	0.66±0.00	0±0 (0±0%)
2	9F0	A	102	-	57,108,108	0.66±0.00	0±0 (0±0%)
2	9F0	A	101	-	57,108,108	0.64±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9F0	B	101	-	-	0±0,24,102,102	0±0,12,12,12
2	9F0	A	102	-	-	0±0,24,102,102	0±0,12,12,12
2	9F0	B	102	-	-	0±0,24,102,102	0±0,12,12,12
2	9F0	A	101	-	-	0±0,24,102,102	0±0,12,12,12

There are no bond-length outliers.

There are no bond-angle outliers.

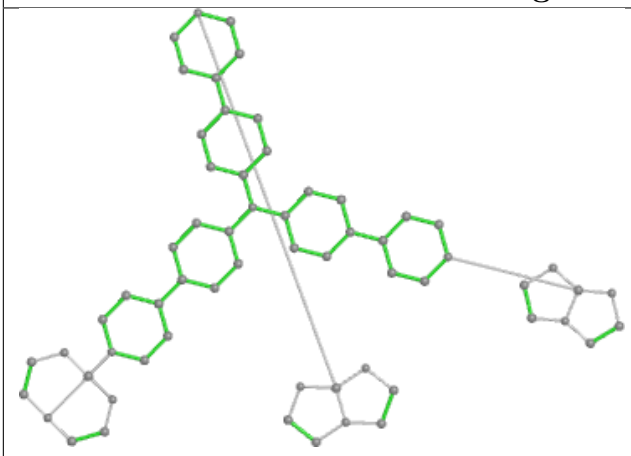
There are no chirality outliers.

There are no torsion outliers.

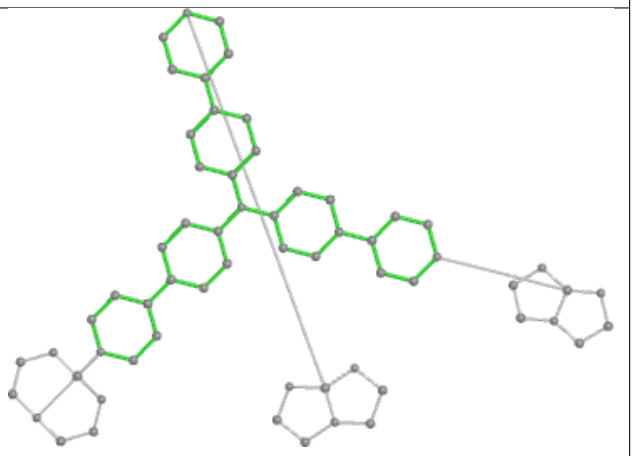
There are no ring outliers.

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

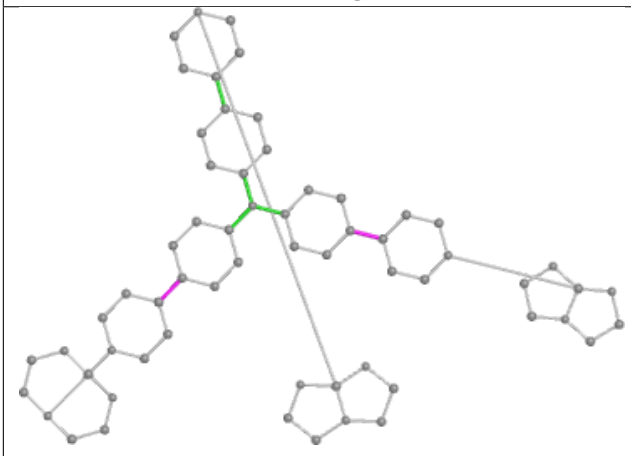
Ligand 9F0 B 101



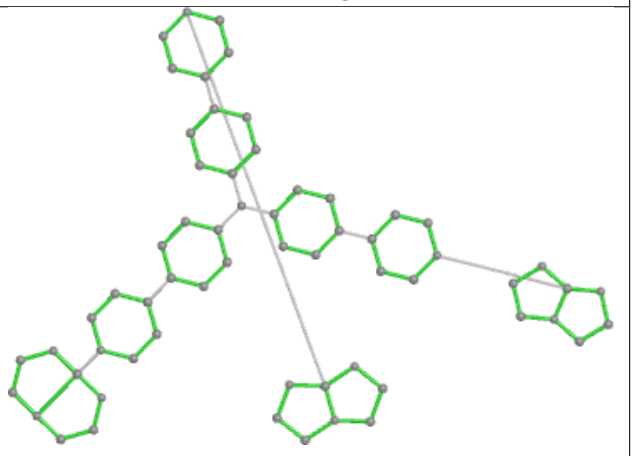
Bond lengths



Bond angles

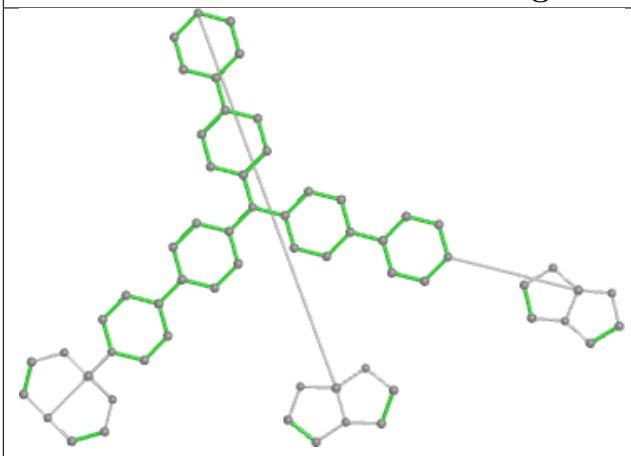


Torsions

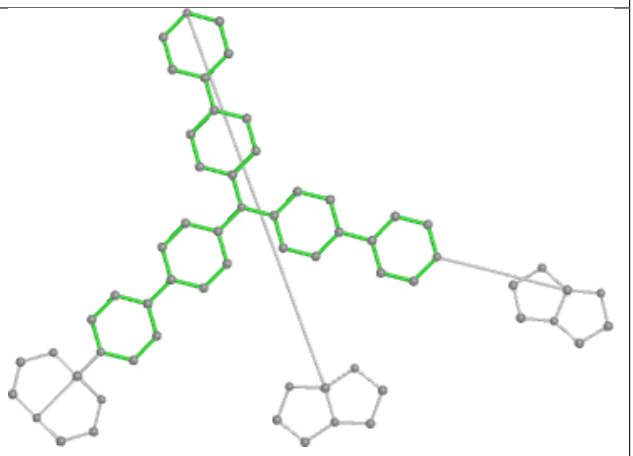


Rings

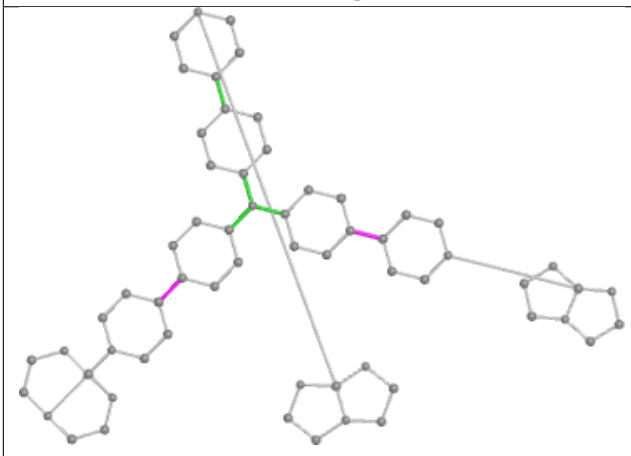
Ligand 9F0 A 102



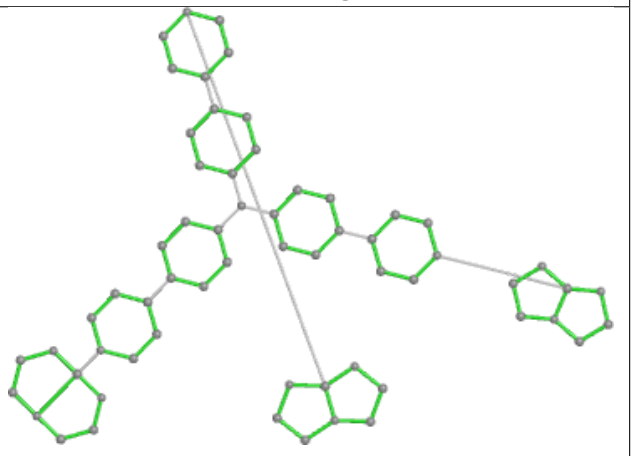
Bond lengths



Bond angles

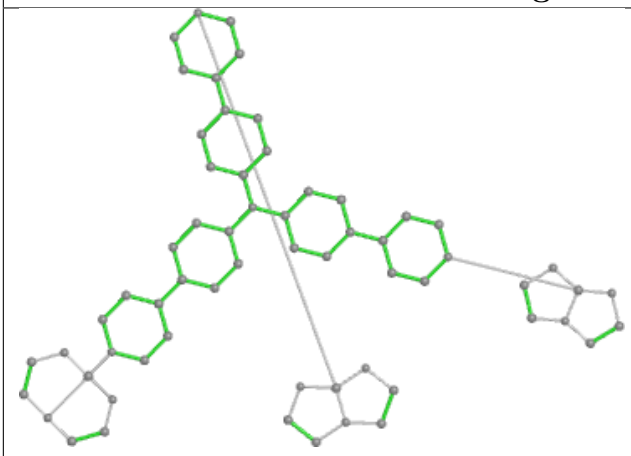


Torsions

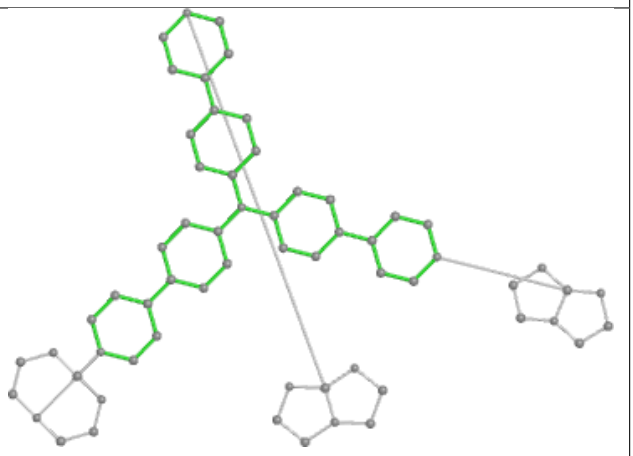


Rings

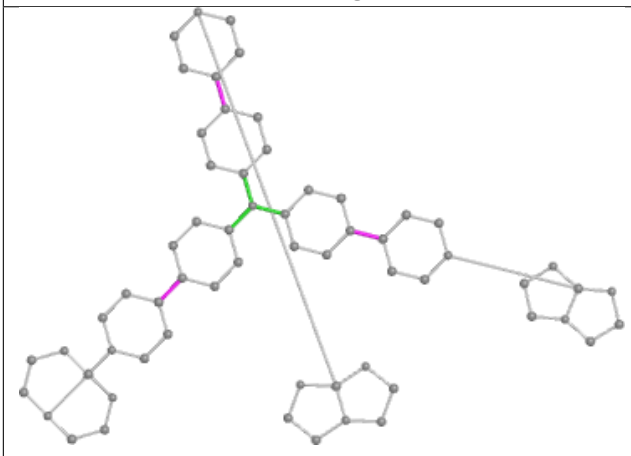
Ligand 9F0 B 102



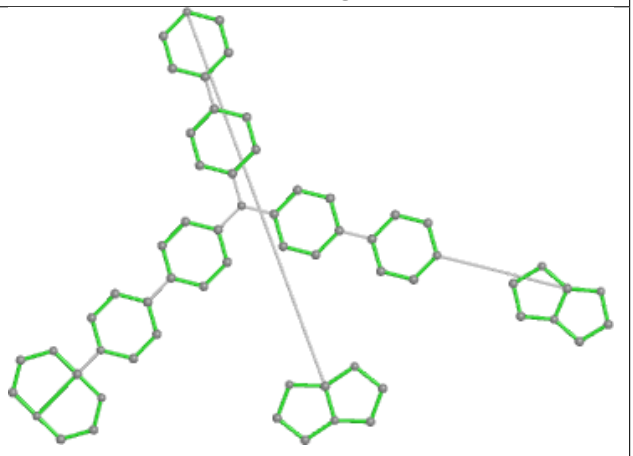
Bond lengths



Bond angles

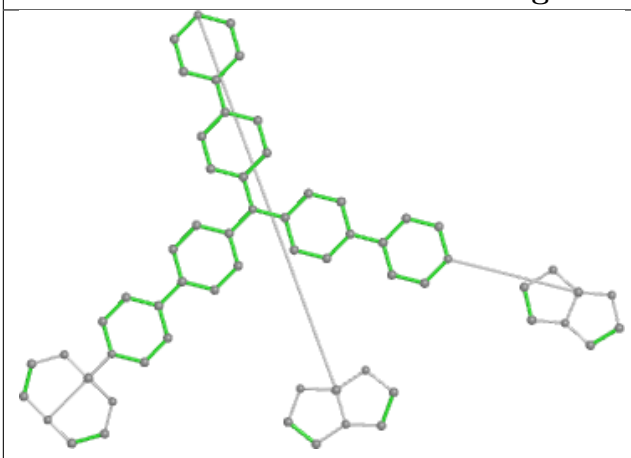


Torsions

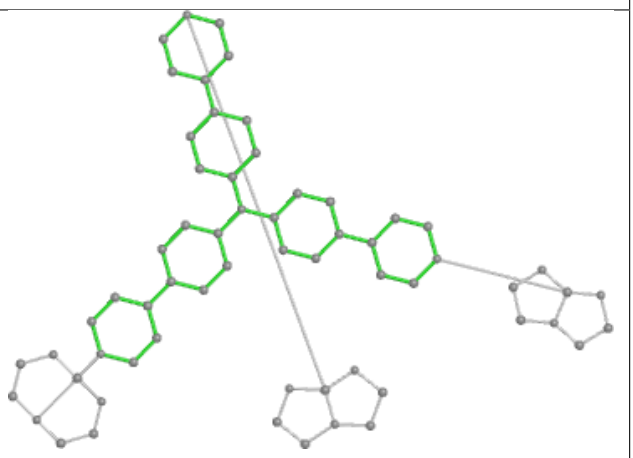


Rings

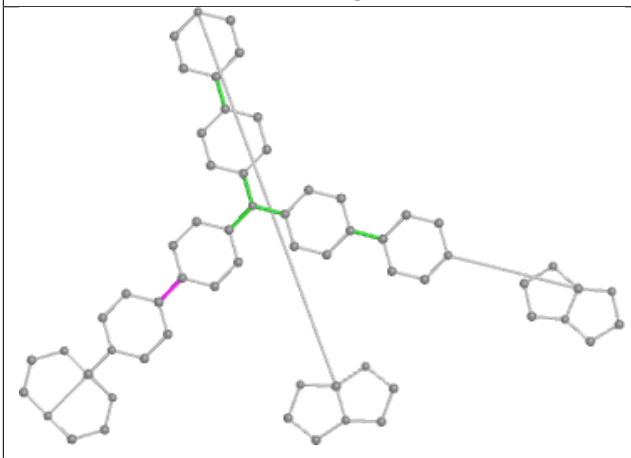
Ligand 9F0 A 101



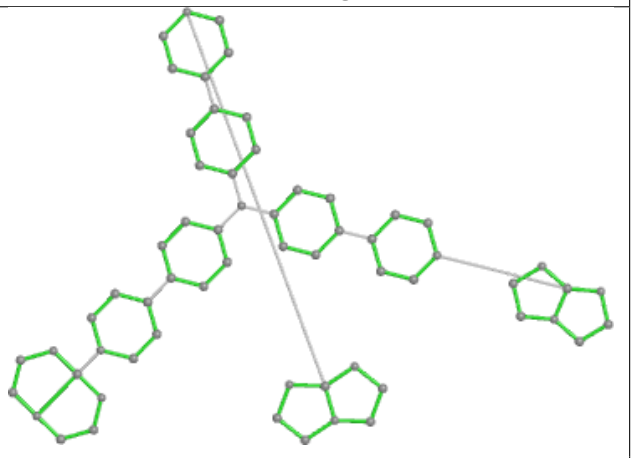
Bond lengths



Bond angles



Torsions



Rings

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 23% for the well-defined parts and 23% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *4-2-chemicalshifts_str.txt*

7.1.1 Bookkeeping

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

Total number of shifts	388
Number of shifts mapped to atoms	388
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 23%, i.e. 244 atoms were assigned a chemical shift out of a possible 1040. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Sugar	182/624 (29%)	182/364 (50%)	0/260 (0%)	0/0 (—%)
Base	62/416 (15%)	62/260 (24%)	0/80 (0%)	0/76 (0%)
Overall	244/1040 (23%)	244/624 (39%)	0/340 (0%)	0/76 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 23%, i.e. 244 atoms were assigned a chemical shift out of a possible 1040. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Sugar	182/624 (29%)	182/364 (50%)	0/260 (0%)	0/0 (—%)
Base	62/416 (15%)	62/260 (24%)	0/80 (0%)	0/76 (0%)
Overall	244/1040 (23%)	244/624 (39%)	0/340 (0%)	0/76 (0%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	760
Intra-residue (|i-j|=0)	289
Sequential (|i-j|=1)	135
Medium range (|i-j|>1 and |i-j|<5)	21
Long range (|i-j|≥5)	315
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	36
Number of unmapped restraints	0
Number of restraints per residue	15.3
Number of long range restraints per residue[1]	6.1

[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)	35.9	0.2
0.2-0.5 (Medium)	64.0	0.5
>0.5 (Large)	24.9	2.92

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.6	8.1
10.0-20.0 (Medium)	0.4	16.9
>20.0 (Large)	None	None

9 Distance violation analysis (i)

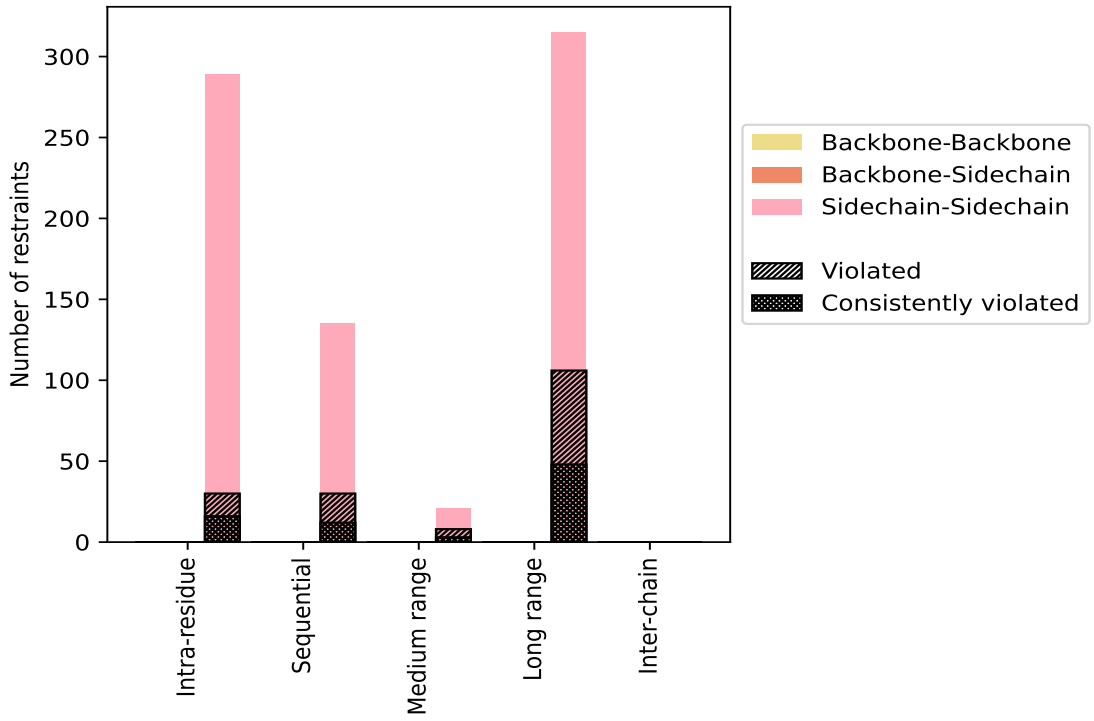
9.1 Summary of distance violations (i)

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 (|i-j|=0)	289	38.0	30	10.4	3.9	16	5.5	2.1
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	289	38.0	30	10.4	3.9	16	5.5	2.1
Sequential (|i-j|=1)	135	17.8	30	22.2	3.9	12	8.9	1.6
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	135	17.8	30	22.2	3.9	12	8.9	1.6
Medium range (|i-j|>1 & |i-j|<5)	21	2.8	8	38.1	1.1	3	14.3	0.4
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	21	2.8	8	38.1	1.1	3	14.3	0.4
Long range (|i-j|≥5)	315	41.4	106	33.7	13.9	48	15.2	6.3
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	315	41.4	106	33.7	13.9	48	15.2	6.3
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	760	100.0	174	22.9	22.9	79	10.4	10.4
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	760	100.0	174	22.9	22.9	79	10.4	10.4

[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

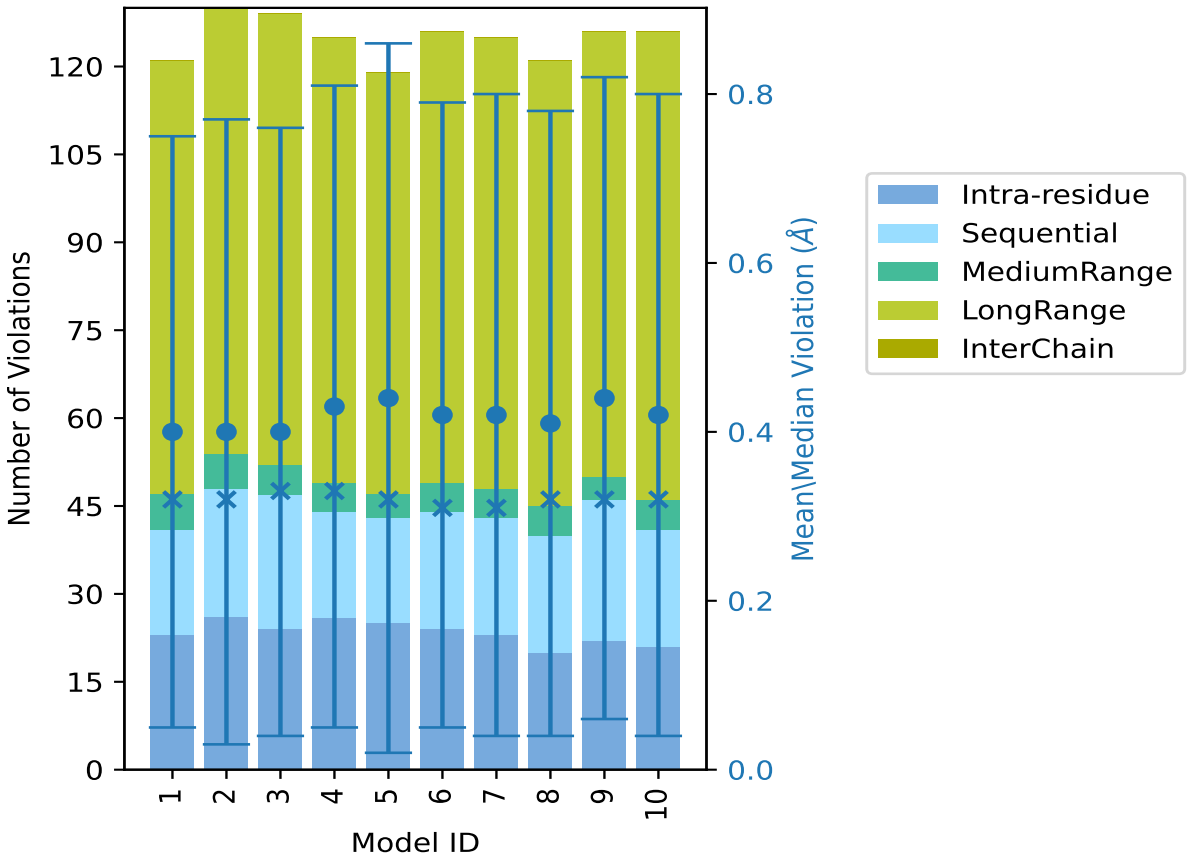
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	23	18	6	74	0	121	0.4	2.37	0.35	0.32
2	26	22	6	76	0	130	0.4	2.76	0.37	0.32
3	24	23	5	77	0	129	0.4	2.53	0.36	0.33
4	26	18	5	76	0	125	0.43	2.79	0.38	0.33
5	25	18	4	72	0	119	0.44	2.92	0.42	0.32
6	24	20	5	77	0	126	0.42	2.41	0.37	0.31
7	23	20	5	77	0	125	0.42	2.37	0.38	0.31
8	20	20	5	76	0	121	0.41	2.38	0.37	0.32
9	22	24	4	76	0	126	0.44	2.4	0.38	0.32
10	21	20	5	80	0	126	0.42	2.38	0.38	0.32

[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, 586(IR:259, SQ:105, MR:13, LR:209, 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	4	2	11	0	18	1	10.0
1	3	0	6	0	10	2	20.0
0	2	0	5	0	7	3	30.0
3	0	0	5	0	8	4	40.0

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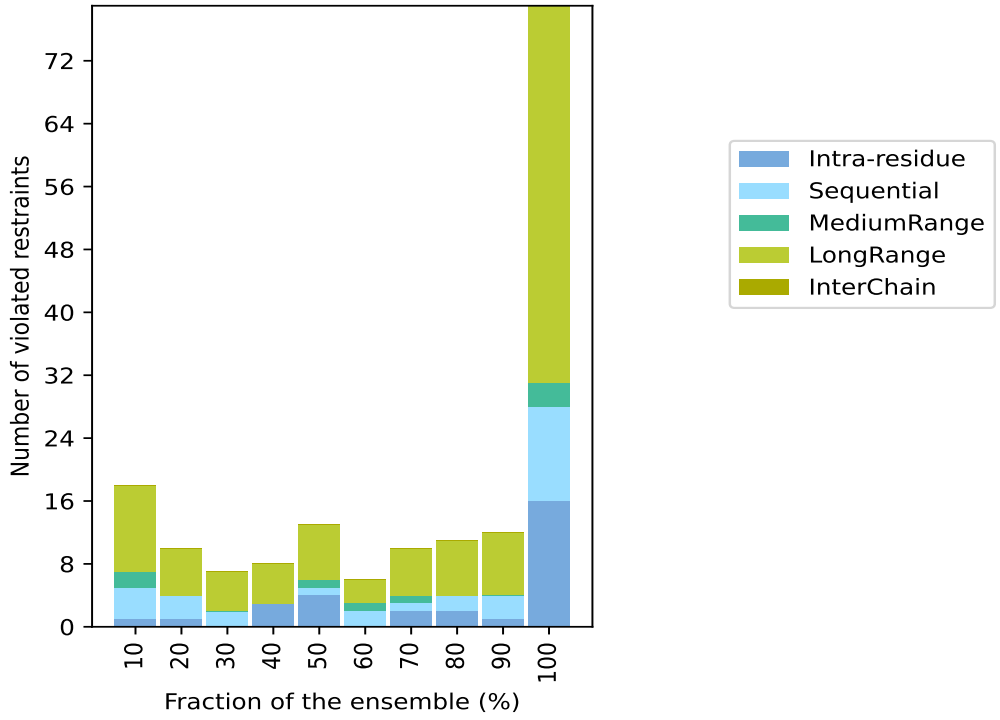
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
4	1	1	7	0	13	5	50.0
0	2	1	3	0	6	6	60.0
2	1	1	6	0	10	7	70.0
2	2	0	7	0	11	8	80.0
1	3	0	8	0	12	9	90.0
16	12	3	48	0	79	10	100.0

[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

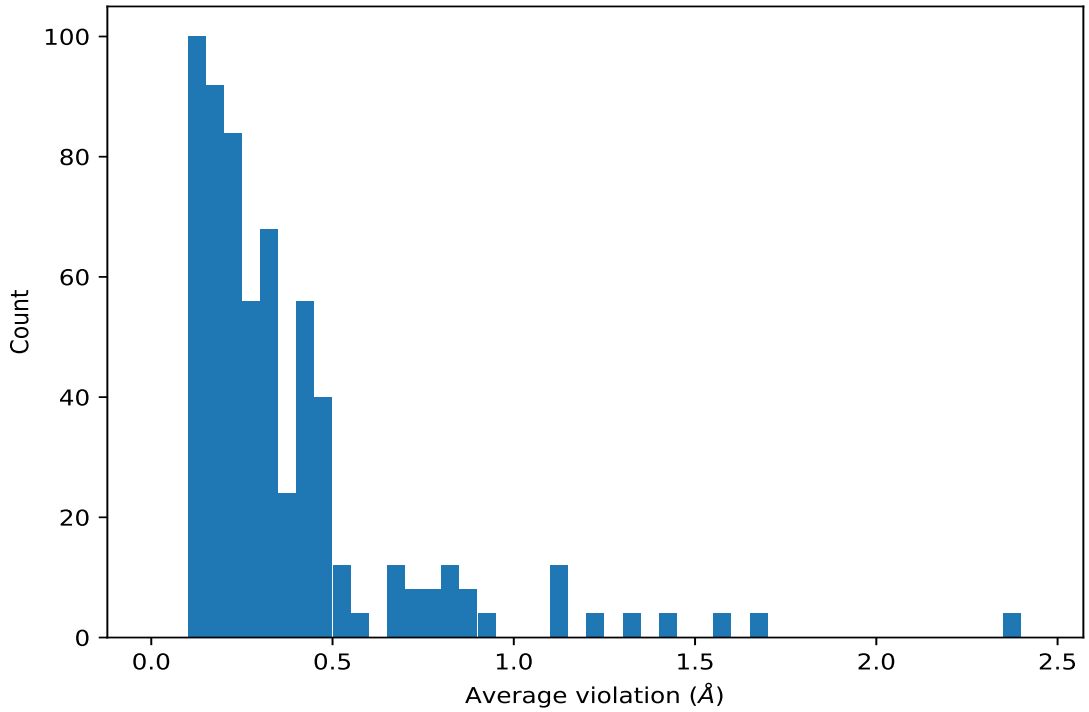
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	10	2.4	0.02	2.4
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	10	2.4	0.02	2.4
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	10	2.4	0.02	2.4
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	10	2.4	0.02	2.4
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	10	1.69	0.94	1.42
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	10	1.69	0.94	1.42
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	10	1.69	0.94	1.42
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	10	1.69	0.94	1.42
(5,59)	1:A:21:DA:H5”	1:A:21:DA:H8	10	1.57	0.02	1.56
(5,59)	1:A:21:DA:H5”	1:B:21:DA:H8	10	1.57	0.02	1.56
(5,59)	1:B:21:DA:H5”	1:A:21:DA:H8	10	1.57	0.02	1.56
(5,59)	1:B:21:DA:H5”	1:B:21:DA:H8	10	1.57	0.02	1.56
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2’	10	1.43	0.51	1.65
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2’	10	1.43	0.51	1.65
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2’	10	1.43	0.51	1.65
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2’	10	1.43	0.51	1.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,250)	1:A:24:DG:H5"	1:A:24:DG:H8	10	1.3	0.02	1.3
(5,250)	1:A:24:DG:H5"	1:B:24:DG:H8	10	1.3	0.02	1.3
(5,250)	1:B:24:DG:H5"	1:A:24:DG:H8	10	1.3	0.02	1.3
(5,250)	1:B:24:DG:H5"	1:B:24:DG:H8	10	1.3	0.02	1.3
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	10	1.11	0.02	1.12
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	10	1.11	0.02	1.12
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	10	1.11	0.02	1.12
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	10	1.11	0.02	1.12
(5,166)	1:A:11:DG:H5"	1:A:11:DG:H8	10	1.1	0.06	1.08
(5,166)	1:A:11:DG:H5"	1:B:11:DG:H8	10	1.1	0.06	1.08
(5,166)	1:B:11:DG:H5"	1:A:11:DG:H8	10	1.1	0.06	1.08
(5,166)	1:B:11:DG:H5"	1:B:11:DG:H8	10	1.1	0.06	1.08
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	10	0.95	0.03	0.95
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	10	0.95	0.03	0.95
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	10	0.95	0.03	0.95
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	10	0.95	0.03	0.95
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2"	10	0.86	0.36	1.06
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2"	10	0.86	0.36	1.06
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2"	10	0.86	0.36	1.06
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2"	10	0.86	0.36	1.06
(5,38)	1:A:19:DT:H3'	1:A:19:DT:H6	10	0.86	0.23	0.86
(5,38)	1:A:19:DT:H3'	1:B:19:DT:H6	10	0.86	0.23	0.86
(5,38)	1:B:19:DT:H3'	1:A:19:DT:H6	10	0.86	0.23	0.86
(5,38)	1:B:19:DT:H3'	1:B:19:DT:H6	10	0.86	0.23	0.86
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	10	0.85	0.02	0.84
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	10	0.85	0.02	0.84
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	10	0.85	0.02	0.84
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	10	0.85	0.02	0.84
(4,49)	1:A:14:DT:H1'	1:A:15:DA:H8	10	0.83	0.26	0.89
(4,49)	1:A:14:DT:H1'	1:B:15:DA:H8	10	0.83	0.26	0.89
(4,49)	1:B:14:DT:H1'	1:A:15:DA:H8	10	0.83	0.26	0.89
(4,49)	1:B:14:DT:H1'	1:B:15:DA:H8	10	0.83	0.26	0.89
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	10	0.79	0.04	0.76
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	10	0.79	0.04	0.76
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	10	0.79	0.04	0.76
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	10	0.79	0.04	0.76
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	10	0.76	0.11	0.78
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	10	0.76	0.11	0.78
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	10	0.76	0.11	0.78
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	10	0.76	0.11	0.78
(5,25)	1:A:8:DT:H3'	1:A:8:DT:H6	10	0.73	0.11	0.76
(5,25)	1:A:8:DT:H3'	1:B:8:DT:H6	10	0.73	0.11	0.76

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,25)	1:B:8:DT:H3'	1:A:8:DT:H6	10	0.73	0.11	0.76
(5,25)	1:B:8:DT:H3'	1:B:8:DT:H6	10	0.73	0.11	0.76
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3'	10	0.71	0.07	0.72
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3'	10	0.71	0.07	0.72
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3'	10	0.71	0.07	0.72
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3'	10	0.71	0.07	0.72
(5,213)	1:A:18:DG:H5"	1:A:18:DG:H8	10	0.7	0.03	0.72
(5,213)	1:A:18:DG:H5"	1:B:18:DG:H8	10	0.7	0.03	0.72
(5,213)	1:B:18:DG:H5"	1:A:18:DG:H8	10	0.7	0.03	0.72
(5,213)	1:B:18:DG:H5"	1:B:18:DG:H8	10	0.7	0.03	0.72
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	10	0.69	0.11	0.71
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	10	0.69	0.11	0.71
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	10	0.69	0.11	0.71
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	10	0.69	0.11	0.71
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5"	10	0.56	0.04	0.56
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5"	10	0.56	0.04	0.56
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5"	10	0.56	0.04	0.56
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5"	10	0.56	0.04	0.56
(4,53)	1:A:14:DT:H4'	1:A:15:DA:H8	10	0.51	0.21	0.44
(4,53)	1:A:14:DT:H4'	1:B:15:DA:H8	10	0.51	0.21	0.44
(4,53)	1:B:14:DT:H4'	1:A:15:DA:H8	10	0.51	0.21	0.44
(4,53)	1:B:14:DT:H4'	1:B:15:DA:H8	10	0.51	0.21	0.44
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	10	0.51	0.01	0.5
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	10	0.51	0.01	0.5
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	10	0.51	0.01	0.5
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	10	0.51	0.01	0.5
(4,67)	1:A:25:DA:H2'	1:A:26:DA:H8	10	0.5	0.02	0.5
(4,67)	1:A:25:DA:H2'	1:B:26:DA:H8	10	0.5	0.02	0.5
(4,67)	1:B:25:DA:H2'	1:A:26:DA:H8	10	0.5	0.02	0.5
(4,67)	1:B:25:DA:H2'	1:B:26:DA:H8	10	0.5	0.02	0.5
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	10	0.49	0.02	0.48
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	10	0.49	0.02	0.48
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	10	0.49	0.02	0.48
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	10	0.49	0.02	0.48
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	10	0.48	0.04	0.48
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	10	0.48	0.04	0.48
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	10	0.48	0.04	0.48
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	10	0.48	0.04	0.48
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	10	0.48	0.25	0.4
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	10	0.48	0.25	0.4
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	10	0.48	0.25	0.4
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	10	0.48	0.25	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	10	0.47	0.04	0.49
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	10	0.47	0.04	0.49
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	10	0.47	0.04	0.49
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	10	0.47	0.04	0.49
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1'	10	0.46	0.04	0.48
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1'	10	0.46	0.04	0.48
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1'	10	0.46	0.04	0.48
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1'	10	0.46	0.04	0.48
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	10	0.46	0.02	0.46
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	10	0.46	0.02	0.46
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	10	0.46	0.02	0.46
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	10	0.46	0.02	0.46
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	10	0.46	0.02	0.46
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	10	0.46	0.02	0.46
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	10	0.46	0.02	0.46
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	10	0.46	0.02	0.46
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	10	0.45	0.25	0.36
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	10	0.45	0.25	0.36
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	10	0.45	0.25	0.36
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	10	0.45	0.25	0.36
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	10	0.45	0.02	0.45
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	10	0.45	0.02	0.45
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	10	0.45	0.02	0.45
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	10	0.45	0.02	0.45
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	10	0.44	0.11	0.46
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	10	0.44	0.11	0.46
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	10	0.44	0.11	0.46
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	10	0.44	0.11	0.46
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	10	0.43	0.04	0.44
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	10	0.43	0.04	0.44
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	10	0.43	0.04	0.44
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	10	0.43	0.04	0.44
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	10	0.42	0.09	0.43
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	10	0.42	0.09	0.43
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	10	0.42	0.09	0.43
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	10	0.42	0.09	0.43
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	10	0.42	0.02	0.42
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	10	0.42	0.02	0.42
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	10	0.42	0.02	0.42
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	10	0.42	0.02	0.42
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	10	0.42	0.06	0.4
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	10	0.42	0.06	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	10	0.42	0.06	0.4
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	10	0.42	0.06	0.4
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	10	0.41	0.05	0.41
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	10	0.41	0.05	0.41
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	10	0.41	0.05	0.41
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	10	0.41	0.05	0.41
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	10	0.4	0.04	0.42
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	10	0.4	0.04	0.42
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	10	0.4	0.04	0.42
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	10	0.4	0.04	0.42
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1'	10	0.4	0.02	0.4
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1'	10	0.4	0.02	0.4
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1'	10	0.4	0.02	0.4
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1'	10	0.4	0.02	0.4
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2"	10	0.4	0.05	0.42
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2"	10	0.4	0.05	0.42
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2"	10	0.4	0.05	0.42
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2"	10	0.4	0.05	0.42
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	10	0.37	0.01	0.37
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	10	0.37	0.01	0.37
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	10	0.37	0.01	0.37
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	10	0.37	0.01	0.37
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	10	0.37	0.05	0.37
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	10	0.37	0.05	0.37
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	10	0.37	0.05	0.37
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	10	0.37	0.05	0.37
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	10	0.37	0.04	0.36
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	10	0.37	0.04	0.36
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	10	0.37	0.04	0.36
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	10	0.37	0.04	0.36
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	10	0.36	0.03	0.36
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	10	0.36	0.03	0.36
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	10	0.36	0.03	0.36
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	10	0.36	0.03	0.36
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	10	0.36	0.03	0.36
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	10	0.36	0.03	0.36
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	10	0.36	0.03	0.36
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	10	0.36	0.03	0.36
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	10	0.35	0.01	0.35
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	10	0.35	0.01	0.35
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	10	0.35	0.01	0.35
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	10	0.35	0.01	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	10	0.35	0.01	0.35
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	10	0.35	0.01	0.35
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	10	0.35	0.01	0.35
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	10	0.35	0.01	0.35
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	10	0.34	0.08	0.35
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	10	0.34	0.08	0.35
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	10	0.34	0.08	0.35
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	10	0.34	0.08	0.35
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	10	0.33	0.05	0.34
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	10	0.33	0.05	0.34
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	10	0.33	0.05	0.34
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	10	0.33	0.05	0.34
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	10	0.33	0.04	0.35
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	10	0.33	0.04	0.35
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	10	0.33	0.04	0.35
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	10	0.33	0.04	0.35
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	10	0.32	0.04	0.33
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	10	0.32	0.04	0.33
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	10	0.32	0.04	0.33
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	10	0.32	0.04	0.33
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	10	0.32	0.01	0.32
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	10	0.32	0.01	0.32
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	10	0.32	0.01	0.32
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	10	0.32	0.01	0.32
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	10	0.32	0.08	0.32
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	10	0.32	0.08	0.32
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	10	0.32	0.08	0.32
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	10	0.32	0.08	0.32
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	10	0.32	0.07	0.34
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	10	0.32	0.07	0.34
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	10	0.32	0.07	0.34
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	10	0.32	0.07	0.34
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	10	0.31	0.01	0.31
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	10	0.31	0.01	0.31
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	10	0.31	0.01	0.31
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	10	0.31	0.01	0.31
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	10	0.31	0.02	0.31
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	10	0.31	0.02	0.31
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	10	0.31	0.02	0.31
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	10	0.31	0.02	0.31
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	10	0.29	0.03	0.28
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	10	0.29	0.03	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	10	0.29	0.03	0.28
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	10	0.29	0.03	0.28
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	10	0.27	0.05	0.25
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	10	0.27	0.05	0.25
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	10	0.27	0.05	0.25
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	10	0.27	0.05	0.25
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	10	0.26	0.03	0.27
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	10	0.26	0.03	0.27
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	10	0.26	0.03	0.27
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	10	0.26	0.03	0.27
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	10	0.26	0.02	0.26
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	10	0.26	0.02	0.26
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	10	0.26	0.02	0.26
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	10	0.26	0.02	0.26
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	10	0.25	0.04	0.24
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	10	0.25	0.04	0.24
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	10	0.25	0.04	0.24
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	10	0.25	0.04	0.24
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	10	0.25	0.03	0.26
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	10	0.25	0.03	0.26
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	10	0.25	0.03	0.26
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	10	0.25	0.03	0.26
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	10	0.25	0.04	0.25
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	10	0.25	0.04	0.25
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	10	0.25	0.04	0.25
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	10	0.25	0.04	0.25
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	10	0.24	0.01	0.24
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	10	0.24	0.01	0.24
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	10	0.24	0.01	0.24
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	10	0.24	0.01	0.24
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	10	0.24	0.03	0.24
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	10	0.24	0.03	0.24
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	10	0.24	0.03	0.24
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	10	0.24	0.03	0.24
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	10	0.23	0.08	0.2
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	10	0.23	0.08	0.2
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	10	0.23	0.08	0.2
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	10	0.23	0.08	0.2
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	10	0.22	0.05	0.22
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	10	0.22	0.05	0.22
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	10	0.22	0.05	0.22
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	10	0.22	0.05	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	10	0.21	0.05	0.21
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	10	0.21	0.05	0.21
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	10	0.21	0.05	0.21
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	10	0.21	0.05	0.21
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	10	0.2	0.01	0.2
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	10	0.2	0.01	0.2
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	10	0.2	0.01	0.2
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	10	0.2	0.01	0.2
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	10	0.2	0.02	0.2
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	10	0.2	0.02	0.2
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	10	0.2	0.02	0.2
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	10	0.2	0.02	0.2
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	10	0.18	0.03	0.18
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	10	0.18	0.03	0.18
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	10	0.18	0.03	0.18
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	10	0.18	0.03	0.18
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	10	0.17	0.01	0.17
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	10	0.17	0.01	0.17
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	10	0.17	0.01	0.17
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	10	0.17	0.01	0.17
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	10	0.17	0.02	0.16
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	10	0.17	0.02	0.16
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	10	0.17	0.02	0.16
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	10	0.17	0.02	0.16
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	10	0.16	0.02	0.16
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	10	0.16	0.02	0.16
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	10	0.16	0.02	0.16
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	10	0.16	0.02	0.16
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	10	0.16	0.03	0.16
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	10	0.16	0.03	0.16
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	10	0.16	0.03	0.16
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	10	0.16	0.03	0.16
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	10	0.16	0.02	0.16
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	10	0.16	0.02	0.16
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	10	0.16	0.02	0.16
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	10	0.16	0.02	0.16
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	10	0.14	0.02	0.14
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	10	0.14	0.02	0.14
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	10	0.14	0.02	0.14
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	10	0.14	0.02	0.14
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	10	0.13	0.01	0.13
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	10	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	10	0.13	0.01	0.13
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	10	0.13	0.01	0.13
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	10	0.13	0.01	0.13
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	10	0.13	0.01	0.13
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	10	0.13	0.01	0.13
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	10	0.13	0.01	0.13
(2,114)	2:A:101:9F0:H26	1:A:8:DT:H2"	9	1.21	0.44	1.53
(2,114)	2:A:101:9F0:H26	1:B:8:DT:H2"	9	1.21	0.44	1.53
(2,114)	2:B:101:9F0:H26	1:A:8:DT:H2"	9	1.21	0.44	1.53
(2,114)	2:B:101:9F0:H26	1:B:8:DT:H2"	9	1.21	0.44	1.53
(4,18)	1:A:8:DT:H2"	1:A:9:DA:H8	9	0.68	0.24	0.73
(4,18)	1:A:8:DT:H2"	1:B:9:DA:H8	9	0.68	0.24	0.73
(4,18)	1:B:8:DT:H2"	1:A:9:DA:H8	9	0.68	0.24	0.73
(4,18)	1:B:8:DT:H2"	1:B:9:DA:H8	9	0.68	0.24	0.73
(2,1)	2:A:101:9F0:H14	1:A:3:DA:H2	9	0.39	0.06	0.41
(2,1)	2:A:101:9F0:H14	1:B:3:DA:H2	9	0.39	0.06	0.41
(2,1)	2:B:101:9F0:H14	1:A:3:DA:H2	9	0.39	0.06	0.41
(2,1)	2:B:101:9F0:H14	1:B:3:DA:H2	9	0.39	0.06	0.41
(4,34)	1:A:21:DA:H2	1:A:10:DG:H1	9	0.35	0.08	0.34
(4,34)	1:A:21:DA:H2	1:B:10:DG:H1	9	0.35	0.08	0.34
(4,34)	1:B:21:DA:H2	1:A:10:DG:H1	9	0.35	0.08	0.34
(4,34)	1:B:21:DA:H2	1:B:10:DG:H1	9	0.35	0.08	0.34
(2,4)	2:A:101:9F0:H14	1:A:9:DA:H2'	9	0.34	0.05	0.36
(2,4)	2:A:101:9F0:H14	1:B:9:DA:H2'	9	0.34	0.05	0.36
(2,4)	2:B:101:9F0:H14	1:A:9:DA:H2'	9	0.34	0.05	0.36
(2,4)	2:B:101:9F0:H14	1:B:9:DA:H2'	9	0.34	0.05	0.36
(3,1)	2:A:102:9F0:H33	1:A:15:DA:N6	9	0.32	0.09	0.35
(3,1)	2:A:102:9F0:H33	1:B:15:DA:N6	9	0.32	0.09	0.35
(3,1)	2:B:102:9F0:H33	1:A:15:DA:N6	9	0.32	0.09	0.35
(3,1)	2:B:102:9F0:H33	1:B:15:DA:N6	9	0.32	0.09	0.35
(4,24)	1:A:20:DT:H6	1:A:21:DA:H8	9	0.32	0.13	0.27
(4,24)	1:A:20:DT:H6	1:B:21:DA:H8	9	0.32	0.13	0.27
(4,24)	1:B:20:DT:H6	1:A:21:DA:H8	9	0.32	0.13	0.27
(4,24)	1:B:20:DT:H6	1:B:21:DA:H8	9	0.32	0.13	0.27
(5,20)	1:A:3:DA:H4'	1:A:3:DA:H1'	9	0.26	0.12	0.35
(5,20)	1:A:3:DA:H4'	1:B:3:DA:H1'	9	0.26	0.12	0.35
(5,20)	1:B:3:DA:H4'	1:A:3:DA:H1'	9	0.26	0.12	0.35
(5,20)	1:B:3:DA:H4'	1:B:3:DA:H1'	9	0.26	0.12	0.35
(4,169)	1:A:17:DG:H2'	1:A:18:DG:H1'	9	0.23	0.05	0.24
(4,169)	1:A:17:DG:H2'	1:B:18:DG:H1'	9	0.23	0.05	0.24
(4,169)	1:B:17:DG:H2'	1:A:18:DG:H1'	9	0.23	0.05	0.24
(4,169)	1:B:17:DG:H2'	1:B:18:DG:H1'	9	0.23	0.05	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,13)	1:A:3:DA:H2	1:A:9:DA:H2	9	0.22	0.06	0.19
(4,13)	1:A:3:DA:H2	1:B:9:DA:H2	9	0.22	0.06	0.19
(4,13)	1:B:3:DA:H2	1:A:9:DA:H2	9	0.22	0.06	0.19
(4,13)	1:B:3:DA:H2	1:B:9:DA:H2	9	0.22	0.06	0.19
(2,79)	2:A:101:9F0:H9	1:A:9:DA:H2	9	0.21	0.03	0.22
(2,79)	2:A:101:9F0:H9	1:B:9:DA:H2	9	0.21	0.03	0.22
(2,79)	2:B:101:9F0:H9	1:A:9:DA:H2	9	0.21	0.03	0.22
(2,79)	2:B:101:9F0:H9	1:B:9:DA:H2	9	0.21	0.03	0.22
(2,164)	2:A:102:9F0:H19	1:A:6:DG:H1	9	0.16	0.02	0.17
(2,164)	2:A:102:9F0:H19	1:B:6:DG:H1	9	0.16	0.02	0.17
(2,164)	2:B:102:9F0:H19	1:A:6:DG:H1	9	0.16	0.02	0.17
(2,164)	2:B:102:9F0:H19	1:B:6:DG:H1	9	0.16	0.02	0.17
(2,118)	2:A:101:9F0:H45	1:A:8:DT:H2”	8	1.12	0.46	1.42
(2,118)	2:A:101:9F0:H45	1:B:8:DT:H2”	8	1.12	0.46	1.42
(2,118)	2:B:101:9F0:H45	1:A:8:DT:H2”	8	1.12	0.46	1.42
(2,118)	2:B:101:9F0:H45	1:B:8:DT:H2”	8	1.12	0.46	1.42
(4,60)	1:A:15:DA:H2”	1:A:16:DG:H1	8	0.4	0.13	0.38
(4,60)	1:A:15:DA:H2”	1:B:16:DG:H1	8	0.4	0.13	0.38
(4,60)	1:B:15:DA:H2”	1:A:16:DG:H1	8	0.4	0.13	0.38
(4,60)	1:B:15:DA:H2”	1:B:16:DG:H1	8	0.4	0.13	0.38
(2,96)	2:A:101:9F0:H6	1:A:9:DA:H3’	8	0.29	0.08	0.28
(2,96)	2:A:101:9F0:H6	1:B:9:DA:H3’	8	0.29	0.08	0.28
(2,96)	2:B:101:9F0:H6	1:A:9:DA:H3’	8	0.29	0.08	0.28
(2,96)	2:B:101:9F0:H6	1:B:9:DA:H3’	8	0.29	0.08	0.28
(2,58)	2:A:101:9F0:H37	1:A:3:DA:H2’	8	0.28	0.04	0.29
(2,58)	2:A:101:9F0:H37	1:B:3:DA:H2’	8	0.28	0.04	0.29
(2,58)	2:B:101:9F0:H37	1:A:3:DA:H2’	8	0.28	0.04	0.29
(2,58)	2:B:101:9F0:H37	1:B:3:DA:H2’	8	0.28	0.04	0.29
(2,184)	2:A:102:9F0:H37	1:A:6:DG:H2’	8	0.24	0.07	0.24
(2,184)	2:A:102:9F0:H37	1:B:6:DG:H2’	8	0.24	0.07	0.24
(2,184)	2:B:102:9F0:H37	1:A:6:DG:H2’	8	0.24	0.07	0.24
(2,184)	2:B:102:9F0:H37	1:B:6:DG:H2’	8	0.24	0.07	0.24
(5,83)	1:A:15:DA:H3’	1:A:15:DA:H8	8	0.24	0.1	0.22
(5,83)	1:A:15:DA:H3’	1:B:15:DA:H8	8	0.24	0.1	0.22
(5,83)	1:B:15:DA:H3’	1:A:15:DA:H8	8	0.24	0.1	0.22
(5,83)	1:B:15:DA:H3’	1:B:15:DA:H8	8	0.24	0.1	0.22
(5,12)	1:A:2:DA:H5”	1:A:2:DA:H8	8	0.2	0.05	0.2
(5,12)	1:A:2:DA:H5”	1:B:2:DA:H8	8	0.2	0.05	0.2
(5,12)	1:B:2:DA:H5”	1:A:2:DA:H8	8	0.2	0.05	0.2
(5,12)	1:B:2:DA:H5”	1:B:2:DA:H8	8	0.2	0.05	0.2
(4,170)	1:A:17:DG:H2”	1:A:18:DG:H1’	8	0.18	0.07	0.16
(4,170)	1:A:17:DG:H2”	1:B:18:DG:H1’	8	0.18	0.07	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,170)	1:B:17:DG:H2"	1:A:18:DG:H1'	8	0.18	0.07	0.16
(4,170)	1:B:17:DG:H2"	1:B:18:DG:H1'	8	0.18	0.07	0.16
(2,12)	2:A:101:9F0:H13	1:A:9:DA:H2"	8	0.16	0.05	0.14
(2,12)	2:A:101:9F0:H13	1:B:9:DA:H2"	8	0.16	0.05	0.14
(2,12)	2:B:101:9F0:H13	1:A:9:DA:H2"	8	0.16	0.05	0.14
(2,12)	2:B:101:9F0:H13	1:B:9:DA:H2"	8	0.16	0.05	0.14
(1,6)	1:A:14:DT:H3	1:A:25:DA:N7	8	0.13	0.01	0.12
(1,6)	1:A:14:DT:H3	1:B:25:DA:N7	8	0.13	0.01	0.12
(1,6)	1:B:14:DT:H3	1:A:25:DA:N7	8	0.13	0.01	0.12
(1,6)	1:B:14:DT:H3	1:B:25:DA:N7	8	0.13	0.01	0.12
(1,34)	1:A:23:DG:N7	1:A:17:DG:N2	8	0.12	0.01	0.12
(1,34)	1:A:23:DG:N7	1:B:17:DG:N2	8	0.12	0.01	0.12
(1,34)	1:B:23:DG:N7	1:A:17:DG:N2	8	0.12	0.01	0.12
(1,34)	1:B:23:DG:N7	1:B:17:DG:N2	8	0.12	0.01	0.12
(4,64)	1:A:15:DA:H4'	1:A:16:DG:H1'	7	0.44	0.24	0.53
(4,64)	1:A:15:DA:H4'	1:B:16:DG:H1'	7	0.44	0.24	0.53
(4,64)	1:B:15:DA:H4'	1:A:16:DG:H1'	7	0.44	0.24	0.53
(4,64)	1:B:15:DA:H4'	1:B:16:DG:H1'	7	0.44	0.24	0.53
(6,39)	2:A:102:9F0:H41	2:A:102:9F0:H34	7	0.27	0.07	0.25
(6,39)	2:A:102:9F0:H41	2:B:102:9F0:H34	7	0.27	0.07	0.25
(6,39)	2:B:102:9F0:H41	2:A:102:9F0:H34	7	0.27	0.07	0.25
(6,39)	2:B:102:9F0:H41	2:B:102:9F0:H34	7	0.27	0.07	0.25
(2,47)	2:A:101:9F0:H19	1:A:21:DA:H2	7	0.27	0.08	0.29
(2,47)	2:A:101:9F0:H19	1:B:21:DA:H2	7	0.27	0.08	0.29
(2,47)	2:B:101:9F0:H19	1:A:21:DA:H2	7	0.27	0.08	0.29
(2,47)	2:B:101:9F0:H19	1:B:21:DA:H2	7	0.27	0.08	0.29
(4,120)	1:A:4:DG:H1	1:A:22:DG:H8	7	0.21	0.08	0.17
(4,120)	1:A:4:DG:H1	1:B:22:DG:H8	7	0.21	0.08	0.17
(4,120)	1:B:4:DG:H1	1:A:22:DG:H8	7	0.21	0.08	0.17
(4,120)	1:B:4:DG:H1	1:B:22:DG:H8	7	0.21	0.08	0.17
(1,29)	1:A:5:DG:N7	1:A:23:DG:H22	7	0.17	0.04	0.19
(1,29)	1:A:5:DG:N7	1:B:23:DG:H22	7	0.17	0.04	0.19
(1,29)	1:B:5:DG:N7	1:A:23:DG:H22	7	0.17	0.04	0.19
(1,29)	1:B:5:DG:N7	1:B:23:DG:H22	7	0.17	0.04	0.19
(2,159)	2:A:102:9F0:H48	1:A:14:DT:H6	7	0.17	0.03	0.17
(2,159)	2:A:102:9F0:H48	1:B:14:DT:H6	7	0.17	0.03	0.17
(2,159)	2:B:102:9F0:H48	1:A:14:DT:H6	7	0.17	0.03	0.17
(2,159)	2:B:102:9F0:H48	1:B:14:DT:H6	7	0.17	0.03	0.17
(1,11)	1:A:4:DG:O6	1:A:10:DG:H1	7	0.15	0.02	0.15
(1,11)	1:A:4:DG:O6	1:B:10:DG:H1	7	0.15	0.02	0.15
(1,11)	1:B:4:DG:O6	1:A:10:DG:H1	7	0.15	0.02	0.15
(1,11)	1:B:4:DG:O6	1:B:10:DG:H1	7	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,58)	1:A:21:DA:H5'	1:A:21:DA:H8	7	0.15	0.04	0.12
(5,58)	1:A:21:DA:H5'	1:B:21:DA:H8	7	0.15	0.04	0.12
(5,58)	1:B:21:DA:H5'	1:A:21:DA:H8	7	0.15	0.04	0.12
(5,58)	1:B:21:DA:H5'	1:B:21:DA:H8	7	0.15	0.04	0.12
(1,54)	1:A:16:DG:N7	1:A:12:DG:N2	7	0.14	0.02	0.15
(1,54)	1:A:16:DG:N7	1:B:12:DG:N2	7	0.14	0.02	0.15
(1,54)	1:B:16:DG:N7	1:A:12:DG:N2	7	0.14	0.02	0.15
(1,54)	1:B:16:DG:N7	1:B:12:DG:N2	7	0.14	0.02	0.15
(1,46)	1:A:6:DG:N7	1:A:24:DG:N2	7	0.12	0.01	0.11
(1,46)	1:A:6:DG:N7	1:B:24:DG:N2	7	0.12	0.01	0.11
(1,46)	1:B:6:DG:N7	1:A:24:DG:N2	7	0.12	0.01	0.11
(1,46)	1:B:6:DG:N7	1:B:24:DG:N2	7	0.12	0.01	0.11
(2,112)	2:A:101:9F0:H26	1:A:8:DT:H1'	6	0.42	0.09	0.46
(2,112)	2:A:101:9F0:H26	1:B:8:DT:H1'	6	0.42	0.09	0.46
(2,112)	2:B:101:9F0:H26	1:A:8:DT:H1'	6	0.42	0.09	0.46
(2,112)	2:B:101:9F0:H26	1:B:8:DT:H1'	6	0.42	0.09	0.46
(4,61)	1:A:15:DA:H2"	1:A:16:DG:H8	6	0.42	0.21	0.36
(4,61)	1:A:15:DA:H2"	1:B:16:DG:H8	6	0.42	0.21	0.36
(4,61)	1:B:15:DA:H2"	1:A:16:DG:H8	6	0.42	0.21	0.36
(4,61)	1:B:15:DA:H2"	1:B:16:DG:H8	6	0.42	0.21	0.36
(4,97)	1:A:26:DA:H8	1:A:14:DT:H3'	6	0.24	0.07	0.23
(4,97)	1:A:26:DA:H8	1:B:14:DT:H3'	6	0.24	0.07	0.23
(4,97)	1:B:26:DA:H8	1:A:14:DT:H3'	6	0.24	0.07	0.23
(4,97)	1:B:26:DA:H8	1:B:14:DT:H3'	6	0.24	0.07	0.23
(2,55)	2:A:101:9F0:H16	1:A:4:DG:H8	6	0.17	0.04	0.17
(2,55)	2:A:101:9F0:H16	1:B:4:DG:H8	6	0.17	0.04	0.17
(2,55)	2:B:101:9F0:H16	1:A:4:DG:H8	6	0.17	0.04	0.17
(2,55)	2:B:101:9F0:H16	1:B:4:DG:H8	6	0.17	0.04	0.17
(4,16)	1:A:8:DT:H1'	1:A:9:DA:H8	6	0.15	0.03	0.16
(4,16)	1:A:8:DT:H1'	1:B:9:DA:H8	6	0.15	0.03	0.16
(4,16)	1:B:8:DT:H1'	1:A:9:DA:H8	6	0.15	0.03	0.16
(4,16)	1:B:8:DT:H1'	1:B:9:DA:H8	6	0.15	0.03	0.16
(4,42)	1:A:21:DA:H2'	1:A:18:DG:H8	6	0.12	0.02	0.12
(4,42)	1:A:21:DA:H2'	1:B:18:DG:H8	6	0.12	0.02	0.12
(4,42)	1:B:21:DA:H2'	1:A:18:DG:H8	6	0.12	0.02	0.12
(4,42)	1:B:21:DA:H2'	1:B:18:DG:H8	6	0.12	0.02	0.12
(4,2)	1:A:1:DA:H8	1:A:2:DA:H2	5	0.8	0.31	0.71
(4,2)	1:A:1:DA:H8	1:B:2:DA:H2	5	0.8	0.31	0.71
(4,2)	1:B:1:DA:H8	1:A:2:DA:H2	5	0.8	0.31	0.71
(4,2)	1:B:1:DA:H8	1:B:2:DA:H2	5	0.8	0.31	0.71
(2,59)	2:A:101:9F0:H37	1:A:3:DA:H3'	5	0.48	0.02	0.47
(2,59)	2:A:101:9F0:H37	1:B:3:DA:H3'	5	0.48	0.02	0.47

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,59)	2:B:101:9F0:H37	1:A:3:DA:H3'	5	0.48	0.02	0.47
(2,59)	2:B:101:9F0:H37	1:B:3:DA:H3'	5	0.48	0.02	0.47
(4,23)	1:A:19:DT:H3'	1:A:21:DA:H8	5	0.42	0.16	0.41
(4,23)	1:A:19:DT:H3'	1:B:21:DA:H8	5	0.42	0.16	0.41
(4,23)	1:B:19:DT:H3'	1:A:21:DA:H8	5	0.42	0.16	0.41
(4,23)	1:B:19:DT:H3'	1:B:21:DA:H8	5	0.42	0.16	0.41
(2,104)	2:A:101:9F0:H27	1:A:8:DT:H2'	5	0.32	0.04	0.3
(2,104)	2:A:101:9F0:H27	1:B:8:DT:H2'	5	0.32	0.04	0.3
(2,104)	2:B:101:9F0:H27	1:A:8:DT:H2'	5	0.32	0.04	0.3
(2,104)	2:B:101:9F0:H27	1:B:8:DT:H2'	5	0.32	0.04	0.3
(2,13)	2:A:101:9F0:H13	1:A:9:DA:H3'	5	0.31	0.03	0.31
(2,13)	2:A:101:9F0:H13	1:B:9:DA:H3'	5	0.31	0.03	0.31
(2,13)	2:B:101:9F0:H13	1:A:9:DA:H3'	5	0.31	0.03	0.31
(2,13)	2:B:101:9F0:H13	1:B:9:DA:H3'	5	0.31	0.03	0.31
(5,15)	1:A:3:DA:H2'	1:A:3:DA:H8	5	0.26	0.03	0.28
(5,15)	1:A:3:DA:H2'	1:B:3:DA:H8	5	0.26	0.03	0.28
(5,15)	1:B:3:DA:H2'	1:A:3:DA:H8	5	0.26	0.03	0.28
(5,15)	1:B:3:DA:H2'	1:B:3:DA:H8	5	0.26	0.03	0.28
(5,71)	1:A:14:DT:H2'	1:A:14:DT:H6	5	0.23	0.05	0.22
(5,71)	1:A:14:DT:H2'	1:B:14:DT:H6	5	0.23	0.05	0.22
(5,71)	1:B:14:DT:H2'	1:A:14:DT:H6	5	0.23	0.05	0.22
(5,71)	1:B:14:DT:H2'	1:B:14:DT:H6	5	0.23	0.05	0.22
(6,16)	2:A:101:9F0:H42	2:A:101:9F0:H34	5	0.22	0.04	0.2
(6,16)	2:A:101:9F0:H42	2:B:101:9F0:H34	5	0.22	0.04	0.2
(6,16)	2:B:101:9F0:H42	2:A:101:9F0:H34	5	0.22	0.04	0.2
(6,16)	2:B:101:9F0:H42	2:B:101:9F0:H34	5	0.22	0.04	0.2
(2,18)	2:A:101:9F0:H11	1:A:21:DA:H2	5	0.2	0.02	0.21
(2,18)	2:A:101:9F0:H11	1:B:21:DA:H2	5	0.2	0.02	0.21
(2,18)	2:B:101:9F0:H11	1:A:21:DA:H2	5	0.2	0.02	0.21
(2,18)	2:B:101:9F0:H11	1:B:21:DA:H2	5	0.2	0.02	0.21
(6,15)	2:A:101:9F0:H41	2:A:101:9F0:H36	5	0.19	0.04	0.18
(6,15)	2:A:101:9F0:H41	2:B:101:9F0:H36	5	0.19	0.04	0.18
(6,15)	2:B:101:9F0:H41	2:A:101:9F0:H36	5	0.19	0.04	0.18
(6,15)	2:B:101:9F0:H41	2:B:101:9F0:H36	5	0.19	0.04	0.18
(2,35)	2:A:101:9F0:H60	1:A:10:DG:H8	5	0.19	0.07	0.16
(2,35)	2:A:101:9F0:H60	1:B:10:DG:H8	5	0.19	0.07	0.16
(2,35)	2:B:101:9F0:H60	1:A:10:DG:H8	5	0.19	0.07	0.16
(2,35)	2:B:101:9F0:H60	1:B:10:DG:H8	5	0.19	0.07	0.16
(2,211)	2:A:102:9F0:H6	1:A:25:DA:H1'	5	0.14	0.03	0.13
(2,211)	2:A:102:9F0:H6	1:B:25:DA:H1'	5	0.14	0.03	0.13
(2,211)	2:B:102:9F0:H6	1:A:25:DA:H1'	5	0.14	0.03	0.13
(2,211)	2:B:102:9F0:H6	1:B:25:DA:H1'	5	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,40)	1:A:17:DG:O6	1:A:11:DG:N1	5	0.11	0.0	0.11
(1,40)	1:A:17:DG:O6	1:B:11:DG:N1	5	0.11	0.0	0.11
(1,40)	1:B:17:DG:O6	1:A:11:DG:N1	5	0.11	0.0	0.11
(1,40)	1:B:17:DG:O6	1:B:11:DG:N1	5	0.11	0.0	0.11
(2,192)	2:A:102:9F0:H34	1:A:12:DG:H3'	4	0.22	0.07	0.24
(2,192)	2:A:102:9F0:H34	1:B:12:DG:H3'	4	0.22	0.07	0.24
(2,192)	2:B:102:9F0:H34	1:A:12:DG:H3'	4	0.22	0.07	0.24
(2,192)	2:B:102:9F0:H34	1:B:12:DG:H3'	4	0.22	0.07	0.24
(2,142)	2:A:102:9F0:H32	1:A:24:DG:H3'	4	0.18	0.02	0.18
(2,142)	2:A:102:9F0:H32	1:B:24:DG:H3'	4	0.18	0.02	0.18
(2,142)	2:B:102:9F0:H32	1:A:24:DG:H3'	4	0.18	0.02	0.18
(2,142)	2:B:102:9F0:H32	1:B:24:DG:H3'	4	0.18	0.02	0.18
(2,152)	2:A:102:9F0:H31	1:A:24:DG:H3'	4	0.17	0.01	0.18
(2,152)	2:A:102:9F0:H31	1:B:24:DG:H3'	4	0.17	0.01	0.18
(2,152)	2:B:102:9F0:H31	1:A:24:DG:H3'	4	0.17	0.01	0.18
(2,152)	2:B:102:9F0:H31	1:B:24:DG:H3'	4	0.17	0.01	0.18
(2,129)	2:A:102:9F0:H10	1:A:25:DA:H2	4	0.16	0.03	0.16
(2,129)	2:A:102:9F0:H10	1:B:25:DA:H2	4	0.16	0.03	0.16
(2,129)	2:B:102:9F0:H10	1:A:25:DA:H2	4	0.16	0.03	0.16
(2,129)	2:B:102:9F0:H10	1:B:25:DA:H2	4	0.16	0.03	0.16
(2,117)	2:A:101:9F0:H45	1:A:8:DT:H2'	4	0.16	0.02	0.16
(2,117)	2:A:101:9F0:H45	1:B:8:DT:H2'	4	0.16	0.02	0.16
(2,117)	2:B:101:9F0:H45	1:A:8:DT:H2'	4	0.16	0.02	0.16
(2,117)	2:B:101:9F0:H45	1:B:8:DT:H2'	4	0.16	0.02	0.16
(5,131)	1:A:6:DG:H2'	1:A:6:DG:H8	4	0.15	0.02	0.15
(5,131)	1:A:6:DG:H2'	1:B:6:DG:H8	4	0.15	0.02	0.15
(5,131)	1:B:6:DG:H2'	1:A:6:DG:H8	4	0.15	0.02	0.15
(5,131)	1:B:6:DG:H2'	1:B:6:DG:H8	4	0.15	0.02	0.15
(5,142)	1:A:6:DG:H5'	1:A:6:DG:H8	4	0.13	0.02	0.13
(5,142)	1:A:6:DG:H5'	1:B:6:DG:H8	4	0.13	0.02	0.13
(5,142)	1:B:6:DG:H5'	1:A:6:DG:H8	4	0.13	0.02	0.13
(5,142)	1:B:6:DG:H5'	1:B:6:DG:H8	4	0.13	0.02	0.13
(5,37)	1:A:19:DT:H2"	1:A:19:DT:H6	4	0.13	0.03	0.12
(5,37)	1:A:19:DT:H2"	1:B:19:DT:H6	4	0.13	0.03	0.12
(5,37)	1:B:19:DT:H2"	1:A:19:DT:H6	4	0.13	0.03	0.12
(5,37)	1:B:19:DT:H2"	1:B:19:DT:H6	4	0.13	0.03	0.12
(2,3)	2:A:101:9F0:H14	1:A:9:DA:H1'	3	0.25	0.01	0.26
(2,3)	2:A:101:9F0:H14	1:B:9:DA:H1'	3	0.25	0.01	0.26
(2,3)	2:B:101:9F0:H14	1:A:9:DA:H1'	3	0.25	0.01	0.26
(2,3)	2:B:101:9F0:H14	1:B:9:DA:H1'	3	0.25	0.01	0.26
(4,21)	1:A:19:DT:H3'	1:A:20:DT:H6	3	0.19	0.04	0.22
(4,21)	1:A:19:DT:H3'	1:B:20:DT:H6	3	0.19	0.04	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,21)	1:B:19:DT:H3'	1:A:20:DT:H6	3	0.19	0.04	0.22
(4,21)	1:B:19:DT:H3'	1:B:20:DT:H6	3	0.19	0.04	0.22
(2,191)	2:A:102:9F0:H34	1:A:12:DG:H2'	3	0.19	0.04	0.19
(2,191)	2:A:102:9F0:H34	1:B:12:DG:H2'	3	0.19	0.04	0.19
(2,191)	2:B:102:9F0:H34	1:A:12:DG:H2'	3	0.19	0.04	0.19
(2,191)	2:B:102:9F0:H34	1:B:12:DG:H2'	3	0.19	0.04	0.19
(2,40)	2:A:101:9F0:H19	1:A:3:DA:H2	3	0.15	0.03	0.14
(2,40)	2:A:101:9F0:H19	1:B:3:DA:H2	3	0.15	0.03	0.14
(2,40)	2:B:101:9F0:H19	1:A:3:DA:H2	3	0.15	0.03	0.14
(2,40)	2:B:101:9F0:H19	1:B:3:DA:H2	3	0.15	0.03	0.14
(1,14)	1:A:22:DG:N7	1:A:4:DG:N2	3	0.14	0.02	0.14
(1,14)	1:A:22:DG:N7	1:B:4:DG:N2	3	0.14	0.02	0.14
(1,14)	1:B:22:DG:N7	1:A:4:DG:N2	3	0.14	0.02	0.14
(1,14)	1:B:22:DG:N7	1:B:4:DG:N2	3	0.14	0.02	0.14
(2,180)	2:A:102:9F0:H18	1:A:13:DT:H1'	3	0.14	0.04	0.12
(2,180)	2:A:102:9F0:H18	1:B:13:DT:H1'	3	0.14	0.04	0.12
(2,180)	2:B:102:9F0:H18	1:A:13:DT:H1'	3	0.14	0.04	0.12
(2,180)	2:B:102:9F0:H18	1:B:13:DT:H1'	3	0.14	0.04	0.12
(4,144)	1:A:5:DG:H2"	1:A:6:DG:H8	3	0.13	0.01	0.13
(4,144)	1:A:5:DG:H2"	1:B:6:DG:H8	3	0.13	0.01	0.13
(4,144)	1:B:5:DG:H2"	1:A:6:DG:H8	3	0.13	0.01	0.13
(4,144)	1:B:5:DG:H2"	1:B:6:DG:H8	3	0.13	0.01	0.13
(2,28)	2:A:101:9F0:H31	1:A:10:DG:H1'	2	0.2	0.02	0.2
(2,28)	2:A:101:9F0:H31	1:B:10:DG:H1'	2	0.2	0.02	0.2
(2,28)	2:B:101:9F0:H31	1:A:10:DG:H1'	2	0.2	0.02	0.2
(2,28)	2:B:101:9F0:H31	1:B:10:DG:H1'	2	0.2	0.02	0.2
(2,108)	2:A:101:9F0:H27	1:A:9:DA:H2'	2	0.2	0.08	0.2
(2,108)	2:A:101:9F0:H27	1:B:9:DA:H2'	2	0.2	0.08	0.2
(2,108)	2:B:101:9F0:H27	1:A:9:DA:H2'	2	0.2	0.08	0.2
(2,108)	2:B:101:9F0:H27	1:B:9:DA:H2'	2	0.2	0.08	0.2
(4,45)	1:A:21:DA:H2"	1:A:22:DG:H1	2	0.16	0.01	0.16
(4,45)	1:A:21:DA:H2"	1:B:22:DG:H1	2	0.16	0.01	0.16
(4,45)	1:B:21:DA:H2"	1:A:22:DG:H1	2	0.16	0.01	0.16
(4,45)	1:B:21:DA:H2"	1:B:22:DG:H1	2	0.16	0.01	0.16
(6,8)	2:A:101:9F0:H47	2:A:101:9F0:H31	2	0.16	0.04	0.16
(6,8)	2:A:101:9F0:H47	2:B:101:9F0:H31	2	0.16	0.04	0.16
(6,8)	2:B:101:9F0:H47	2:A:101:9F0:H31	2	0.16	0.04	0.16
(6,8)	2:B:101:9F0:H47	2:B:101:9F0:H31	2	0.16	0.04	0.16
(4,96)	1:A:26:DA:H8	1:A:14:DT:H2"	2	0.16	0.04	0.16
(4,96)	1:A:26:DA:H8	1:B:14:DT:H2"	2	0.16	0.04	0.16
(4,96)	1:B:26:DA:H8	1:A:14:DT:H2"	2	0.16	0.04	0.16
(4,96)	1:B:26:DA:H8	1:B:14:DT:H2"	2	0.16	0.04	0.16

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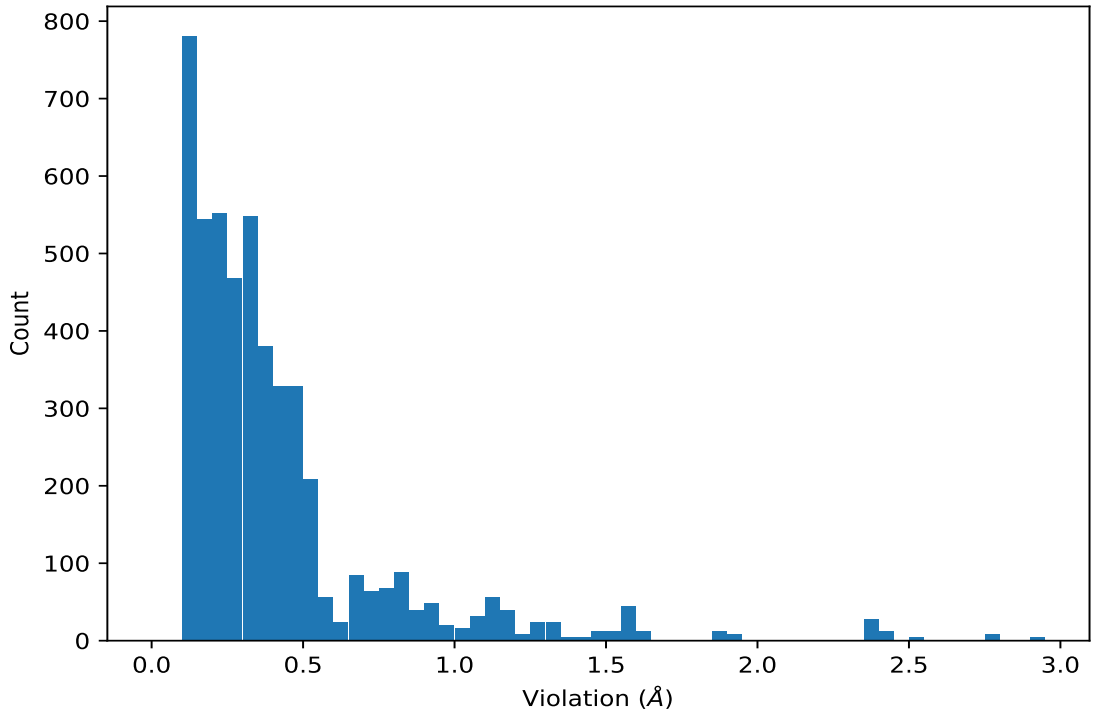
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,5)	2:A:101:9F0:H14	1:A:9:DA:H2"	2	0.14	0.01	0.14
(2,5)	2:A:101:9F0:H14	1:B:9:DA:H2"	2	0.14	0.01	0.14
(2,5)	2:B:101:9F0:H14	1:A:9:DA:H2"	2	0.14	0.01	0.14
(2,5)	2:B:101:9F0:H14	1:B:9:DA:H2"	2	0.14	0.01	0.14
(2,195)	2:A:102:9F0:H34	1:A:13:DT:H1'	2	0.12	0.01	0.12
(2,195)	2:A:102:9F0:H34	1:B:13:DT:H1'	2	0.12	0.01	0.12
(2,195)	2:B:102:9F0:H34	1:A:13:DT:H1'	2	0.12	0.01	0.12
(2,195)	2:B:102:9F0:H34	1:B:13:DT:H1'	2	0.12	0.01	0.12
(4,50)	1:A:14:DT:H1'	1:A:15:DA:H2'	2	0.12	0.01	0.12
(4,50)	1:A:14:DT:H1'	1:B:15:DA:H2'	2	0.12	0.01	0.12
(4,50)	1:B:14:DT:H1'	1:A:15:DA:H2'	2	0.12	0.01	0.12
(4,50)	1:B:14:DT:H1'	1:B:15:DA:H2'	2	0.12	0.01	0.12
(2,122)	2:A:102:9F0:H14	1:A:24:DG:H2'	2	0.12	0.01	0.12
(2,122)	2:A:102:9F0:H14	1:B:24:DG:H2'	2	0.12	0.01	0.12
(2,122)	2:B:102:9F0:H14	1:A:24:DG:H2'	2	0.12	0.01	0.12
(2,122)	2:B:102:9F0:H14	1:B:24:DG:H2'	2	0.12	0.01	0.12
(4,10)	1:A:2:DA:H2"	1:A:3:DA:H8	2	0.11	0.0	0.11
(4,10)	1:A:2:DA:H2"	1:B:3:DA:H8	2	0.11	0.0	0.11
(4,10)	1:B:2:DA:H2"	1:A:3:DA:H8	2	0.11	0.0	0.11
(4,10)	1:B:2:DA:H2"	1:B:3:DA:H8	2	0.11	0.0	0.11

[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)
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	5	2.92
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	5	2.92
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	5	2.92
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	5	2.92
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	4	2.79
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	4	2.79
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	4	2.79
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	4	2.79
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	2	2.76
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	2	2.76
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	2	2.76
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	2	2.76
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	3	2.53
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	3	2.53
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	3	2.53
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	3	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	2	2.44
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	2	2.44
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	2	2.44
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	2	2.44
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	4	2.41
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	4	2.41
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	4	2.41
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	4	2.41
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	6	2.41
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	6	2.41
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	6	2.41
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	6	2.41
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	3	2.4
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	3	2.4
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	3	2.4
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	3	2.4
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	9	2.4
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	9	2.4
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	9	2.4
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	9	2.4
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	5	2.39
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	5	2.39
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	5	2.39
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	5	2.39
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	8	2.38
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	8	2.38
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	8	2.38
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	8	2.38
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	10	2.38
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	10	2.38
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	10	2.38
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	10	2.38
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	1	2.37
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	1	2.37
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	1	2.37
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	1	2.37
(4,77)	1:A:26:DA:H2	1:A:13:DT:C5	7	2.37
(4,77)	1:A:26:DA:H2	1:B:13:DT:C5	7	2.37
(4,77)	1:B:26:DA:H2	1:A:13:DT:C5	7	2.37
(4,77)	1:B:26:DA:H2	1:B:13:DT:C5	7	2.37
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2'	6	1.91
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2'	6	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2'	6	1.91
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2'	6	1.91
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2'	8	1.91
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2'	8	1.91
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2'	8	1.91
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2'	8	1.91
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2'	9	1.89
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2'	9	1.89
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2'	9	1.89
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2'	9	1.89
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2'	7	1.88
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2'	7	1.88
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2'	7	1.88
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2'	7	1.88
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2'	10	1.88
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2'	10	1.88
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2'	10	1.88
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2'	10	1.88
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	1	1.65
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	1	1.65
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	1	1.65
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	1	1.65
(5,59)	1:A:21:DA:H5"	1:A:21:DA:H8	2	1.61
(5,59)	1:A:21:DA:H5"	1:B:21:DA:H8	2	1.61
(5,59)	1:B:21:DA:H5"	1:A:21:DA:H8	2	1.61
(5,59)	1:B:21:DA:H5"	1:B:21:DA:H8	2	1.61
(5,59)	1:A:21:DA:H5"	1:A:21:DA:H8	9	1.61
(5,59)	1:A:21:DA:H5"	1:B:21:DA:H8	9	1.61
(5,59)	1:B:21:DA:H5"	1:A:21:DA:H8	9	1.61
(5,59)	1:B:21:DA:H5"	1:B:21:DA:H8	9	1.61
(5,59)	1:A:21:DA:H5"	1:A:21:DA:H8	4	1.58
(5,59)	1:A:21:DA:H5"	1:B:21:DA:H8	4	1.58
(5,59)	1:B:21:DA:H5"	1:A:21:DA:H8	4	1.58
(5,59)	1:B:21:DA:H5"	1:B:21:DA:H8	4	1.58
(5,59)	1:A:21:DA:H5"	1:A:21:DA:H8	10	1.58
(5,59)	1:A:21:DA:H5"	1:B:21:DA:H8	10	1.58
(5,59)	1:B:21:DA:H5"	1:A:21:DA:H8	10	1.58
(5,59)	1:B:21:DA:H5"	1:B:21:DA:H8	10	1.58
(2,114)	2:A:101:9F0:H26	1:A:8:DT:H2"	7	1.58
(2,114)	2:A:101:9F0:H26	1:B:8:DT:H2"	7	1.58
(2,114)	2:B:101:9F0:H26	1:A:8:DT:H2"	7	1.58
(2,114)	2:B:101:9F0:H26	1:B:8:DT:H2"	7	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	2:A:101:9F0:H26	1:A:8:DT:H2”	10	1.58
(2,114)	2:A:101:9F0:H26	1:B:8:DT:H2”	10	1.58
(2,114)	2:B:101:9F0:H26	1:A:8:DT:H2”	10	1.58
(2,114)	2:B:101:9F0:H26	1:B:8:DT:H2”	10	1.58
(5,59)	1:A:21:DA:H5”	1:A:21:DA:H8	5	1.57
(5,59)	1:A:21:DA:H5”	1:B:21:DA:H8	5	1.57
(5,59)	1:B:21:DA:H5”	1:A:21:DA:H8	5	1.57
(5,59)	1:B:21:DA:H5”	1:B:21:DA:H8	5	1.57
(2,114)	2:A:101:9F0:H26	1:A:8:DT:H2”	8	1.57
(2,114)	2:A:101:9F0:H26	1:B:8:DT:H2”	8	1.57
(2,114)	2:B:101:9F0:H26	1:A:8:DT:H2”	8	1.57
(2,114)	2:B:101:9F0:H26	1:B:8:DT:H2”	8	1.57
(2,114)	2:A:101:9F0:H26	1:A:8:DT:H2”	9	1.57
(2,114)	2:A:101:9F0:H26	1:B:8:DT:H2”	9	1.57
(2,114)	2:B:101:9F0:H26	1:A:8:DT:H2”	9	1.57
(2,114)	2:B:101:9F0:H26	1:B:8:DT:H2”	9	1.57
(5,59)	1:A:21:DA:H5”	1:A:21:DA:H8	3	1.56
(5,59)	1:A:21:DA:H5”	1:B:21:DA:H8	3	1.56
(5,59)	1:B:21:DA:H5”	1:A:21:DA:H8	3	1.56
(5,59)	1:B:21:DA:H5”	1:B:21:DA:H8	3	1.56
(5,59)	1:A:21:DA:H5”	1:A:21:DA:H8	6	1.56
(5,59)	1:A:21:DA:H5”	1:B:21:DA:H8	6	1.56
(5,59)	1:B:21:DA:H5”	1:A:21:DA:H8	6	1.56
(5,59)	1:B:21:DA:H5”	1:B:21:DA:H8	6	1.56
(5,59)	1:A:21:DA:H5”	1:A:21:DA:H8	7	1.56
(5,59)	1:A:21:DA:H5”	1:B:21:DA:H8	7	1.56
(5,59)	1:B:21:DA:H5”	1:A:21:DA:H8	7	1.56
(5,59)	1:B:21:DA:H5”	1:B:21:DA:H8	7	1.56
(5,59)	1:A:21:DA:H5”	1:A:21:DA:H8	1	1.55
(5,59)	1:A:21:DA:H5”	1:B:21:DA:H8	1	1.55
(5,59)	1:B:21:DA:H5”	1:A:21:DA:H8	1	1.55
(5,59)	1:B:21:DA:H5”	1:B:21:DA:H8	1	1.55
(5,59)	1:A:21:DA:H5”	1:A:21:DA:H8	8	1.54
(5,59)	1:A:21:DA:H5”	1:B:21:DA:H8	8	1.54
(5,59)	1:B:21:DA:H5”	1:A:21:DA:H8	8	1.54
(5,59)	1:B:21:DA:H5”	1:B:21:DA:H8	8	1.54
(2,114)	2:A:101:9F0:H26	1:A:8:DT:H2”	6	1.53
(2,114)	2:A:101:9F0:H26	1:B:8:DT:H2”	6	1.53
(2,114)	2:B:101:9F0:H26	1:A:8:DT:H2”	6	1.53
(2,114)	2:B:101:9F0:H26	1:B:8:DT:H2”	6	1.53
(2,118)	2:A:101:9F0:H45	1:A:8:DT:H2”	8	1.52
(2,118)	2:A:101:9F0:H45	1:B:8:DT:H2”	8	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	2:B:101:9F0:H45	1:A:8:DT:H2”	8	1.52
(2,118)	2:B:101:9F0:H45	1:B:8:DT:H2”	8	1.52
(2,118)	2:A:101:9F0:H45	1:A:8:DT:H2”	7	1.49
(2,118)	2:A:101:9F0:H45	1:B:8:DT:H2”	7	1.49
(2,118)	2:B:101:9F0:H45	1:A:8:DT:H2”	7	1.49
(2,118)	2:B:101:9F0:H45	1:B:8:DT:H2”	7	1.49
(2,118)	2:A:101:9F0:H45	1:A:8:DT:H2”	10	1.49
(2,118)	2:A:101:9F0:H45	1:B:8:DT:H2”	10	1.49
(2,118)	2:B:101:9F0:H45	1:A:8:DT:H2”	10	1.49
(2,118)	2:B:101:9F0:H45	1:B:8:DT:H2”	10	1.49
(2,118)	2:A:101:9F0:H45	1:A:8:DT:H2”	9	1.47
(2,118)	2:A:101:9F0:H45	1:B:8:DT:H2”	9	1.47
(2,118)	2:B:101:9F0:H45	1:A:8:DT:H2”	9	1.47
(2,118)	2:B:101:9F0:H45	1:B:8:DT:H2”	9	1.47
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2’	5	1.43
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2’	5	1.43
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2’	5	1.43
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2’	5	1.43
(2,118)	2:A:101:9F0:H45	1:A:8:DT:H2”	6	1.36
(2,118)	2:A:101:9F0:H45	1:B:8:DT:H2”	6	1.36
(2,118)	2:B:101:9F0:H45	1:A:8:DT:H2”	6	1.36
(2,118)	2:B:101:9F0:H45	1:B:8:DT:H2”	6	1.36
(5,250)	1:A:24:DG:H5”	1:A:24:DG:H8	7	1.33
(5,250)	1:A:24:DG:H5”	1:B:24:DG:H8	7	1.33
(5,250)	1:B:24:DG:H5”	1:A:24:DG:H8	7	1.33
(5,250)	1:B:24:DG:H5”	1:B:24:DG:H8	7	1.33
(5,250)	1:A:24:DG:H5”	1:A:24:DG:H8	1	1.32
(5,250)	1:A:24:DG:H5”	1:B:24:DG:H8	1	1.32
(5,250)	1:B:24:DG:H5”	1:A:24:DG:H8	1	1.32
(5,250)	1:B:24:DG:H5”	1:B:24:DG:H8	1	1.32
(5,250)	1:A:24:DG:H5”	1:A:24:DG:H8	10	1.32
(5,250)	1:A:24:DG:H5”	1:B:24:DG:H8	10	1.32
(5,250)	1:B:24:DG:H5”	1:A:24:DG:H8	10	1.32
(5,250)	1:B:24:DG:H5”	1:B:24:DG:H8	10	1.32
(5,250)	1:A:24:DG:H5”	1:A:24:DG:H8	9	1.31
(5,250)	1:A:24:DG:H5”	1:B:24:DG:H8	9	1.31
(5,250)	1:B:24:DG:H5”	1:A:24:DG:H8	9	1.31
(5,250)	1:B:24:DG:H5”	1:B:24:DG:H8	9	1.31
(5,250)	1:A:24:DG:H5”	1:A:24:DG:H8	5	1.3
(5,250)	1:A:24:DG:H5”	1:B:24:DG:H8	5	1.3
(5,250)	1:B:24:DG:H5”	1:A:24:DG:H8	5	1.3
(5,250)	1:B:24:DG:H5”	1:B:24:DG:H8	5	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,250)	1:A:24:DG:H5”	1:A:24:DG:H8	6	1.3
(5,250)	1:A:24:DG:H5”	1:B:24:DG:H8	6	1.3
(5,250)	1:B:24:DG:H5”	1:A:24:DG:H8	6	1.3
(5,250)	1:B:24:DG:H5”	1:B:24:DG:H8	6	1.3
(5,250)	1:A:24:DG:H5”	1:A:24:DG:H8	2	1.28
(5,250)	1:A:24:DG:H5”	1:B:24:DG:H8	2	1.28
(5,250)	1:B:24:DG:H5”	1:A:24:DG:H8	2	1.28
(5,250)	1:B:24:DG:H5”	1:B:24:DG:H8	2	1.28
(5,250)	1:A:24:DG:H5”	1:A:24:DG:H8	8	1.28
(5,250)	1:A:24:DG:H5”	1:B:24:DG:H8	8	1.28
(5,250)	1:B:24:DG:H5”	1:A:24:DG:H8	8	1.28
(5,250)	1:B:24:DG:H5”	1:B:24:DG:H8	8	1.28
(5,250)	1:A:24:DG:H5”	1:A:24:DG:H8	4	1.27
(5,250)	1:A:24:DG:H5”	1:B:24:DG:H8	4	1.27
(5,250)	1:B:24:DG:H5”	1:A:24:DG:H8	4	1.27
(5,250)	1:B:24:DG:H5”	1:B:24:DG:H8	4	1.27
(5,38)	1:A:19:DT:H3’	1:A:19:DT:H6	9	1.25
(5,38)	1:A:19:DT:H3’	1:B:19:DT:H6	9	1.25
(5,38)	1:B:19:DT:H3’	1:A:19:DT:H6	9	1.25
(5,38)	1:B:19:DT:H3’	1:B:19:DT:H6	9	1.25
(5,250)	1:A:24:DG:H5”	1:A:24:DG:H8	3	1.25
(5,250)	1:A:24:DG:H5”	1:B:24:DG:H8	3	1.25
(5,250)	1:B:24:DG:H5”	1:A:24:DG:H8	3	1.25
(5,250)	1:B:24:DG:H5”	1:B:24:DG:H8	3	1.25
(4,2)	1:A:1:DA:H8	1:A:2:DA:H2	5	1.25
(4,2)	1:A:1:DA:H8	1:B:2:DA:H2	5	1.25
(4,2)	1:B:1:DA:H8	1:A:2:DA:H2	5	1.25
(4,2)	1:B:1:DA:H8	1:B:2:DA:H2	5	1.25
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	1	1.24
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	1	1.24
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	1	1.24
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	1	1.24
(4,49)	1:A:14:DT:H1’	1:A:15:DA:H8	5	1.22
(4,49)	1:A:14:DT:H1’	1:B:15:DA:H8	5	1.22
(4,49)	1:B:14:DT:H1’	1:A:15:DA:H8	5	1.22
(4,49)	1:B:14:DT:H1’	1:B:15:DA:H8	5	1.22
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	1	1.2
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	1	1.2
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	1	1.2
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	1	1.2
(5,166)	1:A:11:DG:H5”	1:A:11:DG:H8	5	1.2
(5,166)	1:A:11:DG:H5”	1:B:11:DG:H8	5	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,166)	1:B:11:DG:H5”	1:A:11:DG:H8	5	1.2
(5,166)	1:B:11:DG:H5”	1:B:11:DG:H8	5	1.2
(4,49)	1:A:14:DT:H1’	1:A:15:DA:H8	4	1.19
(4,49)	1:A:14:DT:H1’	1:B:15:DA:H8	4	1.19
(4,49)	1:B:14:DT:H1’	1:A:15:DA:H8	4	1.19
(4,49)	1:B:14:DT:H1’	1:B:15:DA:H8	4	1.19
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2”	6	1.19
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2”	6	1.19
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2”	6	1.19
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2”	6	1.19
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	7	1.18
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	7	1.18
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	7	1.18
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	7	1.18
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2”	7	1.18
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2”	7	1.18
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2”	7	1.18
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2”	7	1.18
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2”	9	1.17
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2”	9	1.17
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2”	9	1.17
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2”	9	1.17
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2”	10	1.17
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2”	10	1.17
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2”	10	1.17
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2”	10	1.17
(5,166)	1:A:11:DG:H5”	1:A:11:DG:H8	1	1.16
(5,166)	1:A:11:DG:H5”	1:B:11:DG:H8	1	1.16
(5,166)	1:B:11:DG:H5”	1:A:11:DG:H8	1	1.16
(5,166)	1:B:11:DG:H5”	1:B:11:DG:H8	1	1.16
(5,166)	1:A:11:DG:H5”	1:A:11:DG:H8	7	1.16
(5,166)	1:A:11:DG:H5”	1:B:11:DG:H8	7	1.16
(5,166)	1:B:11:DG:H5”	1:A:11:DG:H8	7	1.16
(5,166)	1:B:11:DG:H5”	1:B:11:DG:H8	7	1.16
(2,114)	2:A:101:9F0:H26	1:A:8:DT:H2”	5	1.15
(2,114)	2:A:101:9F0:H26	1:B:8:DT:H2”	5	1.15
(2,114)	2:B:101:9F0:H26	1:A:8:DT:H2”	5	1.15
(2,114)	2:B:101:9F0:H26	1:B:8:DT:H2”	5	1.15
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2”	8	1.15
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2”	8	1.15
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2”	8	1.15
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2”	8	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,38)	1:A:19:DT:H3'	1:A:19:DT:H6	10	1.14
(5,38)	1:A:19:DT:H3'	1:B:19:DT:H6	10	1.14
(5,38)	1:B:19:DT:H3'	1:A:19:DT:H6	10	1.14
(5,38)	1:B:19:DT:H3'	1:B:19:DT:H6	10	1.14
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	5	1.14
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	5	1.14
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	5	1.14
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	5	1.14
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2'	4	1.14
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2'	4	1.14
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2'	4	1.14
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2'	4	1.14
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	3	1.13
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	3	1.13
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	3	1.13
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	3	1.13
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	9	1.13
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	9	1.13
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	9	1.13
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	9	1.13
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	6	1.12
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	6	1.12
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	6	1.12
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	6	1.12
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	7	1.12
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	7	1.12
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	7	1.12
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	7	1.12
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	9	1.12
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	9	1.12
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	9	1.12
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	9	1.12
(5,166)	1:A:11:DG:H5"	1:A:11:DG:H8	2	1.11
(5,166)	1:A:11:DG:H5"	1:B:11:DG:H8	2	1.11
(5,166)	1:B:11:DG:H5"	1:A:11:DG:H8	2	1.11
(5,166)	1:B:11:DG:H5"	1:B:11:DG:H8	2	1.11
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	1	1.11
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	1	1.11
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	1	1.11
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	1	1.11
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	4	1.1
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	4	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	4	1.1
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	4	1.1
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	8	1.1
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	8	1.1
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	8	1.1
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	8	1.1
(5,166)	1:A:11:DG:H5"	1:A:11:DG:H8	10	1.09
(5,166)	1:A:11:DG:H5"	1:B:11:DG:H8	10	1.09
(5,166)	1:B:11:DG:H5"	1:A:11:DG:H8	10	1.09
(5,166)	1:B:11:DG:H5"	1:B:11:DG:H8	10	1.09
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	10	1.09
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	10	1.09
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	10	1.09
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	10	1.09
(5,166)	1:A:11:DG:H5"	1:A:11:DG:H8	8	1.08
(5,166)	1:A:11:DG:H5"	1:B:11:DG:H8	8	1.08
(5,166)	1:B:11:DG:H5"	1:A:11:DG:H8	8	1.08
(5,166)	1:B:11:DG:H5"	1:B:11:DG:H8	8	1.08
(4,87)	1:A:26:DA:H2	1:A:13:DT:H2'	2	1.08
(4,87)	1:A:26:DA:H2	1:B:13:DT:H2'	2	1.08
(4,87)	1:B:26:DA:H2	1:A:13:DT:H2'	2	1.08
(4,87)	1:B:26:DA:H2	1:B:13:DT:H2'	2	1.08
(5,166)	1:A:11:DG:H5"	1:A:11:DG:H8	6	1.07
(5,166)	1:A:11:DG:H5"	1:B:11:DG:H8	6	1.07
(5,166)	1:B:11:DG:H5"	1:A:11:DG:H8	6	1.07
(5,166)	1:B:11:DG:H5"	1:B:11:DG:H8	6	1.07
(5,166)	1:A:11:DG:H5"	1:A:11:DG:H8	9	1.07
(5,166)	1:A:11:DG:H5"	1:B:11:DG:H8	9	1.07
(5,166)	1:B:11:DG:H5"	1:A:11:DG:H8	9	1.07
(5,166)	1:B:11:DG:H5"	1:B:11:DG:H8	9	1.07
(4,2)	1:A:1:DA:H8	1:A:2:DA:H2	3	1.07
(4,2)	1:A:1:DA:H8	1:B:2:DA:H2	3	1.07
(4,2)	1:B:1:DA:H8	1:A:2:DA:H2	3	1.07
(4,2)	1:B:1:DA:H8	1:B:2:DA:H2	3	1.07
(4,49)	1:A:14:DT:H1'	1:A:15:DA:H8	2	1.06
(4,49)	1:A:14:DT:H1'	1:B:15:DA:H8	2	1.06
(4,49)	1:B:14:DT:H1'	1:A:15:DA:H8	2	1.06
(4,49)	1:B:14:DT:H1'	1:B:15:DA:H8	2	1.06
(5,166)	1:A:11:DG:H5"	1:A:11:DG:H8	3	1.04
(5,166)	1:A:11:DG:H5"	1:B:11:DG:H8	3	1.04
(5,166)	1:B:11:DG:H5"	1:A:11:DG:H8	3	1.04
(5,166)	1:B:11:DG:H5"	1:B:11:DG:H8	3	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,38)	1:A:19:DT:H3'	1:A:19:DT:H6	6	1.01
(5,38)	1:A:19:DT:H3'	1:B:19:DT:H6	6	1.01
(5,38)	1:B:19:DT:H3'	1:A:19:DT:H6	6	1.01
(5,38)	1:B:19:DT:H3'	1:B:19:DT:H6	6	1.01
(5,166)	1:A:11:DG:H5"	1:A:11:DG:H8	4	1.01
(5,166)	1:A:11:DG:H5"	1:B:11:DG:H8	4	1.01
(5,166)	1:B:11:DG:H5"	1:A:11:DG:H8	4	1.01
(5,166)	1:B:11:DG:H5"	1:B:11:DG:H8	4	1.01
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	2	1.01
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	2	1.01
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	2	1.01
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	2	1.01
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2'	3	0.98
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2'	3	0.98
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2'	3	0.98
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2'	3	0.98
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	5	0.97
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	5	0.97
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	5	0.97
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	5	0.97
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	6	0.97
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	6	0.97
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	6	0.97
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	6	0.97
(5,38)	1:A:19:DT:H3'	1:A:19:DT:H6	7	0.96
(5,38)	1:A:19:DT:H3'	1:B:19:DT:H6	7	0.96
(5,38)	1:B:19:DT:H3'	1:A:19:DT:H6	7	0.96
(5,38)	1:B:19:DT:H3'	1:B:19:DT:H6	7	0.96
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2"	5	0.96
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2"	5	0.96
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2"	5	0.96
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2"	5	0.96
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	1	0.95
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	1	0.95
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	1	0.95
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	1	0.95
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	4	0.95
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	4	0.95
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	4	0.95
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	4	0.95
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	7	0.95
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	7	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	7	0.95
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	7	0.95
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	10	0.95
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	10	0.95
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	10	0.95
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	10	0.95
(5,38)	1:A:19:DT:H3'	1:A:19:DT:H6	8	0.94
(5,38)	1:A:19:DT:H3'	1:B:19:DT:H6	8	0.94
(5,38)	1:B:19:DT:H3'	1:A:19:DT:H6	8	0.94
(5,38)	1:B:19:DT:H3'	1:B:19:DT:H6	8	0.94
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	3	0.94
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	3	0.94
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	3	0.94
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	3	0.94
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	9	0.93
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	9	0.93
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	9	0.93
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	9	0.93
(4,18)	1:A:8:DT:H2"	1:A:9:DA:H8	9	0.93
(4,18)	1:A:8:DT:H2"	1:B:9:DA:H8	9	0.93
(4,18)	1:B:8:DT:H2"	1:A:9:DA:H8	9	0.93
(4,18)	1:B:8:DT:H2"	1:B:9:DA:H8	9	0.93
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	10	0.92
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	10	0.92
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	10	0.92
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	10	0.92
(4,18)	1:A:8:DT:H2"	1:A:9:DA:H8	8	0.91
(4,18)	1:A:8:DT:H2"	1:B:9:DA:H8	8	0.91
(4,18)	1:B:8:DT:H2"	1:A:9:DA:H8	8	0.91
(4,18)	1:B:8:DT:H2"	1:B:9:DA:H8	8	0.91
(4,68)	1:A:25:DA:H2"	1:A:26:DA:H8	8	0.9
(4,68)	1:A:25:DA:H2"	1:B:26:DA:H8	8	0.9
(4,68)	1:B:25:DA:H2"	1:A:26:DA:H8	8	0.9
(4,68)	1:B:25:DA:H2"	1:B:26:DA:H8	8	0.9
(4,49)	1:A:14:DT:H1'	1:A:15:DA:H8	6	0.9
(4,49)	1:A:14:DT:H1'	1:B:15:DA:H8	6	0.9
(4,49)	1:B:14:DT:H1'	1:A:15:DA:H8	6	0.9
(4,49)	1:B:14:DT:H1'	1:B:15:DA:H8	6	0.9
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	10	0.89
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	10	0.89
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	10	0.89
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	10	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,53)	1:A:14:DT:H4'	1:A:15:DA:H8	4	0.89
(4,53)	1:A:14:DT:H4'	1:B:15:DA:H8	4	0.89
(4,53)	1:B:14:DT:H4'	1:A:15:DA:H8	4	0.89
(4,53)	1:B:14:DT:H4'	1:B:15:DA:H8	4	0.89
(4,49)	1:A:14:DT:H1'	1:A:15:DA:H8	3	0.89
(4,49)	1:A:14:DT:H1'	1:B:15:DA:H8	3	0.89
(4,49)	1:B:14:DT:H1'	1:A:15:DA:H8	3	0.89
(4,49)	1:B:14:DT:H1'	1:B:15:DA:H8	3	0.89
(4,49)	1:A:14:DT:H1'	1:A:15:DA:H8	7	0.89
(4,49)	1:A:14:DT:H1'	1:B:15:DA:H8	7	0.89
(4,49)	1:B:14:DT:H1'	1:A:15:DA:H8	7	0.89
(4,49)	1:B:14:DT:H1'	1:B:15:DA:H8	7	0.89
(4,18)	1:A:8:DT:H2"	1:A:9:DA:H8	10	0.89
(4,18)	1:A:8:DT:H2"	1:B:9:DA:H8	10	0.89
(4,18)	1:B:8:DT:H2"	1:A:9:DA:H8	10	0.89
(4,18)	1:B:8:DT:H2"	1:B:9:DA:H8	10	0.89
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	2	0.89
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	2	0.89
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	2	0.89
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	2	0.89
(5,25)	1:A:8:DT:H3'	1:A:8:DT:H6	7	0.88
(5,25)	1:A:8:DT:H3'	1:B:8:DT:H6	7	0.88
(5,25)	1:B:8:DT:H3'	1:A:8:DT:H6	7	0.88
(5,25)	1:B:8:DT:H3'	1:B:8:DT:H6	7	0.88
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	9	0.87
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	9	0.87
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	9	0.87
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	9	0.87
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	4	0.87
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	4	0.87
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	4	0.87
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	4	0.87
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	5	0.86
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	5	0.86
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	5	0.86
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	5	0.86
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	2	0.85
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	2	0.85
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	2	0.85
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	2	0.85
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	7	0.85
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	7	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	7	0.85
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	7	0.85
(5,25)	1:A:8:DT:H3'	1:A:8:DT:H6	1	0.85
(5,25)	1:A:8:DT:H3'	1:B:8:DT:H6	1	0.85
(5,25)	1:B:8:DT:H3'	1:A:8:DT:H6	1	0.85
(5,25)	1:B:8:DT:H3'	1:B:8:DT:H6	1	0.85
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	6	0.85
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	6	0.85
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	6	0.85
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	6	0.85
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	10	0.85
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	10	0.85
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	10	0.85
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	10	0.85
(4,53)	1:A:14:DT:H4'	1:A:15:DA:H8	5	0.84
(4,53)	1:A:14:DT:H4'	1:B:15:DA:H8	5	0.84
(4,53)	1:B:14:DT:H4'	1:A:15:DA:H8	5	0.84
(4,53)	1:B:14:DT:H4'	1:B:15:DA:H8	5	0.84
(4,18)	1:A:8:DT:H2"	1:A:9:DA:H8	7	0.84
(4,18)	1:A:8:DT:H2"	1:B:9:DA:H8	7	0.84
(4,18)	1:B:8:DT:H2"	1:A:9:DA:H8	7	0.84
(4,18)	1:B:8:DT:H2"	1:B:9:DA:H8	7	0.84
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	1	0.84
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	1	0.84
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	1	0.84
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	1	0.84
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	4	0.84
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	4	0.84
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	4	0.84
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	4	0.84
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	7	0.84
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	7	0.84
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	7	0.84
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	7	0.84
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	7	0.84
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	7	0.84
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	7	0.84
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	7	0.84
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	1	0.83
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	1	0.83
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	1	0.83
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	1	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	3	0.83
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	3	0.83
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	3	0.83
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	3	0.83
(2,186)	2:A:102:9F0:H33	1:A:12:DG:H8	8	0.83
(2,186)	2:A:102:9F0:H33	1:B:12:DG:H8	8	0.83
(2,186)	2:B:102:9F0:H33	1:A:12:DG:H8	8	0.83
(2,186)	2:B:102:9F0:H33	1:B:12:DG:H8	8	0.83
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	6	0.83
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	6	0.83
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	6	0.83
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	6	0.83
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	10	0.82
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	10	0.82
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	10	0.82
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	10	0.82
(5,25)	1:A:8:DT:H3'	1:A:8:DT:H6	8	0.82
(5,25)	1:A:8:DT:H3'	1:B:8:DT:H6	8	0.82
(5,25)	1:B:8:DT:H3'	1:A:8:DT:H6	8	0.82
(5,25)	1:B:8:DT:H3'	1:B:8:DT:H6	8	0.82
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3'	5	0.82
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3'	5	0.82
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3'	5	0.82
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3'	5	0.82
(4,64)	1:A:15:DA:H4'	1:A:16:DG:H1'	2	0.81
(4,64)	1:A:15:DA:H4'	1:B:16:DG:H1'	2	0.81
(4,64)	1:B:15:DA:H4'	1:A:16:DG:H1'	2	0.81
(4,64)	1:B:15:DA:H4'	1:B:16:DG:H1'	2	0.81
(2,114)	2:A:101:9F0:H26	1:A:8:DT:H2"	4	0.81
(2,114)	2:A:101:9F0:H26	1:B:8:DT:H2"	4	0.81
(2,114)	2:B:101:9F0:H26	1:A:8:DT:H2"	4	0.81
(2,114)	2:B:101:9F0:H26	1:B:8:DT:H2"	4	0.81
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	9	0.8
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	9	0.8
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	9	0.8
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	9	0.8
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3'	4	0.8
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3'	4	0.8
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3'	4	0.8
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3'	4	0.8
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	5	0.79
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	5	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	5	0.79
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	5	0.79
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	2	0.78
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	2	0.78
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	2	0.78
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	2	0.78
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	7	0.78
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	7	0.78
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	7	0.78
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	7	0.78
(5,38)	1:A:19:DT:H3'	1:A:19:DT:H6	3	0.78
(5,38)	1:A:19:DT:H3'	1:B:19:DT:H6	3	0.78
(5,38)	1:B:19:DT:H3'	1:A:19:DT:H6	3	0.78
(5,38)	1:B:19:DT:H3'	1:B:19:DT:H6	3	0.78
(5,25)	1:A:8:DT:H3'	1:A:8:DT:H6	5	0.78
(5,25)	1:A:8:DT:H3'	1:B:8:DT:H6	5	0.78
(5,25)	1:B:8:DT:H3'	1:A:8:DT:H6	5	0.78
(5,25)	1:B:8:DT:H3'	1:B:8:DT:H6	5	0.78
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3'	3	0.78
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3'	3	0.78
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3'	3	0.78
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3'	3	0.78
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	1	0.77
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	1	0.77
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	1	0.77
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	1	0.77
(5,25)	1:A:8:DT:H3'	1:A:8:DT:H6	10	0.77
(5,25)	1:A:8:DT:H3'	1:B:8:DT:H6	10	0.77
(5,25)	1:B:8:DT:H3'	1:A:8:DT:H6	10	0.77
(5,25)	1:B:8:DT:H3'	1:B:8:DT:H6	10	0.77
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	3	0.77
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	3	0.77
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	3	0.77
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	3	0.77
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	3	0.76
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	3	0.76
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	3	0.76
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	3	0.76
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	1	0.76
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	1	0.76
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	1	0.76
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	2	0.76
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	2	0.76
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	2	0.76
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	2	0.76
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	8	0.76
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	8	0.76
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	8	0.76
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	8	0.76
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	10	0.76
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	10	0.76
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	10	0.76
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	10	0.76
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	5	0.75
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	5	0.75
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	5	0.75
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	5	0.75
(5,38)	1:A:19:DT:H3'	1:A:19:DT:H6	1	0.75
(5,38)	1:A:19:DT:H3'	1:B:19:DT:H6	1	0.75
(5,38)	1:B:19:DT:H3'	1:A:19:DT:H6	1	0.75
(5,38)	1:B:19:DT:H3'	1:B:19:DT:H6	1	0.75
(2,118)	2:A:101:9F0:H45	1:A:8:DT:H2"	5	0.75
(2,118)	2:A:101:9F0:H45	1:B:8:DT:H2"	5	0.75
(2,118)	2:B:101:9F0:H45	1:A:8:DT:H2"	5	0.75
(2,118)	2:B:101:9F0:H45	1:B:8:DT:H2"	5	0.75
(5,25)	1:A:8:DT:H3'	1:A:8:DT:H6	9	0.74
(5,25)	1:A:8:DT:H3'	1:B:8:DT:H6	9	0.74
(5,25)	1:B:8:DT:H3'	1:A:8:DT:H6	9	0.74
(5,25)	1:B:8:DT:H3'	1:B:8:DT:H6	9	0.74
(5,213)	1:A:18:DG:H5"	1:A:18:DG:H8	9	0.74
(5,213)	1:A:18:DG:H5"	1:B:18:DG:H8	9	0.74
(5,213)	1:B:18:DG:H5"	1:A:18:DG:H8	9	0.74
(5,213)	1:B:18:DG:H5"	1:B:18:DG:H8	9	0.74
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3'	6	0.74
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3'	6	0.74
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3'	6	0.74
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3'	6	0.74
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	9	0.73
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	9	0.73
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	9	0.73
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	9	0.73
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3'	2	0.73
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3'	2	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3'	2	0.73
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3'	2	0.73
(4,18)	1:A:8:DT:H2"	1:A:9:DA:H8	6	0.73
(4,18)	1:A:8:DT:H2"	1:B:9:DA:H8	6	0.73
(4,18)	1:B:8:DT:H2"	1:A:9:DA:H8	6	0.73
(4,18)	1:B:8:DT:H2"	1:B:9:DA:H8	6	0.73
(2,179)	2:A:102:9F0:H16	1:A:13:DT:C5	9	0.73
(2,179)	2:A:102:9F0:H16	1:B:13:DT:C5	9	0.73
(2,179)	2:B:102:9F0:H16	1:A:13:DT:C5	9	0.73
(2,179)	2:B:102:9F0:H16	1:B:13:DT:C5	9	0.73
(5,213)	1:A:18:DG:H5"	1:A:18:DG:H8	1	0.72
(5,213)	1:A:18:DG:H5"	1:B:18:DG:H8	1	0.72
(5,213)	1:B:18:DG:H5"	1:A:18:DG:H8	1	0.72
(5,213)	1:B:18:DG:H5"	1:B:18:DG:H8	1	0.72
(5,213)	1:A:18:DG:H5"	1:A:18:DG:H8	3	0.72
(5,213)	1:A:18:DG:H5"	1:B:18:DG:H8	3	0.72
(5,213)	1:B:18:DG:H5"	1:A:18:DG:H8	3	0.72
(5,213)	1:B:18:DG:H5"	1:B:18:DG:H8	3	0.72
(5,213)	1:A:18:DG:H5"	1:A:18:DG:H8	5	0.72
(5,213)	1:A:18:DG:H5"	1:B:18:DG:H8	5	0.72
(5,213)	1:B:18:DG:H5"	1:A:18:DG:H8	5	0.72
(5,213)	1:B:18:DG:H5"	1:B:18:DG:H8	5	0.72
(5,213)	1:A:18:DG:H5"	1:A:18:DG:H8	8	0.72
(5,213)	1:A:18:DG:H5"	1:B:18:DG:H8	8	0.72
(5,213)	1:B:18:DG:H5"	1:A:18:DG:H8	8	0.72
(5,213)	1:B:18:DG:H5"	1:B:18:DG:H8	8	0.72
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	6	0.72
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	6	0.72
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	6	0.72
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	6	0.72
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	4	0.71
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	4	0.71
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	4	0.71
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	4	0.71
(5,213)	1:A:18:DG:H5"	1:A:18:DG:H8	7	0.71
(5,213)	1:A:18:DG:H5"	1:B:18:DG:H8	7	0.71
(5,213)	1:B:18:DG:H5"	1:A:18:DG:H8	7	0.71
(5,213)	1:B:18:DG:H5"	1:B:18:DG:H8	7	0.71
(4,2)	1:A:1:DA:H8	1:A:2:DA:H2	1	0.71
(4,2)	1:A:1:DA:H8	1:B:2:DA:H2	1	0.71
(4,2)	1:B:1:DA:H8	1:A:2:DA:H2	1	0.71
(4,2)	1:B:1:DA:H8	1:B:2:DA:H2	1	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2'	2	0.71
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2'	2	0.71
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2'	2	0.71
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2'	2	0.71
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3'	7	0.7
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3'	7	0.7
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3'	7	0.7
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3'	7	0.7
(4,61)	1:A:15:DA:H2"	1:A:16:DG:H8	4	0.7
(4,61)	1:A:15:DA:H2"	1:B:16:DG:H8	4	0.7
(4,61)	1:B:15:DA:H2"	1:A:16:DG:H8	4	0.7
(4,61)	1:B:15:DA:H2"	1:B:16:DG:H8	4	0.7
(4,23)	1:A:19:DT:H3'	1:A:21:DA:H8	4	0.7
(4,23)	1:A:19:DT:H3'	1:B:21:DA:H8	4	0.7
(4,23)	1:B:19:DT:H3'	1:A:21:DA:H8	4	0.7
(4,23)	1:B:19:DT:H3'	1:B:21:DA:H8	4	0.7
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	3	0.69
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	3	0.69
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	3	0.69
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	3	0.69
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	5	0.69
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	5	0.69
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	5	0.69
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	5	0.69
(4,61)	1:A:15:DA:H2"	1:A:16:DG:H8	9	0.69
(4,61)	1:A:15:DA:H2"	1:B:16:DG:H8	9	0.69
(4,61)	1:B:15:DA:H2"	1:A:16:DG:H8	9	0.69
(4,61)	1:B:15:DA:H2"	1:B:16:DG:H8	9	0.69
(2,114)	2:A:101:9F0:H26	1:A:8:DT:H2"	3	0.69
(2,114)	2:A:101:9F0:H26	1:B:8:DT:H2"	3	0.69
(2,114)	2:B:101:9F0:H26	1:A:8:DT:H2"	3	0.69
(2,114)	2:B:101:9F0:H26	1:B:8:DT:H2"	3	0.69
(5,25)	1:A:8:DT:H3'	1:A:8:DT:H6	6	0.67
(5,25)	1:A:8:DT:H3'	1:B:8:DT:H6	6	0.67
(5,25)	1:B:8:DT:H3'	1:A:8:DT:H6	6	0.67
(5,25)	1:B:8:DT:H3'	1:B:8:DT:H6	6	0.67
(5,213)	1:A:18:DG:H5"	1:A:18:DG:H8	2	0.67
(5,213)	1:A:18:DG:H5"	1:B:18:DG:H8	2	0.67
(5,213)	1:B:18:DG:H5"	1:A:18:DG:H8	2	0.67
(5,213)	1:B:18:DG:H5"	1:B:18:DG:H8	2	0.67
(5,213)	1:A:18:DG:H5"	1:A:18:DG:H8	4	0.67
(5,213)	1:A:18:DG:H5"	1:B:18:DG:H8	4	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,213)	1:B:18:DG:H5”	1:A:18:DG:H8	4	0.67
(5,213)	1:B:18:DG:H5”	1:B:18:DG:H8	4	0.67
(5,213)	1:A:18:DG:H5”	1:A:18:DG:H8	10	0.67
(5,213)	1:A:18:DG:H5”	1:B:18:DG:H8	10	0.67
(5,213)	1:B:18:DG:H5”	1:A:18:DG:H8	10	0.67
(5,213)	1:B:18:DG:H5”	1:B:18:DG:H8	10	0.67
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3’	8	0.67
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3’	8	0.67
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3’	8	0.67
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3’	8	0.67
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	6	0.66
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	6	0.66
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	6	0.66
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	6	0.66
(5,25)	1:A:8:DT:H3’	1:A:8:DT:H6	4	0.66
(5,25)	1:A:8:DT:H3’	1:B:8:DT:H6	4	0.66
(5,25)	1:B:8:DT:H3’	1:A:8:DT:H6	4	0.66
(5,25)	1:B:8:DT:H3’	1:B:8:DT:H6	4	0.66
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3’	9	0.66
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3’	9	0.66
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3’	9	0.66
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3’	9	0.66
(4,64)	1:A:15:DA:H4’	1:A:16:DG:H1’	10	0.66
(4,64)	1:A:15:DA:H4’	1:B:16:DG:H1’	10	0.66
(4,64)	1:B:15:DA:H4’	1:A:16:DG:H1’	10	0.66
(4,64)	1:B:15:DA:H4’	1:B:16:DG:H1’	10	0.66
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2”	4	0.66
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2”	4	0.66
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2”	4	0.66
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2”	4	0.66
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	4	0.65
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	4	0.65
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	4	0.65
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	4	0.65
(5,38)	1:A:19:DT:H3’	1:A:19:DT:H6	2	0.65
(5,38)	1:A:19:DT:H3’	1:B:19:DT:H6	2	0.65
(5,38)	1:B:19:DT:H3’	1:A:19:DT:H6	2	0.65
(5,38)	1:B:19:DT:H3’	1:B:19:DT:H6	2	0.65
(5,213)	1:A:18:DG:H5”	1:A:18:DG:H8	6	0.65
(5,213)	1:A:18:DG:H5”	1:B:18:DG:H8	6	0.65
(5,213)	1:B:18:DG:H5”	1:A:18:DG:H8	6	0.65
(5,213)	1:B:18:DG:H5”	1:B:18:DG:H8	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,53)	1:A:14:DT:H4'	1:A:15:DA:H8	2	0.65
(4,53)	1:A:14:DT:H4'	1:B:15:DA:H8	2	0.65
(4,53)	1:B:14:DT:H4'	1:A:15:DA:H8	2	0.65
(4,53)	1:B:14:DT:H4'	1:B:15:DA:H8	2	0.65
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3'	1	0.63
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3'	1	0.63
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3'	1	0.63
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3'	1	0.63
(4,49)	1:A:14:DT:H1'	1:A:15:DA:H8	8	0.63
(4,49)	1:A:14:DT:H1'	1:B:15:DA:H8	8	0.63
(4,49)	1:B:14:DT:H1'	1:A:15:DA:H8	8	0.63
(4,49)	1:B:14:DT:H1'	1:B:15:DA:H8	8	0.63
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5"	4	0.63
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5"	4	0.63
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5"	4	0.63
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5"	4	0.63
(5,38)	1:A:19:DT:H3'	1:A:19:DT:H6	4	0.62
(5,38)	1:A:19:DT:H3'	1:B:19:DT:H6	4	0.62
(5,38)	1:B:19:DT:H3'	1:A:19:DT:H6	4	0.62
(5,38)	1:B:19:DT:H3'	1:B:19:DT:H6	4	0.62
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5"	2	0.62
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5"	2	0.62
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5"	2	0.62
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5"	2	0.62
(5,25)	1:A:8:DT:H3'	1:A:8:DT:H6	3	0.61
(5,25)	1:A:8:DT:H3'	1:B:8:DT:H6	3	0.61
(5,25)	1:B:8:DT:H3'	1:A:8:DT:H6	3	0.61
(5,25)	1:B:8:DT:H3'	1:B:8:DT:H6	3	0.61
(4,89)	1:A:26:DA:H2	1:A:13:DT:H3'	10	0.6
(4,89)	1:A:26:DA:H2	1:B:13:DT:H3'	10	0.6
(4,89)	1:B:26:DA:H2	1:A:13:DT:H3'	10	0.6
(4,89)	1:B:26:DA:H2	1:B:13:DT:H3'	10	0.6
(4,60)	1:A:15:DA:H2"	1:A:16:DG:H1	9	0.6
(4,60)	1:A:15:DA:H2"	1:B:16:DG:H1	9	0.6
(4,60)	1:B:15:DA:H2"	1:A:16:DG:H1	9	0.6
(4,60)	1:B:15:DA:H2"	1:B:16:DG:H1	9	0.6
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5"	6	0.6
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5"	6	0.6
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5"	6	0.6
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5"	6	0.6
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5"	9	0.6
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5"	9	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5”	9	0.6
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5”	9	0.6
(2,113)	2:A:101:9F0:H26	1:A:8:DT:H2’	1	0.59
(2,113)	2:A:101:9F0:H26	1:B:8:DT:H2’	1	0.59
(2,113)	2:B:101:9F0:H26	1:A:8:DT:H2’	1	0.59
(2,113)	2:B:101:9F0:H26	1:B:8:DT:H2’	1	0.59
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	6	0.58
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	6	0.58
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	6	0.58
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	6	0.58
(4,18)	1:A:8:DT:H2”	1:A:9:DA:H8	5	0.58
(4,18)	1:A:8:DT:H2”	1:B:9:DA:H8	5	0.58
(4,18)	1:B:8:DT:H2”	1:A:9:DA:H8	5	0.58
(4,18)	1:B:8:DT:H2”	1:B:9:DA:H8	5	0.58
(4,18)	1:A:8:DT:H2”	1:A:9:DA:H8	4	0.57
(4,18)	1:A:8:DT:H2”	1:B:9:DA:H8	4	0.57
(4,18)	1:B:8:DT:H2”	1:A:9:DA:H8	4	0.57
(4,18)	1:B:8:DT:H2”	1:B:9:DA:H8	4	0.57
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5”	1	0.56
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5”	1	0.56
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5”	1	0.56
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5”	1	0.56
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2”	3	0.56
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2”	3	0.56
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2”	3	0.56
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2”	3	0.56
(4,60)	1:A:15:DA:H2”	1:A:16:DG:H1	2	0.55
(4,60)	1:A:15:DA:H2”	1:B:16:DG:H1	2	0.55
(4,60)	1:B:15:DA:H2”	1:A:16:DG:H1	2	0.55
(4,60)	1:B:15:DA:H2”	1:B:16:DG:H1	2	0.55
(4,53)	1:A:14:DT:H4’	1:A:15:DA:H8	3	0.55
(4,53)	1:A:14:DT:H4’	1:B:15:DA:H8	3	0.55
(4,53)	1:B:14:DT:H4’	1:A:15:DA:H8	3	0.55
(4,53)	1:B:14:DT:H4’	1:B:15:DA:H8	3	0.55
(4,24)	1:A:20:DT:H6	1:A:21:DA:H8	6	0.55
(4,24)	1:A:20:DT:H6	1:B:21:DA:H8	6	0.55
(4,24)	1:B:20:DT:H6	1:A:21:DA:H8	6	0.55
(4,24)	1:B:20:DT:H6	1:B:21:DA:H8	6	0.55
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5”	8	0.55
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5”	8	0.55
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5”	8	0.55
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5”	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5”	10	0.54
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5”	10	0.54
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5”	10	0.54
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5”	10	0.54
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	7	0.54
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	7	0.54
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	7	0.54
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	7	0.54
(4,67)	1:A:25:DA:H2’	1:A:26:DA:H8	6	0.53
(4,67)	1:A:25:DA:H2’	1:B:26:DA:H8	6	0.53
(4,67)	1:B:25:DA:H2’	1:A:26:DA:H8	6	0.53
(4,67)	1:B:25:DA:H2’	1:B:26:DA:H8	6	0.53
(4,67)	1:A:25:DA:H2’	1:A:26:DA:H8	7	0.53
(4,67)	1:A:25:DA:H2’	1:B:26:DA:H8	7	0.53
(4,67)	1:B:25:DA:H2’	1:A:26:DA:H8	7	0.53
(4,67)	1:B:25:DA:H2’	1:B:26:DA:H8	7	0.53
(4,64)	1:A:15:DA:H4’	1:A:16:DG:H1’	1	0.53
(4,64)	1:A:15:DA:H4’	1:B:16:DG:H1’	1	0.53
(4,64)	1:B:15:DA:H4’	1:A:16:DG:H1’	1	0.53
(4,64)	1:B:15:DA:H4’	1:B:16:DG:H1’	1	0.53
(4,64)	1:A:15:DA:H4’	1:A:16:DG:H1’	3	0.53
(4,64)	1:A:15:DA:H4’	1:B:16:DG:H1’	3	0.53
(4,64)	1:B:15:DA:H4’	1:A:16:DG:H1’	3	0.53
(4,64)	1:B:15:DA:H4’	1:B:16:DG:H1’	3	0.53
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5”	3	0.53
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5”	3	0.53
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5”	3	0.53
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5”	3	0.53
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5”	5	0.53
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5”	5	0.53
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5”	5	0.53
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5”	5	0.53
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	5	0.53
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	5	0.53
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	5	0.53
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	5	0.53
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	2	0.53
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	2	0.53
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	2	0.53
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	2	0.53
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	10	0.53
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	10	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	10	0.53
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	10	0.53
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	8	0.53
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	8	0.53
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	8	0.53
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	8	0.53
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	9	0.53
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	9	0.53
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	9	0.53
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	9	0.53
(5,25)	1:A:8:DT:H3’	1:A:8:DT:H6	2	0.52
(5,25)	1:A:8:DT:H3’	1:B:8:DT:H6	2	0.52
(5,25)	1:B:8:DT:H3’	1:A:8:DT:H6	2	0.52
(5,25)	1:B:8:DT:H3’	1:B:8:DT:H6	2	0.52
(4,67)	1:A:25:DA:H2’	1:A:26:DA:H8	5	0.52
(4,67)	1:A:25:DA:H2’	1:B:26:DA:H8	5	0.52
(4,67)	1:B:25:DA:H2’	1:A:26:DA:H8	5	0.52
(4,67)	1:B:25:DA:H2’	1:B:26:DA:H8	5	0.52
(4,49)	1:A:14:DT:H1’	1:A:15:DA:H8	9	0.52
(4,49)	1:A:14:DT:H1’	1:B:15:DA:H8	9	0.52
(4,49)	1:B:14:DT:H1’	1:A:15:DA:H8	9	0.52
(4,49)	1:B:14:DT:H1’	1:B:15:DA:H8	9	0.52
(4,49)	1:A:14:DT:H1’	1:A:15:DA:H8	10	0.52
(4,49)	1:A:14:DT:H1’	1:B:15:DA:H8	10	0.52
(4,49)	1:B:14:DT:H1’	1:A:15:DA:H8	10	0.52
(4,49)	1:B:14:DT:H1’	1:B:15:DA:H8	10	0.52
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1’	2	0.52
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1’	2	0.52
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1’	2	0.52
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1’	2	0.52
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1’	5	0.52
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1’	5	0.52
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1’	5	0.52
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1’	5	0.52
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	1	0.52
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	1	0.52
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	1	0.52
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	1	0.52
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	10	0.52
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	10	0.52
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	10	0.52
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	2	0.52
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	2	0.52
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	2	0.52
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	2	0.52
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	1	0.52
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	1	0.52
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	1	0.52
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	1	0.52
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	5	0.52
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	5	0.52
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	5	0.52
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	5	0.52
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	1	0.52
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	1	0.52
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	1	0.52
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	1	0.52
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	10	0.52
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	10	0.52
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	10	0.52
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	10	0.52
(2,112)	2:A:101:9F0:H26	1:A:8:DT:H1'	10	0.52
(2,112)	2:A:101:9F0:H26	1:B:8:DT:H1'	10	0.52
(2,112)	2:B:101:9F0:H26	1:A:8:DT:H1'	10	0.52
(2,112)	2:B:101:9F0:H26	1:B:8:DT:H1'	10	0.52
(4,24)	1:A:20:DT:H6	1:A:21:DA:H8	9	0.51
(4,24)	1:A:20:DT:H6	1:B:21:DA:H8	9	0.51
(4,24)	1:B:20:DT:H6	1:A:21:DA:H8	9	0.51
(4,24)	1:B:20:DT:H6	1:B:21:DA:H8	9	0.51
(4,18)	1:A:8:DT:H2"	1:A:9:DA:H8	3	0.51
(4,18)	1:A:8:DT:H2"	1:B:9:DA:H8	3	0.51
(4,18)	1:B:8:DT:H2"	1:A:9:DA:H8	3	0.51
(4,18)	1:B:8:DT:H2"	1:B:9:DA:H8	3	0.51
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	7	0.51
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	7	0.51
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	7	0.51
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	7	0.51
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	9	0.51
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	9	0.51
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	9	0.51
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	9	0.51
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	7	0.51
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	7	0.51
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	7	0.51
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	9	0.51
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	9	0.51
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	9	0.51
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	9	0.51
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	4	0.51
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	4	0.51
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	4	0.51
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	4	0.51
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	7	0.51
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	7	0.51
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	7	0.51
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	7	0.51
(5,38)	1:A:19:DT:H3'	1:A:19:DT:H6	5	0.5
(5,38)	1:A:19:DT:H3'	1:B:19:DT:H6	5	0.5
(5,38)	1:B:19:DT:H3'	1:A:19:DT:H6	5	0.5
(5,38)	1:B:19:DT:H3'	1:B:19:DT:H6	5	0.5
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	2	0.5
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	2	0.5
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	2	0.5
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	2	0.5
(4,67)	1:A:25:DA:H2'	1:A:26:DA:H8	2	0.5
(4,67)	1:A:25:DA:H2'	1:B:26:DA:H8	2	0.5
(4,67)	1:B:25:DA:H2'	1:A:26:DA:H8	2	0.5
(4,67)	1:B:25:DA:H2'	1:B:26:DA:H8	2	0.5
(4,67)	1:A:25:DA:H2'	1:A:26:DA:H8	10	0.5
(4,67)	1:A:25:DA:H2'	1:B:26:DA:H8	10	0.5
(4,67)	1:B:25:DA:H2'	1:A:26:DA:H8	10	0.5
(4,67)	1:B:25:DA:H2'	1:B:26:DA:H8	10	0.5
(4,60)	1:A:15:DA:H2"	1:A:16:DG:H1	10	0.5
(4,60)	1:A:15:DA:H2"	1:B:16:DG:H1	10	0.5
(4,60)	1:B:15:DA:H2"	1:A:16:DG:H1	10	0.5
(4,60)	1:B:15:DA:H2"	1:B:16:DG:H1	10	0.5
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	2	0.5
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	2	0.5
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	2	0.5
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	2	0.5
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	4	0.5
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	4	0.5
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	4	0.5
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,59)	2:A:101:9F0:H37	1:A:3:DA:H3'	8	0.5
(2,59)	2:A:101:9F0:H37	1:B:3:DA:H3'	8	0.5
(2,59)	2:B:101:9F0:H37	1:A:3:DA:H3'	8	0.5
(2,59)	2:B:101:9F0:H37	1:B:3:DA:H3'	8	0.5
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	3	0.5
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	3	0.5
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	3	0.5
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	3	0.5
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	6	0.5
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	6	0.5
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	6	0.5
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	6	0.5
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	2	0.5
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	2	0.5
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	2	0.5
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	2	0.5
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	6	0.5
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	6	0.5
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	6	0.5
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	6	0.5
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	4	0.5
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	4	0.5
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	4	0.5
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	4	0.5
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	5	0.5
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	5	0.5
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	5	0.5
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	5	0.5
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	6	0.5
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	6	0.5
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	6	0.5
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	6	0.5
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	8	0.5
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	8	0.5
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	8	0.5
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	8	0.5
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	2	0.5
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	2	0.5
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	2	0.5
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	2	0.5
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	2	0.49
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	2	0.49
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	2	0.49
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	7	0.49
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	7	0.49
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	7	0.49
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	7	0.49
(4,67)	1:A:25:DA:H2'	1:A:26:DA:H8	9	0.49
(4,67)	1:A:25:DA:H2'	1:B:26:DA:H8	9	0.49
(4,67)	1:B:25:DA:H2'	1:A:26:DA:H8	9	0.49
(4,67)	1:B:25:DA:H2'	1:B:26:DA:H8	9	0.49
(4,49)	1:A:14:DT:H1'	1:A:15:DA:H8	1	0.49
(4,49)	1:A:14:DT:H1'	1:B:15:DA:H8	1	0.49
(4,49)	1:B:14:DT:H1'	1:A:15:DA:H8	1	0.49
(4,49)	1:B:14:DT:H1'	1:B:15:DA:H8	1	0.49
(4,2)	1:A:1:DA:H8	1:A:2:DA:H2	9	0.49
(4,2)	1:A:1:DA:H8	1:B:2:DA:H2	9	0.49
(4,2)	1:B:1:DA:H8	1:A:2:DA:H2	9	0.49
(4,2)	1:B:1:DA:H8	1:B:2:DA:H2	9	0.49
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	2	0.49
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	2	0.49
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	2	0.49
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	2	0.49
(2,59)	2:A:101:9F0:H37	1:A:3:DA:H3'	9	0.49
(2,59)	2:A:101:9F0:H37	1:B:3:DA:H3'	9	0.49
(2,59)	2:B:101:9F0:H37	1:A:3:DA:H3'	9	0.49
(2,59)	2:B:101:9F0:H37	1:B:3:DA:H3'	9	0.49
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	2	0.49
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	2	0.49
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	2	0.49
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	2	0.49
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	5	0.49
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	5	0.49
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	5	0.49
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	5	0.49
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	10	0.49
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	10	0.49
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	10	0.49
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	10	0.49
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1'	3	0.49
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1'	3	0.49
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1'	3	0.49
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1'	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1'	7	0.49
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1'	7	0.49
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1'	7	0.49
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1'	7	0.49
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	4	0.49
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	4	0.49
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	4	0.49
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	4	0.49
(2,149)	2:A:102:9F0:H32	1:A:25:DA:H8	3	0.49
(2,149)	2:A:102:9F0:H32	1:B:25:DA:H8	3	0.49
(2,149)	2:B:102:9F0:H32	1:A:25:DA:H8	3	0.49
(2,149)	2:B:102:9F0:H32	1:B:25:DA:H8	3	0.49
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	6	0.49
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	6	0.49
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	6	0.49
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	6	0.49
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	3	0.49
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	3	0.49
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	3	0.49
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	3	0.49
(2,112)	2:A:101:9F0:H26	1:A:8:DT:H1'	7	0.49
(2,112)	2:A:101:9F0:H26	1:B:8:DT:H1'	7	0.49
(2,112)	2:B:101:9F0:H26	1:A:8:DT:H1'	7	0.49
(2,112)	2:B:101:9F0:H26	1:B:8:DT:H1'	7	0.49
(6,32)	2:A:102:9F0:H47	2:A:102:9F0:H31	8	0.48
(6,32)	2:A:102:9F0:H47	2:B:102:9F0:H31	8	0.48
(6,32)	2:B:102:9F0:H47	2:A:102:9F0:H31	8	0.48
(6,32)	2:B:102:9F0:H47	2:B:102:9F0:H31	8	0.48
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	6	0.48
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	6	0.48
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	6	0.48
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	6	0.48
(4,67)	1:A:25:DA:H2'	1:A:26:DA:H8	1	0.48
(4,67)	1:A:25:DA:H2'	1:B:26:DA:H8	1	0.48
(4,67)	1:B:25:DA:H2'	1:A:26:DA:H8	1	0.48
(4,67)	1:B:25:DA:H2'	1:B:26:DA:H8	1	0.48
(4,67)	1:A:25:DA:H2'	1:A:26:DA:H8	3	0.48
(4,67)	1:A:25:DA:H2'	1:B:26:DA:H8	3	0.48
(4,67)	1:B:25:DA:H2'	1:A:26:DA:H8	3	0.48
(4,67)	1:B:25:DA:H2'	1:B:26:DA:H8	3	0.48
(4,67)	1:A:25:DA:H2'	1:A:26:DA:H8	8	0.48
(4,67)	1:A:25:DA:H2'	1:B:26:DA:H8	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,67)	1:B:25:DA:H2'	1:A:26:DA:H8	8	0.48
(4,67)	1:B:25:DA:H2'	1:B:26:DA:H8	8	0.48
(4,23)	1:A:19:DT:H3'	1:A:21:DA:H8	2	0.48
(4,23)	1:A:19:DT:H3'	1:B:21:DA:H8	2	0.48
(4,23)	1:B:19:DT:H3'	1:A:21:DA:H8	2	0.48
(4,23)	1:B:19:DT:H3'	1:B:21:DA:H8	2	0.48
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	5	0.48
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	5	0.48
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	5	0.48
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	5	0.48
(2,70)	2:A:101:9F0:H34	1:A:22:DG:H5"	7	0.48
(2,70)	2:A:101:9F0:H34	1:B:22:DG:H5"	7	0.48
(2,70)	2:B:101:9F0:H34	1:A:22:DG:H5"	7	0.48
(2,70)	2:B:101:9F0:H34	1:B:22:DG:H5"	7	0.48
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1'	6	0.48
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1'	6	0.48
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1'	6	0.48
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1'	6	0.48
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	3	0.48
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	3	0.48
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	3	0.48
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	3	0.48
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	4	0.48
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	4	0.48
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	4	0.48
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	4	0.48
(2,118)	2:A:101:9F0:H45	1:A:8:DT:H2"	4	0.48
(2,118)	2:A:101:9F0:H45	1:B:8:DT:H2"	4	0.48
(2,118)	2:B:101:9F0:H45	1:A:8:DT:H2"	4	0.48
(2,118)	2:B:101:9F0:H45	1:B:8:DT:H2"	4	0.48
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	4	0.47
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	4	0.47
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	4	0.47
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	4	0.47
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	4	0.47
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	4	0.47
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	4	0.47
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	4	0.47
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	6	0.47
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	6	0.47
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	6	0.47
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:A:21:DA:H2	1:A:10:DG:H1	2	0.47
(4,34)	1:A:21:DA:H2	1:B:10:DG:H1	2	0.47
(4,34)	1:B:21:DA:H2	1:A:10:DG:H1	2	0.47
(4,34)	1:B:21:DA:H2	1:B:10:DG:H1	2	0.47
(4,34)	1:A:21:DA:H2	1:A:10:DG:H1	4	0.47
(4,34)	1:A:21:DA:H2	1:B:10:DG:H1	4	0.47
(4,34)	1:B:21:DA:H2	1:A:10:DG:H1	4	0.47
(4,34)	1:B:21:DA:H2	1:B:10:DG:H1	4	0.47
(4,2)	1:A:1:DA:H8	1:A:2:DA:H2	4	0.47
(4,2)	1:A:1:DA:H8	1:B:2:DA:H2	4	0.47
(4,2)	1:B:1:DA:H8	1:A:2:DA:H2	4	0.47
(4,2)	1:B:1:DA:H8	1:B:2:DA:H2	4	0.47
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	4	0.47
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	4	0.47
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	4	0.47
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	4	0.47
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	4	0.47
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	4	0.47
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	4	0.47
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	4	0.47
(2,59)	2:A:101:9F0:H37	1:A:3:DA:H3'	6	0.47
(2,59)	2:A:101:9F0:H37	1:B:3:DA:H3'	6	0.47
(2,59)	2:B:101:9F0:H37	1:A:3:DA:H3'	6	0.47
(2,59)	2:B:101:9F0:H37	1:B:3:DA:H3'	6	0.47
(2,59)	2:A:101:9F0:H37	1:A:3:DA:H3'	10	0.47
(2,59)	2:A:101:9F0:H37	1:B:3:DA:H3'	10	0.47
(2,59)	2:B:101:9F0:H37	1:A:3:DA:H3'	10	0.47
(2,59)	2:B:101:9F0:H37	1:B:3:DA:H3'	10	0.47
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	1	0.47
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	1	0.47
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	1	0.47
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	1	0.47
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	4	0.47
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	4	0.47
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	4	0.47
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	4	0.47
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	9	0.47
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	9	0.47
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	9	0.47
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	9	0.47
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1'	4	0.47
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1'	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1'	4	0.47
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1'	4	0.47
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	4	0.47
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	4	0.47
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	4	0.47
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	4	0.47
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	5	0.47
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	5	0.47
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	5	0.47
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	5	0.47
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	6	0.47
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	6	0.47
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	6	0.47
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	6	0.47
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	7	0.47
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	7	0.47
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	7	0.47
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	7	0.47
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	2	0.47
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	2	0.47
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	2	0.47
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	2	0.47
(2,112)	2:A:101:9F0:H26	1:A:8:DT:H1'	9	0.47
(2,112)	2:A:101:9F0:H26	1:B:8:DT:H1'	9	0.47
(2,112)	2:B:101:9F0:H26	1:A:8:DT:H1'	9	0.47
(2,112)	2:B:101:9F0:H26	1:B:8:DT:H1'	9	0.47
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	5	0.46
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	5	0.46
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	5	0.46
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	5	0.46
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	7	0.46
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	7	0.46
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	7	0.46
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	7	0.46
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	9	0.46
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	9	0.46
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	9	0.46
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	9	0.46
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	10	0.46
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	10	0.46
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	10	0.46
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	4	0.46
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	4	0.46
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	4	0.46
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	4	0.46
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	3	0.46
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	3	0.46
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	3	0.46
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	3	0.46
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	9	0.46
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	9	0.46
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	9	0.46
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	9	0.46
(4,67)	1:A:25:DA:H2'	1:A:26:DA:H8	4	0.46
(4,67)	1:A:25:DA:H2'	1:B:26:DA:H8	4	0.46
(4,67)	1:B:25:DA:H2'	1:A:26:DA:H8	4	0.46
(4,67)	1:B:25:DA:H2'	1:B:26:DA:H8	4	0.46
(4,53)	1:A:14:DT:H4'	1:A:15:DA:H8	7	0.46
(4,53)	1:A:14:DT:H4'	1:B:15:DA:H8	7	0.46
(4,53)	1:B:14:DT:H4'	1:A:15:DA:H8	7	0.46
(4,53)	1:B:14:DT:H4'	1:B:15:DA:H8	7	0.46
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	9	0.46
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	9	0.46
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	9	0.46
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	9	0.46
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	4	0.46
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	4	0.46
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	4	0.46
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	4	0.46
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	5	0.46
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	5	0.46
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	5	0.46
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	5	0.46
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	6	0.46
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	6	0.46
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	6	0.46
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	6	0.46
(2,1)	2:A:101:9F0:H14	1:A:3:DA:H2	6	0.46
(2,1)	2:A:101:9F0:H14	1:B:3:DA:H2	6	0.46
(2,1)	2:B:101:9F0:H14	1:A:3:DA:H2	6	0.46
(2,1)	2:B:101:9F0:H14	1:B:3:DA:H2	6	0.46
(2,1)	2:A:101:9F0:H14	1:A:3:DA:H2	7	0.46
(2,1)	2:A:101:9F0:H14	1:B:3:DA:H2	7	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	2:B:101:9F0:H14	1:A:3:DA:H2	7	0.46
(2,1)	2:B:101:9F0:H14	1:B:3:DA:H2	7	0.46
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	1	0.45
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	1	0.45
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	1	0.45
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	1	0.45
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2"	1	0.45
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2"	1	0.45
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2"	1	0.45
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2"	1	0.45
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2"	10	0.45
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2"	10	0.45
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2"	10	0.45
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2"	10	0.45
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	5	0.45
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	5	0.45
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	5	0.45
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	5	0.45
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	3	0.45
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	3	0.45
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	3	0.45
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	3	0.45
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	5	0.45
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	5	0.45
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	5	0.45
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	5	0.45
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	10	0.45
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	10	0.45
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	10	0.45
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	10	0.45
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	3	0.45
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	3	0.45
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	3	0.45
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	3	0.45
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	2	0.45
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	2	0.45
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	2	0.45
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	2	0.45
(2,59)	2:A:101:9F0:H37	1:A:3:DA:H3'	7	0.45
(2,59)	2:A:101:9F0:H37	1:B:3:DA:H3'	7	0.45
(2,59)	2:B:101:9F0:H37	1:A:3:DA:H3'	7	0.45
(2,59)	2:B:101:9F0:H37	1:B:3:DA:H3'	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	2	0.45
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	2	0.45
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	2	0.45
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	2	0.45
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	7	0.45
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	7	0.45
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	7	0.45
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	7	0.45
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	10	0.45
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	10	0.45
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	10	0.45
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	10	0.45
(2,187)	2:A:102:9F0:H33	1:A:13:DT:H6	8	0.45
(2,187)	2:A:102:9F0:H33	1:B:13:DT:H6	8	0.45
(2,187)	2:B:102:9F0:H33	1:A:13:DT:H6	8	0.45
(2,187)	2:B:102:9F0:H33	1:B:13:DT:H6	8	0.45
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	4	0.45
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	4	0.45
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	4	0.45
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	4	0.45
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	5	0.45
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	5	0.45
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	5	0.45
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	5	0.45
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	6	0.45
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	6	0.45
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	6	0.45
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	6	0.45
(2,112)	2:A:101:9F0:H26	1:A:8:DT:H1'	8	0.45
(2,112)	2:A:101:9F0:H26	1:B:8:DT:H1'	8	0.45
(2,112)	2:B:101:9F0:H26	1:A:8:DT:H1'	8	0.45
(2,112)	2:B:101:9F0:H26	1:B:8:DT:H1'	8	0.45
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	3	0.44
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	3	0.44
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	3	0.44
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	3	0.44
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	6	0.44
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	6	0.44
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	6	0.44
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	6	0.44
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	8	0.44
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	8	0.44
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	8	0.44
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	10	0.44
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	10	0.44
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	10	0.44
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	10	0.44
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	7	0.44
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	7	0.44
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	7	0.44
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	7	0.44
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	4	0.44
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	4	0.44
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	4	0.44
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	4	0.44
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	3	0.44
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	3	0.44
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	3	0.44
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	3	0.44
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	10	0.44
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	10	0.44
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	10	0.44
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	10	0.44
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	10	0.44
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	10	0.44
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	10	0.44
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	10	0.44
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	10	0.44
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	10	0.44
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	10	0.44
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	10	0.44
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	1	0.44
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	1	0.44
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	1	0.44
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	1	0.44
(2,1)	2:A:101:9F0:H14	1:A:3:DA:H2	9	0.44
(2,1)	2:A:101:9F0:H14	1:B:3:DA:H2	9	0.44
(2,1)	2:B:101:9F0:H14	1:A:3:DA:H2	9	0.44
(2,1)	2:B:101:9F0:H14	1:B:3:DA:H2	9	0.44
(6,31)	2:A:102:9F0:H92	2:A:102:9F0:H29	8	0.43
(6,31)	2:A:102:9F0:H92	2:B:102:9F0:H29	8	0.43
(6,31)	2:B:102:9F0:H92	2:A:102:9F0:H29	8	0.43
(6,31)	2:B:102:9F0:H92	2:B:102:9F0:H29	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,237)	1:A:23:DG:H5"	1:A:23:DG:H8	8	0.43
(5,237)	1:A:23:DG:H5"	1:B:23:DG:H8	8	0.43
(5,237)	1:B:23:DG:H5"	1:A:23:DG:H8	8	0.43
(5,237)	1:B:23:DG:H5"	1:B:23:DG:H8	8	0.43
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	2	0.43
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	2	0.43
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	2	0.43
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	2	0.43
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2"	3	0.43
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2"	3	0.43
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2"	3	0.43
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2"	3	0.43
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	1	0.43
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	1	0.43
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	1	0.43
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	1	0.43
(4,74)	1:A:26:DA:H2	1:A:13:DT:C5	7	0.43
(4,74)	1:A:26:DA:H2	1:B:13:DT:C5	7	0.43
(4,74)	1:B:26:DA:H2	1:A:13:DT:C5	7	0.43
(4,74)	1:B:26:DA:H2	1:B:13:DT:C5	7	0.43
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	4	0.43
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	4	0.43
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	4	0.43
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	4	0.43
(4,53)	1:A:14:DT:H4'	1:A:15:DA:H8	6	0.43
(4,53)	1:A:14:DT:H4'	1:B:15:DA:H8	6	0.43
(4,53)	1:B:14:DT:H4'	1:A:15:DA:H8	6	0.43
(4,53)	1:B:14:DT:H4'	1:B:15:DA:H8	6	0.43
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	5	0.43
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	5	0.43
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	5	0.43
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	5	0.43
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	6	0.43
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	6	0.43
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	6	0.43
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	6	0.43
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	9	0.43
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	9	0.43
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	9	0.43
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	9	0.43
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1'	9	0.43
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1'	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1'	9	0.43
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1'	9	0.43
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	8	0.43
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	8	0.43
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	8	0.43
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	8	0.43
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	2	0.43
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	2	0.43
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	2	0.43
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	2	0.43
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	7	0.43
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	7	0.43
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	7	0.43
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	7	0.43
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	9	0.43
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	9	0.43
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	9	0.43
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	9	0.43
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	2	0.43
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	2	0.43
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	2	0.43
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	2	0.43
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	3	0.43
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	3	0.43
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	3	0.43
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	3	0.43
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	4	0.43
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	4	0.43
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	4	0.43
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	4	0.43
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2"	7	0.42
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2"	7	0.42
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2"	7	0.42
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2"	7	0.42
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2"	9	0.42
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2"	9	0.42
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2"	9	0.42
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2"	9	0.42
(4,60)	1:A:15:DA:H2"	1:A:16:DG:H1	1	0.42
(4,60)	1:A:15:DA:H2"	1:B:16:DG:H1	1	0.42
(4,60)	1:B:15:DA:H2"	1:A:16:DG:H1	1	0.42
(4,60)	1:B:15:DA:H2"	1:B:16:DG:H1	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	2	0.42
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	2	0.42
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	2	0.42
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	2	0.42
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	1	0.42
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	1	0.42
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	1	0.42
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	1	0.42
(3,1)	2:A:102:9F0:H33	1:A:15:DA:N6	9	0.42
(3,1)	2:A:102:9F0:H33	1:B:15:DA:N6	9	0.42
(3,1)	2:B:102:9F0:H33	1:A:15:DA:N6	9	0.42
(3,1)	2:B:102:9F0:H33	1:B:15:DA:N6	9	0.42
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	3	0.42
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	3	0.42
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	3	0.42
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	3	0.42
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1'	2	0.42
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1'	2	0.42
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1'	2	0.42
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1'	2	0.42
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1'	5	0.42
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1'	5	0.42
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1'	5	0.42
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1'	5	0.42
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	1	0.42
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	1	0.42
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	1	0.42
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	1	0.42
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1'	1	0.42
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1'	1	0.42
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1'	1	0.42
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1'	1	0.42
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1'	10	0.42
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1'	10	0.42
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1'	10	0.42
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1'	10	0.42
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	6	0.42
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	6	0.42
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	6	0.42
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	6	0.42
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	5	0.42
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	5	0.42
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	5	0.42
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	8	0.42
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	8	0.42
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	8	0.42
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	8	0.42
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	9	0.42
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	9	0.42
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	9	0.42
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	9	0.42
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	10	0.42
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	10	0.42
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	10	0.42
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	10	0.42
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	2	0.41
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	2	0.41
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	2	0.41
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	2	0.41
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	3	0.41
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	3	0.41
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	3	0.41
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	3	0.41
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2”	8	0.41
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2”	8	0.41
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2”	8	0.41
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2”	8	0.41
(4,61)	1:A:15:DA:H2”	1:A:16:DG:H8	6	0.41
(4,61)	1:A:15:DA:H2”	1:B:16:DG:H8	6	0.41
(4,61)	1:B:15:DA:H2”	1:A:16:DG:H8	6	0.41
(4,61)	1:B:15:DA:H2”	1:B:16:DG:H8	6	0.41
(4,23)	1:A:19:DT:H3’	1:A:21:DA:H8	5	0.41
(4,23)	1:A:19:DT:H3’	1:B:21:DA:H8	5	0.41
(4,23)	1:B:19:DT:H3’	1:A:21:DA:H8	5	0.41
(4,23)	1:B:19:DT:H3’	1:B:21:DA:H8	5	0.41
(2,96)	2:A:101:9F0:H6	1:A:9:DA:H3’	1	0.41
(2,96)	2:A:101:9F0:H6	1:B:9:DA:H3’	1	0.41
(2,96)	2:B:101:9F0:H6	1:A:9:DA:H3’	1	0.41
(2,96)	2:B:101:9F0:H6	1:B:9:DA:H3’	1	0.41
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1’	1	0.41
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1’	1	0.41
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1’	1	0.41
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1’	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1'	4	0.41
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1'	4	0.41
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1'	4	0.41
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1'	4	0.41
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	4	0.41
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	4	0.41
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	4	0.41
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	4	0.41
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	7	0.41
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	7	0.41
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	7	0.41
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	7	0.41
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	5	0.41
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	5	0.41
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	5	0.41
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	5	0.41
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	2	0.41
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	2	0.41
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	2	0.41
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	2	0.41
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	9	0.41
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	9	0.41
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	9	0.41
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	9	0.41
(2,138)	2:A:102:9F0:H32	1:A:24:DG:H8	7	0.41
(2,138)	2:A:102:9F0:H32	1:B:24:DG:H8	7	0.41
(2,138)	2:B:102:9F0:H32	1:A:24:DG:H8	7	0.41
(2,138)	2:B:102:9F0:H32	1:B:24:DG:H8	7	0.41
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	1	0.41
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	1	0.41
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	1	0.41
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	1	0.41
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	3	0.41
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	3	0.41
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	3	0.41
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	3	0.41
(2,114)	2:A:101:9F0:H26	1:A:8:DT:H2"	2	0.41
(2,114)	2:A:101:9F0:H26	1:B:8:DT:H2"	2	0.41
(2,114)	2:B:101:9F0:H26	1:A:8:DT:H2"	2	0.41
(2,114)	2:B:101:9F0:H26	1:B:8:DT:H2"	2	0.41
(2,1)	2:A:101:9F0:H14	1:A:3:DA:H2	1	0.41
(2,1)	2:A:101:9F0:H14	1:B:3:DA:H2	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	2:B:101:9F0:H14	1:A:3:DA:H2	1	0.41
(2,1)	2:B:101:9F0:H14	1:B:3:DA:H2	1	0.41
(2,1)	2:A:101:9F0:H14	1:A:3:DA:H2	8	0.41
(2,1)	2:A:101:9F0:H14	1:B:3:DA:H2	8	0.41
(2,1)	2:B:101:9F0:H14	1:A:3:DA:H2	8	0.41
(2,1)	2:B:101:9F0:H14	1:B:3:DA:H2	8	0.41
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	4	0.4
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	4	0.4
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	4	0.4
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	4	0.4
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	6	0.4
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	6	0.4
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	6	0.4
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	6	0.4
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	1	0.4
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	1	0.4
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	1	0.4
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	1	0.4
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	8	0.4
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	8	0.4
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	8	0.4
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	8	0.4
(3,1)	2:A:102:9F0:H33	1:A:15:DA:N6	3	0.4
(3,1)	2:A:102:9F0:H33	1:B:15:DA:N6	3	0.4
(3,1)	2:B:102:9F0:H33	1:A:15:DA:N6	3	0.4
(3,1)	2:B:102:9F0:H33	1:B:15:DA:N6	3	0.4
(3,1)	2:A:102:9F0:H33	1:A:15:DA:N6	4	0.4
(3,1)	2:A:102:9F0:H33	1:B:15:DA:N6	4	0.4
(3,1)	2:B:102:9F0:H33	1:A:15:DA:N6	4	0.4
(3,1)	2:B:102:9F0:H33	1:B:15:DA:N6	4	0.4
(2,4)	2:A:101:9F0:H14	1:A:9:DA:H2'	4	0.4
(2,4)	2:A:101:9F0:H14	1:B:9:DA:H2'	4	0.4
(2,4)	2:B:101:9F0:H14	1:A:9:DA:H2'	4	0.4
(2,4)	2:B:101:9F0:H14	1:B:9:DA:H2'	4	0.4
(2,4)	2:A:101:9F0:H14	1:A:9:DA:H2'	9	0.4
(2,4)	2:A:101:9F0:H14	1:B:9:DA:H2'	9	0.4
(2,4)	2:B:101:9F0:H14	1:A:9:DA:H2'	9	0.4
(2,4)	2:B:101:9F0:H14	1:B:9:DA:H2'	9	0.4
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1'	3	0.4
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1'	3	0.4
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1'	3	0.4
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1'	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1'	6	0.4
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1'	6	0.4
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1'	6	0.4
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1'	6	0.4
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1'	10	0.4
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1'	10	0.4
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1'	10	0.4
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1'	10	0.4
(2,193)	2:A:102:9F0:H34	1:A:13:DT:H6	8	0.4
(2,193)	2:A:102:9F0:H34	1:B:13:DT:H6	8	0.4
(2,193)	2:B:102:9F0:H34	1:A:13:DT:H6	8	0.4
(2,193)	2:B:102:9F0:H34	1:B:13:DT:H6	8	0.4
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	3	0.4
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	3	0.4
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	3	0.4
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	3	0.4
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	6	0.4
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	6	0.4
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	6	0.4
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	6	0.4
(2,104)	2:A:101:9F0:H27	1:A:8:DT:H2'	6	0.4
(2,104)	2:A:101:9F0:H27	1:B:8:DT:H2'	6	0.4
(2,104)	2:B:101:9F0:H27	1:A:8:DT:H2'	6	0.4
(2,104)	2:B:101:9F0:H27	1:B:8:DT:H2'	6	0.4
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	8	0.39
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	8	0.39
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	8	0.39
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	8	0.39
(5,83)	1:A:15:DA:H3'	1:A:15:DA:H8	9	0.39
(5,83)	1:A:15:DA:H3'	1:B:15:DA:H8	9	0.39
(5,83)	1:B:15:DA:H3'	1:A:15:DA:H8	9	0.39
(5,83)	1:B:15:DA:H3'	1:B:15:DA:H8	9	0.39
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2"	2	0.39
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2"	2	0.39
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2"	2	0.39
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2"	2	0.39
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	1	0.39
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	1	0.39
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	1	0.39
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	1	0.39
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	2	0.39
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	2	0.39
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	2	0.39
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	9	0.39
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	9	0.39
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	9	0.39
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	9	0.39
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1'	9	0.39
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1'	9	0.39
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1'	9	0.39
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1'	9	0.39
(2,205)	2:A:102:9F0:H5	1:A:25:DA:H2	8	0.39
(2,205)	2:A:102:9F0:H5	1:B:25:DA:H2	8	0.39
(2,205)	2:B:102:9F0:H5	1:A:25:DA:H2	8	0.39
(2,205)	2:B:102:9F0:H5	1:B:25:DA:H2	8	0.39
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	9	0.39
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	9	0.39
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	9	0.39
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	9	0.39
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	6	0.39
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	6	0.39
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	6	0.39
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	6	0.39
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	7	0.39
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	7	0.39
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	7	0.39
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	7	0.39
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	6	0.39
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	6	0.39
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	6	0.39
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	6	0.39
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	8	0.39
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	8	0.39
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	8	0.39
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	8	0.39
(6,39)	2:A:102:9F0:H41	2:A:102:9F0:H34	8	0.38
(6,39)	2:A:102:9F0:H41	2:B:102:9F0:H34	8	0.38
(6,39)	2:B:102:9F0:H41	2:A:102:9F0:H34	8	0.38
(6,39)	2:B:102:9F0:H41	2:B:102:9F0:H34	8	0.38
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	5	0.38
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	5	0.38
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	5	0.38
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	7	0.38
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	7	0.38
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	7	0.38
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	7	0.38
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	9	0.38
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	9	0.38
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	9	0.38
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	9	0.38
(6,24)	2:A:101:9F0:H43	2:A:101:9F0:H24	10	0.38
(6,24)	2:A:101:9F0:H43	2:B:101:9F0:H24	10	0.38
(6,24)	2:B:101:9F0:H43	2:A:101:9F0:H24	10	0.38
(6,24)	2:B:101:9F0:H43	2:B:101:9F0:H24	10	0.38
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	2	0.38
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	2	0.38
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	2	0.38
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	2	0.38
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	3	0.38
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	3	0.38
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	3	0.38
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	3	0.38
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	4	0.38
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	4	0.38
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	4	0.38
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	4	0.38
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	10	0.38
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	10	0.38
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	10	0.38
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	10	0.38
(4,34)	1:A:21:DA:H2	1:A:10:DG:H1	5	0.38
(4,34)	1:A:21:DA:H2	1:B:10:DG:H1	5	0.38
(4,34)	1:B:21:DA:H2	1:A:10:DG:H1	5	0.38
(4,34)	1:B:21:DA:H2	1:B:10:DG:H1	5	0.38
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	4	0.38
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	4	0.38
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	4	0.38
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	4	0.38
(3,1)	2:A:102:9F0:H33	1:A:15:DA:N6	5	0.38
(3,1)	2:A:102:9F0:H33	1:B:15:DA:N6	5	0.38
(3,1)	2:B:102:9F0:H33	1:A:15:DA:N6	5	0.38
(3,1)	2:B:102:9F0:H33	1:B:15:DA:N6	5	0.38
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	1	0.38
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	1	0.38
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	1	0.38
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1'	7	0.38
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1'	7	0.38
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1'	7	0.38
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1'	7	0.38
(2,189)	2:A:102:9F0:H33	1:A:13:DT:H1'	8	0.38
(2,189)	2:A:102:9F0:H33	1:B:13:DT:H1'	8	0.38
(2,189)	2:B:102:9F0:H33	1:A:13:DT:H1'	8	0.38
(2,189)	2:B:102:9F0:H33	1:B:13:DT:H1'	8	0.38
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	10	0.38
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	10	0.38
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	10	0.38
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	10	0.38
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	1	0.38
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	1	0.38
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	1	0.38
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	1	0.38
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	5	0.38
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	5	0.38
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	5	0.38
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	5	0.38
(2,118)	2:A:101:9F0:H45	1:A:8:DT:H2"	3	0.38
(2,118)	2:A:101:9F0:H45	1:B:8:DT:H2"	3	0.38
(2,118)	2:B:101:9F0:H45	1:A:8:DT:H2"	3	0.38
(2,118)	2:B:101:9F0:H45	1:B:8:DT:H2"	3	0.38
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2"	2	0.38
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2"	2	0.38
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2"	2	0.38
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2"	2	0.38
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	5	0.38
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	5	0.38
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	5	0.38
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	5	0.38
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	9	0.38
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	9	0.38
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	9	0.38
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	9	0.38
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	6	0.37
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	6	0.37
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	6	0.37
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,83)	1:A:15:DA:H3'	1:A:15:DA:H8	7	0.37
(5,83)	1:A:15:DA:H3'	1:B:15:DA:H8	7	0.37
(5,83)	1:B:15:DA:H3'	1:A:15:DA:H8	7	0.37
(5,83)	1:B:15:DA:H3'	1:B:15:DA:H8	7	0.37
(5,20)	1:A:3:DA:H4'	1:A:3:DA:H1'	1	0.37
(5,20)	1:A:3:DA:H4'	1:B:3:DA:H1'	1	0.37
(5,20)	1:B:3:DA:H4'	1:A:3:DA:H1'	1	0.37
(5,20)	1:B:3:DA:H4'	1:B:3:DA:H1'	1	0.37
(5,20)	1:A:3:DA:H4'	1:A:3:DA:H1'	2	0.37
(5,20)	1:A:3:DA:H4'	1:B:3:DA:H1'	2	0.37
(5,20)	1:B:3:DA:H4'	1:A:3:DA:H1'	2	0.37
(5,20)	1:B:3:DA:H4'	1:B:3:DA:H1'	2	0.37
(5,20)	1:A:3:DA:H4'	1:A:3:DA:H1'	3	0.37
(5,20)	1:A:3:DA:H4'	1:B:3:DA:H1'	3	0.37
(5,20)	1:B:3:DA:H4'	1:A:3:DA:H1'	3	0.37
(5,20)	1:B:3:DA:H4'	1:B:3:DA:H1'	3	0.37
(5,20)	1:A:3:DA:H4'	1:A:3:DA:H1'	5	0.37
(5,20)	1:A:3:DA:H4'	1:B:3:DA:H1'	5	0.37
(5,20)	1:B:3:DA:H4'	1:A:3:DA:H1'	5	0.37
(5,20)	1:B:3:DA:H4'	1:B:3:DA:H1'	5	0.37
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	5	0.37
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	5	0.37
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	5	0.37
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	5	0.37
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	10	0.37
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	10	0.37
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	10	0.37
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	10	0.37
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	1	0.37
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	1	0.37
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	1	0.37
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	1	0.37
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	2	0.37
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	2	0.37
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	2	0.37
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	2	0.37
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2"	6	0.37
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2"	6	0.37
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2"	6	0.37
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2"	6	0.37
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	9	0.37
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	9	0.37
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	9	0.37
(4,53)	1:A:14:DT:H4'	1:A:15:DA:H8	1	0.37
(4,53)	1:A:14:DT:H4'	1:B:15:DA:H8	1	0.37
(4,53)	1:B:14:DT:H4'	1:A:15:DA:H8	1	0.37
(4,53)	1:B:14:DT:H4'	1:B:15:DA:H8	1	0.37
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	10	0.37
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	10	0.37
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	10	0.37
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	10	0.37
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	8	0.37
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	8	0.37
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	8	0.37
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	8	0.37
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	7	0.37
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	7	0.37
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	7	0.37
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	7	0.37
(2,96)	2:A:101:9F0:H6	1:A:9:DA:H3'	3	0.37
(2,96)	2:A:101:9F0:H6	1:B:9:DA:H3'	3	0.37
(2,96)	2:B:101:9F0:H6	1:A:9:DA:H3'	3	0.37
(2,96)	2:B:101:9F0:H6	1:B:9:DA:H3'	3	0.37
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	6	0.37
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	6	0.37
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	6	0.37
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	6	0.37
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	8	0.37
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	8	0.37
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	8	0.37
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	8	0.37
(2,47)	2:A:101:9F0:H19	1:A:21:DA:H2	10	0.37
(2,47)	2:A:101:9F0:H19	1:B:21:DA:H2	10	0.37
(2,47)	2:B:101:9F0:H19	1:A:21:DA:H2	10	0.37
(2,47)	2:B:101:9F0:H19	1:B:21:DA:H2	10	0.37
(2,4)	2:A:101:9F0:H14	1:A:9:DA:H2'	8	0.37
(2,4)	2:A:101:9F0:H14	1:B:9:DA:H2'	8	0.37
(2,4)	2:B:101:9F0:H14	1:A:9:DA:H2'	8	0.37
(2,4)	2:B:101:9F0:H14	1:B:9:DA:H2'	8	0.37
(2,4)	2:A:101:9F0:H14	1:A:9:DA:H2'	10	0.37
(2,4)	2:A:101:9F0:H14	1:B:9:DA:H2'	10	0.37
(2,4)	2:B:101:9F0:H14	1:A:9:DA:H2'	10	0.37
(2,4)	2:B:101:9F0:H14	1:B:9:DA:H2'	10	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	7	0.37
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	7	0.37
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	7	0.37
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	7	0.37
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	1	0.37
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	1	0.37
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	1	0.37
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	1	0.37
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	6	0.37
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	6	0.37
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	6	0.37
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	6	0.37
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	1	0.37
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	1	0.37
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	1	0.37
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	1	0.37
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	8	0.37
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	8	0.37
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	8	0.37
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	8	0.37
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	9	0.37
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	9	0.37
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	9	0.37
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	9	0.37
(2,1)	2:A:101:9F0:H14	1:A:3:DA:H2	5	0.37
(2,1)	2:A:101:9F0:H14	1:B:3:DA:H2	5	0.37
(2,1)	2:B:101:9F0:H14	1:A:3:DA:H2	5	0.37
(2,1)	2:B:101:9F0:H14	1:B:3:DA:H2	5	0.37
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	1	0.37
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	1	0.37
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	1	0.37
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	1	0.37
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	3	0.37
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	3	0.37
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	3	0.37
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	3	0.37
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	4	0.37
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	4	0.37
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	4	0.37
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	4	0.37
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	6	0.37
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	6	0.37
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	6	0.37
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	7	0.37
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	7	0.37
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	7	0.37
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	7	0.37
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	10	0.37
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	10	0.37
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	10	0.37
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	10	0.37
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	8	0.36
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	8	0.36
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	8	0.36
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	8	0.36
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	1	0.36
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	1	0.36
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	1	0.36
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	1	0.36
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	3	0.36
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	3	0.36
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	3	0.36
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	3	0.36
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	10	0.36
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	10	0.36
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	10	0.36
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	10	0.36
(4,170)	1:A:17:DG:H2"	1:A:18:DG:H1'	9	0.36
(4,170)	1:A:17:DG:H2"	1:B:18:DG:H1'	9	0.36
(4,170)	1:B:17:DG:H2"	1:A:18:DG:H1'	9	0.36
(4,170)	1:B:17:DG:H2"	1:B:18:DG:H1'	9	0.36
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	2	0.36
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	2	0.36
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	2	0.36
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	2	0.36
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	6	0.36
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	6	0.36
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	6	0.36
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	6	0.36
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	7	0.36
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	7	0.36
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	7	0.36
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,128)	1:A:6:DG:H1	1:A:12:DG:H8	3	0.36
(4,128)	1:A:6:DG:H1	1:B:12:DG:H8	3	0.36
(4,128)	1:B:6:DG:H1	1:A:12:DG:H8	3	0.36
(4,128)	1:B:6:DG:H1	1:B:12:DG:H8	3	0.36
(2,96)	2:A:101:9F0:H6	1:A:9:DA:H3'	4	0.36
(2,96)	2:A:101:9F0:H6	1:B:9:DA:H3'	4	0.36
(2,96)	2:B:101:9F0:H6	1:A:9:DA:H3'	4	0.36
(2,96)	2:B:101:9F0:H6	1:B:9:DA:H3'	4	0.36
(2,4)	2:A:101:9F0:H14	1:A:9:DA:H2'	7	0.36
(2,4)	2:A:101:9F0:H14	1:B:9:DA:H2'	7	0.36
(2,4)	2:B:101:9F0:H14	1:A:9:DA:H2'	7	0.36
(2,4)	2:B:101:9F0:H14	1:B:9:DA:H2'	7	0.36
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	8	0.36
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	8	0.36
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	8	0.36
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	8	0.36
(2,184)	2:A:102:9F0:H37	1:A:6:DG:H2'	8	0.36
(2,184)	2:A:102:9F0:H37	1:B:6:DG:H2'	8	0.36
(2,184)	2:B:102:9F0:H37	1:A:6:DG:H2'	8	0.36
(2,184)	2:B:102:9F0:H37	1:B:6:DG:H2'	8	0.36
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	3	0.36
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	3	0.36
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	3	0.36
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	3	0.36
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	5	0.36
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	5	0.36
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	5	0.36
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	5	0.36
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	4	0.36
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	4	0.36
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	4	0.36
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	4	0.36
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	1	0.36
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	1	0.36
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	1	0.36
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	1	0.36
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	3	0.36
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	3	0.36
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	3	0.36
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	3	0.36
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	9	0.36
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	9	0.36
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	9	0.36
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	2	0.36
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	2	0.36
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	2	0.36
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	2	0.36
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	3	0.36
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	3	0.36
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	3	0.36
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	3	0.36
(2,120)	2:A:102:9F0:H14	1:A:24:DG:H1	7	0.36
(2,120)	2:A:102:9F0:H14	1:B:24:DG:H1	7	0.36
(2,120)	2:B:102:9F0:H14	1:A:24:DG:H1	7	0.36
(2,120)	2:B:102:9F0:H14	1:B:24:DG:H1	7	0.36
(2,112)	2:A:101:9F0:H26	1:A:8:DT:H1'	6	0.36
(2,112)	2:A:101:9F0:H26	1:B:8:DT:H1'	6	0.36
(2,112)	2:B:101:9F0:H26	1:A:8:DT:H1'	6	0.36
(2,112)	2:B:101:9F0:H26	1:B:8:DT:H1'	6	0.36
(2,1)	2:A:101:9F0:H14	1:A:3:DA:H2	10	0.36
(2,1)	2:A:101:9F0:H14	1:B:3:DA:H2	10	0.36
(2,1)	2:B:101:9F0:H14	1:A:3:DA:H2	10	0.36
(2,1)	2:B:101:9F0:H14	1:B:3:DA:H2	10	0.36
(1,4)	1:A:13:DT:O2	1:A:25:DA:N6	2	0.36
(1,4)	1:A:13:DT:O2	1:B:25:DA:N6	2	0.36
(1,4)	1:B:13:DT:O2	1:A:25:DA:N6	2	0.36
(1,4)	1:B:13:DT:O2	1:B:25:DA:N6	2	0.36
(6,39)	2:A:102:9F0:H41	2:A:102:9F0:H34	1	0.35
(6,39)	2:A:102:9F0:H41	2:B:102:9F0:H34	1	0.35
(6,39)	2:B:102:9F0:H41	2:A:102:9F0:H34	1	0.35
(6,39)	2:B:102:9F0:H41	2:B:102:9F0:H34	1	0.35
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	5	0.35
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	5	0.35
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	5	0.35
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	5	0.35
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	7	0.35
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	7	0.35
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	7	0.35
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	7	0.35
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	9	0.35
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	9	0.35
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	9	0.35
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,23)	2:A:101:9F0:H90	2:A:101:9F0:H26	10	0.35
(6,23)	2:A:101:9F0:H90	2:B:101:9F0:H26	10	0.35
(6,23)	2:B:101:9F0:H90	2:A:101:9F0:H26	10	0.35
(6,23)	2:B:101:9F0:H90	2:B:101:9F0:H26	10	0.35
(5,20)	1:A:3:DA:H4'	1:A:3:DA:H1'	4	0.35
(5,20)	1:A:3:DA:H4'	1:B:3:DA:H1'	4	0.35
(5,20)	1:B:3:DA:H4'	1:A:3:DA:H1'	4	0.35
(5,20)	1:B:3:DA:H4'	1:B:3:DA:H1'	4	0.35
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	5	0.35
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	5	0.35
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	5	0.35
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	5	0.35
(4,97)	1:A:26:DA:H8	1:A:14:DT:H3'	3	0.35
(4,97)	1:A:26:DA:H8	1:B:14:DT:H3'	3	0.35
(4,97)	1:B:26:DA:H8	1:A:14:DT:H3'	3	0.35
(4,97)	1:B:26:DA:H8	1:B:14:DT:H3'	3	0.35
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	3	0.35
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	3	0.35
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	3	0.35
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	3	0.35
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	4	0.35
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	4	0.35
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	4	0.35
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	4	0.35
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	6	0.35
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	6	0.35
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	6	0.35
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	6	0.35
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	7	0.35
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	7	0.35
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	7	0.35
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	7	0.35
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	9	0.35
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	9	0.35
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	9	0.35
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	9	0.35
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2"	5	0.35
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2"	5	0.35
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2"	5	0.35
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2"	5	0.35
(4,34)	1:A:21:DA:H2	1:A:10:DG:H1	8	0.35
(4,34)	1:A:21:DA:H2	1:B:10:DG:H1	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:B:21:DA:H2	1:A:10:DG:H1	8	0.35
(4,34)	1:B:21:DA:H2	1:B:10:DG:H1	8	0.35
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	6	0.35
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	6	0.35
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	6	0.35
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	6	0.35
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	9	0.35
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	9	0.35
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	9	0.35
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	9	0.35
(4,24)	1:A:20:DT:H6	1:A:21:DA:H8	10	0.35
(4,24)	1:A:20:DT:H6	1:B:21:DA:H8	10	0.35
(4,24)	1:B:20:DT:H6	1:A:21:DA:H8	10	0.35
(4,24)	1:B:20:DT:H6	1:B:21:DA:H8	10	0.35
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	8	0.35
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	8	0.35
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	8	0.35
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	8	0.35
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	2	0.35
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	2	0.35
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	2	0.35
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	2	0.35
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	4	0.35
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	4	0.35
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	4	0.35
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	4	0.35
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	5	0.35
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	5	0.35
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	5	0.35
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	5	0.35
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	8	0.35
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	8	0.35
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	8	0.35
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	8	0.35
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	9	0.35
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	9	0.35
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	9	0.35
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	9	0.35
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	10	0.35
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	10	0.35
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	10	0.35
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	6	0.35
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	6	0.35
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	6	0.35
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	6	0.35
(3,1)	2:A:102:9F0:H33	1:A:15:DA:N6	8	0.35
(3,1)	2:A:102:9F0:H33	1:B:15:DA:N6	8	0.35
(3,1)	2:B:102:9F0:H33	1:A:15:DA:N6	8	0.35
(3,1)	2:B:102:9F0:H33	1:B:15:DA:N6	8	0.35
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	5	0.35
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	5	0.35
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	5	0.35
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	5	0.35
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	10	0.35
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	10	0.35
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	10	0.35
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	10	0.35
(2,207)	2:A:102:9F0:H5	1:A:25:DA:H1'	8	0.35
(2,207)	2:A:102:9F0:H5	1:B:25:DA:H1'	8	0.35
(2,207)	2:B:102:9F0:H5	1:A:25:DA:H1'	8	0.35
(2,207)	2:B:102:9F0:H5	1:B:25:DA:H1'	8	0.35
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	1	0.35
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	1	0.35
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	1	0.35
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	1	0.35
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	3	0.35
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	3	0.35
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	3	0.35
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	3	0.35
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	5	0.35
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	5	0.35
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	5	0.35
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	5	0.35
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	6	0.35
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	6	0.35
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	6	0.35
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	6	0.35
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	3	0.35
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	3	0.35
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	3	0.35
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	3	0.35
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	10	0.35
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	10	0.35
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	10	0.35
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	2	0.35
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	2	0.35
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	2	0.35
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	2	0.35
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	3	0.34
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	3	0.34
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	3	0.34
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	3	0.34
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	7	0.34
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	7	0.34
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	7	0.34
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	7	0.34
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	8	0.34
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	8	0.34
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	8	0.34
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	8	0.34
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	5	0.34
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	5	0.34
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	5	0.34
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	5	0.34
(4,9)	1:A:2:DA:H2'	1:A:3:DA:H8	8	0.34
(4,9)	1:A:2:DA:H2'	1:B:3:DA:H8	8	0.34
(4,9)	1:B:2:DA:H2'	1:A:3:DA:H8	8	0.34
(4,9)	1:B:2:DA:H2'	1:B:3:DA:H8	8	0.34
(4,53)	1:A:14:DT:H4'	1:A:15:DA:H8	10	0.34
(4,53)	1:A:14:DT:H4'	1:B:15:DA:H8	10	0.34
(4,53)	1:B:14:DT:H4'	1:A:15:DA:H8	10	0.34
(4,53)	1:B:14:DT:H4'	1:B:15:DA:H8	10	0.34
(4,34)	1:A:21:DA:H2	1:A:10:DG:H1	1	0.34
(4,34)	1:A:21:DA:H2	1:B:10:DG:H1	1	0.34
(4,34)	1:B:21:DA:H2	1:A:10:DG:H1	1	0.34
(4,34)	1:B:21:DA:H2	1:B:10:DG:H1	1	0.34
(4,34)	1:A:21:DA:H2	1:A:10:DG:H1	3	0.34
(4,34)	1:A:21:DA:H2	1:B:10:DG:H1	3	0.34
(4,34)	1:B:21:DA:H2	1:A:10:DG:H1	3	0.34
(4,34)	1:B:21:DA:H2	1:B:10:DG:H1	3	0.34
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	3	0.34
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	3	0.34
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	3	0.34
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	8	0.34
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	8	0.34
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	8	0.34
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	8	0.34
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	1	0.34
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	1	0.34
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	1	0.34
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	1	0.34
(4,142)	1:A:5:DG:H2'	1:A:6:DG:H8	3	0.34
(4,142)	1:A:5:DG:H2'	1:B:6:DG:H8	3	0.34
(4,142)	1:B:5:DG:H2'	1:A:6:DG:H8	3	0.34
(4,142)	1:B:5:DG:H2'	1:B:6:DG:H8	3	0.34
(4,120)	1:A:4:DG:H1	1:A:22:DG:H8	2	0.34
(4,120)	1:A:4:DG:H1	1:B:22:DG:H8	2	0.34
(4,120)	1:B:4:DG:H1	1:A:22:DG:H8	2	0.34
(4,120)	1:B:4:DG:H1	1:B:22:DG:H8	2	0.34
(4,120)	1:A:4:DG:H1	1:A:22:DG:H8	4	0.34
(4,120)	1:A:4:DG:H1	1:B:22:DG:H8	4	0.34
(4,120)	1:B:4:DG:H1	1:A:22:DG:H8	4	0.34
(4,120)	1:B:4:DG:H1	1:B:22:DG:H8	4	0.34
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	9	0.34
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	9	0.34
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	9	0.34
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	9	0.34
(2,47)	2:A:101:9F0:H19	1:A:21:DA:H2	7	0.34
(2,47)	2:A:101:9F0:H19	1:B:21:DA:H2	7	0.34
(2,47)	2:B:101:9F0:H19	1:A:21:DA:H2	7	0.34
(2,47)	2:B:101:9F0:H19	1:B:21:DA:H2	7	0.34
(2,47)	2:A:101:9F0:H19	1:A:21:DA:H2	9	0.34
(2,47)	2:A:101:9F0:H19	1:B:21:DA:H2	9	0.34
(2,47)	2:B:101:9F0:H19	1:A:21:DA:H2	9	0.34
(2,47)	2:B:101:9F0:H19	1:B:21:DA:H2	9	0.34
(2,4)	2:A:101:9F0:H14	1:A:9:DA:H2'	6	0.34
(2,4)	2:A:101:9F0:H14	1:B:9:DA:H2'	6	0.34
(2,4)	2:B:101:9F0:H14	1:A:9:DA:H2'	6	0.34
(2,4)	2:B:101:9F0:H14	1:B:9:DA:H2'	6	0.34
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	2	0.34
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	2	0.34
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	2	0.34
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	2	0.34
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	8	0.34
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	8	0.34
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	8	0.34
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	2	0.34
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	2	0.34
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	2	0.34
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	2	0.34
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	8	0.34
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	8	0.34
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	8	0.34
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	8	0.34
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	1	0.34
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	1	0.34
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	1	0.34
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	1	0.34
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	10	0.34
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	10	0.34
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	10	0.34
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	10	0.34
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	3	0.34
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	3	0.34
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	3	0.34
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	3	0.34
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	7	0.34
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	7	0.34
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	7	0.34
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	7	0.34
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	9	0.34
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	9	0.34
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	9	0.34
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	9	0.34
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	4	0.34
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	4	0.34
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	4	0.34
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	4	0.34
(2,13)	2:A:101:9F0:H13	1:A:9:DA:H3'	7	0.34
(2,13)	2:A:101:9F0:H13	1:B:9:DA:H3'	7	0.34
(2,13)	2:B:101:9F0:H13	1:A:9:DA:H3'	7	0.34
(2,13)	2:B:101:9F0:H13	1:B:9:DA:H3'	7	0.34
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	3	0.34
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	3	0.34
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	3	0.34
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	4	0.34
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	4	0.34
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	4	0.34
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	4	0.34
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	1	0.33
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	1	0.33
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	1	0.33
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	1	0.33
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	2	0.33
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	2	0.33
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	2	0.33
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	2	0.33
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	8	0.33
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	8	0.33
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	8	0.33
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	8	0.33
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	9	0.33
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	9	0.33
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	9	0.33
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	9	0.33
(4,60)	1:A:15:DA:H2"	1:A:16:DG:H1	8	0.33
(4,60)	1:A:15:DA:H2"	1:B:16:DG:H1	8	0.33
(4,60)	1:B:15:DA:H2"	1:A:16:DG:H1	8	0.33
(4,60)	1:B:15:DA:H2"	1:B:16:DG:H1	8	0.33
(4,34)	1:A:21:DA:H2	1:A:10:DG:H1	6	0.33
(4,34)	1:A:21:DA:H2	1:B:10:DG:H1	6	0.33
(4,34)	1:B:21:DA:H2	1:A:10:DG:H1	6	0.33
(4,34)	1:B:21:DA:H2	1:B:10:DG:H1	6	0.33
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	1	0.33
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	1	0.33
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	1	0.33
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	1	0.33
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	2	0.33
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	2	0.33
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	2	0.33
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	2	0.33
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	4	0.33
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	4	0.33
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	4	0.33
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	4	0.33
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	10	0.33
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	10	0.33
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	10	0.33
(4,24)	1:A:20:DT:H6	1:A:21:DA:H8	2	0.33
(4,24)	1:A:20:DT:H6	1:B:21:DA:H8	2	0.33
(4,24)	1:B:20:DT:H6	1:A:21:DA:H8	2	0.33
(4,24)	1:B:20:DT:H6	1:B:21:DA:H8	2	0.33
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	3	0.33
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	3	0.33
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	3	0.33
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	3	0.33
(2,58)	2:A:101:9F0:H37	1:A:3:DA:H2'	2	0.33
(2,58)	2:A:101:9F0:H37	1:B:3:DA:H2'	2	0.33
(2,58)	2:B:101:9F0:H37	1:A:3:DA:H2'	2	0.33
(2,58)	2:B:101:9F0:H37	1:B:3:DA:H2'	2	0.33
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	10	0.33
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	10	0.33
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	10	0.33
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	10	0.33
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	3	0.33
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	3	0.33
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	3	0.33
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	3	0.33
(2,13)	2:A:101:9F0:H13	1:A:9:DA:H3'	8	0.33
(2,13)	2:A:101:9F0:H13	1:B:9:DA:H3'	8	0.33
(2,13)	2:B:101:9F0:H13	1:A:9:DA:H3'	8	0.33
(2,13)	2:B:101:9F0:H13	1:B:9:DA:H3'	8	0.33
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	6	0.33
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	6	0.33
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	6	0.33
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	6	0.33
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	7	0.33
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	7	0.33
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	7	0.33
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	7	0.33
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	4	0.33
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	4	0.33
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	4	0.33
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	4	0.33
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	7	0.33
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	7	0.33
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	7	0.33
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	2	0.33
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	2	0.33
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	2	0.33
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	2	0.33
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	5	0.33
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	5	0.33
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	5	0.33
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	5	0.33
(5,71)	1:A:14:DT:H2'	1:A:14:DT:H6	5	0.32
(5,71)	1:A:14:DT:H2'	1:B:14:DT:H6	5	0.32
(5,71)	1:B:14:DT:H2'	1:A:14:DT:H6	5	0.32
(5,71)	1:B:14:DT:H2'	1:B:14:DT:H6	5	0.32
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	2	0.32
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	2	0.32
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	2	0.32
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	2	0.32
(4,53)	1:A:14:DT:H4'	1:A:15:DA:H8	9	0.32
(4,53)	1:A:14:DT:H4'	1:B:15:DA:H8	9	0.32
(4,53)	1:B:14:DT:H4'	1:A:15:DA:H8	9	0.32
(4,53)	1:B:14:DT:H4'	1:B:15:DA:H8	9	0.32
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	5	0.32
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	5	0.32
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	5	0.32
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	5	0.32
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	9	0.32
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	9	0.32
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	9	0.32
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	9	0.32
(4,122)	1:A:18:DG:H1	1:A:10:DG:H8	10	0.32
(4,122)	1:A:18:DG:H1	1:B:10:DG:H8	10	0.32
(4,122)	1:B:18:DG:H1	1:A:10:DG:H8	10	0.32
(4,122)	1:B:18:DG:H1	1:B:10:DG:H8	10	0.32
(2,58)	2:A:101:9F0:H37	1:A:3:DA:H2'	9	0.32
(2,58)	2:A:101:9F0:H37	1:B:3:DA:H2'	9	0.32
(2,58)	2:B:101:9F0:H37	1:A:3:DA:H2'	9	0.32
(2,58)	2:B:101:9F0:H37	1:B:3:DA:H2'	9	0.32
(2,4)	2:A:101:9F0:H14	1:A:9:DA:H2'	1	0.32
(2,4)	2:A:101:9F0:H14	1:B:9:DA:H2'	1	0.32
(2,4)	2:B:101:9F0:H14	1:A:9:DA:H2'	1	0.32
(2,4)	2:B:101:9F0:H14	1:B:9:DA:H2'	1	0.32
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	4	0.32
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	4	0.32
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	4	0.32
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	1	0.32
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	1	0.32
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	1	0.32
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	1	0.32
(2,134)	2:A:102:9F0:H11	1:A:14:DT:H3	8	0.32
(2,134)	2:A:102:9F0:H11	1:B:14:DT:H3	8	0.32
(2,134)	2:B:102:9F0:H11	1:A:14:DT:H3	8	0.32
(2,134)	2:B:102:9F0:H11	1:B:14:DT:H3	8	0.32
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	5	0.32
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	5	0.32
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	5	0.32
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	5	0.32
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	2	0.32
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	2	0.32
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	2	0.32
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	2	0.32
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	2	0.32
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	2	0.32
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	2	0.32
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	2	0.32
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	10	0.32
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	10	0.32
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	10	0.32
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	10	0.32
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	1	0.32
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	1	0.32
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	1	0.32
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	1	0.32
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	6	0.32
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	6	0.32
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	6	0.32
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	6	0.32
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	7	0.32
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	7	0.32
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	7	0.32
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	7	0.32
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	8	0.32
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	8	0.32
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	8	0.32
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	3	0.31
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	3	0.31
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	3	0.31
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	3	0.31
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	4	0.31
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	4	0.31
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	4	0.31
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	4	0.31
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	5	0.31
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	5	0.31
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	5	0.31
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	5	0.31
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	6	0.31
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	6	0.31
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	6	0.31
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	6	0.31
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	10	0.31
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	10	0.31
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	10	0.31
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	10	0.31
(5,191)	1:A:17:DG:H2"	1:A:17:DG:H8	6	0.31
(5,191)	1:A:17:DG:H2"	1:B:17:DG:H8	6	0.31
(5,191)	1:B:17:DG:H2"	1:A:17:DG:H8	6	0.31
(5,191)	1:B:17:DG:H2"	1:B:17:DG:H8	6	0.31
(4,69)	1:A:25:DA:H3'	1:A:26:DA:H8	8	0.31
(4,69)	1:A:25:DA:H3'	1:B:26:DA:H8	8	0.31
(4,69)	1:B:25:DA:H3'	1:A:26:DA:H8	8	0.31
(4,69)	1:B:25:DA:H3'	1:B:26:DA:H8	8	0.31
(4,61)	1:A:15:DA:H2"	1:A:16:DG:H8	7	0.31
(4,61)	1:A:15:DA:H2"	1:B:16:DG:H8	7	0.31
(4,61)	1:B:15:DA:H2"	1:A:16:DG:H8	7	0.31
(4,61)	1:B:15:DA:H2"	1:B:16:DG:H8	7	0.31
(4,169)	1:A:17:DG:H2'	1:A:18:DG:H1'	9	0.31
(4,169)	1:A:17:DG:H2'	1:B:18:DG:H1'	9	0.31
(4,169)	1:B:17:DG:H2'	1:A:18:DG:H1'	9	0.31
(4,169)	1:B:17:DG:H2'	1:B:18:DG:H1'	9	0.31
(2,96)	2:A:101:9F0:H6	1:A:9:DA:H3'	2	0.31
(2,96)	2:A:101:9F0:H6	1:B:9:DA:H3'	2	0.31
(2,96)	2:B:101:9F0:H6	1:A:9:DA:H3'	2	0.31
(2,96)	2:B:101:9F0:H6	1:B:9:DA:H3'	2	0.31
(2,35)	2:A:101:9F0:H60	1:A:10:DG:H8	3	0.31
(2,35)	2:A:101:9F0:H60	1:B:10:DG:H8	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	2:B:101:9F0:H60	1:A:10:DG:H8	3	0.31
(2,35)	2:B:101:9F0:H60	1:B:10:DG:H8	3	0.31
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	9	0.31
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	9	0.31
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	9	0.31
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	9	0.31
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	10	0.31
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	10	0.31
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	10	0.31
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	10	0.31
(2,192)	2:A:102:9F0:H34	1:A:12:DG:H3'	2	0.31
(2,192)	2:A:102:9F0:H34	1:B:12:DG:H3'	2	0.31
(2,192)	2:B:102:9F0:H34	1:A:12:DG:H3'	2	0.31
(2,192)	2:B:102:9F0:H34	1:B:12:DG:H3'	2	0.31
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	6	0.31
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	6	0.31
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	6	0.31
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	6	0.31
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	7	0.31
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	7	0.31
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	7	0.31
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	7	0.31
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	9	0.31
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	9	0.31
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	9	0.31
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	9	0.31
(2,146)	2:A:102:9F0:H32	1:A:14:DT:C5	5	0.31
(2,146)	2:A:102:9F0:H32	1:B:14:DT:C5	5	0.31
(2,146)	2:B:102:9F0:H32	1:A:14:DT:C5	5	0.31
(2,146)	2:B:102:9F0:H32	1:B:14:DT:C5	5	0.31
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	6	0.31
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	6	0.31
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	6	0.31
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	6	0.31
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	5	0.31
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	5	0.31
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	5	0.31
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	5	0.31
(2,13)	2:A:101:9F0:H13	1:A:9:DA:H3'	9	0.31
(2,13)	2:A:101:9F0:H13	1:B:9:DA:H3'	9	0.31
(2,13)	2:B:101:9F0:H13	1:A:9:DA:H3'	9	0.31
(2,13)	2:B:101:9F0:H13	1:B:9:DA:H3'	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	2:A:101:9F0:H13	1:A:9:DA:H3'	10	0.31
(2,13)	2:A:101:9F0:H13	1:B:9:DA:H3'	10	0.31
(2,13)	2:B:101:9F0:H13	1:A:9:DA:H3'	10	0.31
(2,13)	2:B:101:9F0:H13	1:B:9:DA:H3'	10	0.31
(2,104)	2:A:101:9F0:H27	1:A:8:DT:H2'	9	0.31
(2,104)	2:A:101:9F0:H27	1:B:8:DT:H2'	9	0.31
(2,104)	2:B:101:9F0:H27	1:A:8:DT:H2'	9	0.31
(2,104)	2:B:101:9F0:H27	1:B:8:DT:H2'	9	0.31
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	4	0.31
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	4	0.31
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	4	0.31
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	4	0.31
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	5	0.31
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	5	0.31
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	5	0.31
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	5	0.31
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	6	0.31
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	6	0.31
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	6	0.31
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	6	0.31
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	9	0.31
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	9	0.31
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	9	0.31
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	9	0.31
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	10	0.31
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	10	0.31
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	10	0.31
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	10	0.31
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	9	0.3
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	9	0.3
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	9	0.3
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	9	0.3
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	5	0.3
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	5	0.3
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	5	0.3
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	5	0.3
(4,13)	1:A:3:DA:H2	1:A:9:DA:H2	4	0.3
(4,13)	1:A:3:DA:H2	1:B:9:DA:H2	4	0.3
(4,13)	1:B:3:DA:H2	1:A:9:DA:H2	4	0.3
(4,13)	1:B:3:DA:H2	1:B:9:DA:H2	4	0.3
(4,13)	1:A:3:DA:H2	1:A:9:DA:H2	6	0.3
(4,13)	1:A:3:DA:H2	1:B:9:DA:H2	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,13)	1:B:3:DA:H2	1:A:9:DA:H2	6	0.3
(4,13)	1:B:3:DA:H2	1:B:9:DA:H2	6	0.3
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	1	0.3
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	1	0.3
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	1	0.3
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	1	0.3
(2,58)	2:A:101:9F0:H37	1:A:3:DA:H2'	10	0.3
(2,58)	2:A:101:9F0:H37	1:B:3:DA:H2'	10	0.3
(2,58)	2:B:101:9F0:H37	1:A:3:DA:H2'	10	0.3
(2,58)	2:B:101:9F0:H37	1:B:3:DA:H2'	10	0.3
(2,4)	2:A:101:9F0:H14	1:A:9:DA:H2'	3	0.3
(2,4)	2:A:101:9F0:H14	1:B:9:DA:H2'	3	0.3
(2,4)	2:B:101:9F0:H14	1:A:9:DA:H2'	3	0.3
(2,4)	2:B:101:9F0:H14	1:B:9:DA:H2'	3	0.3
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	10	0.3
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	10	0.3
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	10	0.3
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	10	0.3
(2,104)	2:A:101:9F0:H27	1:A:8:DT:H2'	8	0.3
(2,104)	2:A:101:9F0:H27	1:B:8:DT:H2'	8	0.3
(2,104)	2:B:101:9F0:H27	1:A:8:DT:H2'	8	0.3
(2,104)	2:B:101:9F0:H27	1:B:8:DT:H2'	8	0.3
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	1	0.3
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	1	0.3
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	1	0.3
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	1	0.3
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	4	0.3
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	4	0.3
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	4	0.3
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	4	0.3
(1,22)	1:A:10:DG:N7	1:A:18:DG:N2	9	0.3
(1,22)	1:A:10:DG:N7	1:B:18:DG:N2	9	0.3
(1,22)	1:B:10:DG:N7	1:A:18:DG:N2	9	0.3
(1,22)	1:B:10:DG:N7	1:B:18:DG:N2	9	0.3
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	2	0.3
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	2	0.3
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	2	0.3
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	2	0.3
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	4	0.3
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	4	0.3
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	4	0.3
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,16)	2:A:101:9F0:H42	2:A:101:9F0:H34	4	0.29
(6,16)	2:A:101:9F0:H42	2:B:101:9F0:H34	4	0.29
(6,16)	2:B:101:9F0:H42	2:A:101:9F0:H34	4	0.29
(6,16)	2:B:101:9F0:H42	2:B:101:9F0:H34	4	0.29
(5,228)	1:A:23:DG:H2'	1:A:23:DG:H8	7	0.29
(5,228)	1:A:23:DG:H2'	1:B:23:DG:H8	7	0.29
(5,228)	1:B:23:DG:H2'	1:A:23:DG:H8	7	0.29
(5,228)	1:B:23:DG:H2'	1:B:23:DG:H8	7	0.29
(5,15)	1:A:3:DA:H2'	1:A:3:DA:H8	1	0.29
(5,15)	1:A:3:DA:H2'	1:B:3:DA:H8	1	0.29
(5,15)	1:B:3:DA:H2'	1:A:3:DA:H8	1	0.29
(5,15)	1:B:3:DA:H2'	1:B:3:DA:H8	1	0.29
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	2	0.29
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	2	0.29
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	2	0.29
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	2	0.29
(4,169)	1:A:17:DG:H2'	1:A:18:DG:H1'	6	0.29
(4,169)	1:A:17:DG:H2'	1:B:18:DG:H1'	6	0.29
(4,169)	1:B:17:DG:H2'	1:A:18:DG:H1'	6	0.29
(4,169)	1:B:17:DG:H2'	1:B:18:DG:H1'	6	0.29
(2,58)	2:A:101:9F0:H37	1:A:3:DA:H2'	8	0.29
(2,58)	2:A:101:9F0:H37	1:B:3:DA:H2'	8	0.29
(2,58)	2:B:101:9F0:H37	1:A:3:DA:H2'	8	0.29
(2,58)	2:B:101:9F0:H37	1:B:3:DA:H2'	8	0.29
(2,47)	2:A:101:9F0:H19	1:A:21:DA:H2	6	0.29
(2,47)	2:A:101:9F0:H19	1:B:21:DA:H2	6	0.29
(2,47)	2:B:101:9F0:H19	1:A:21:DA:H2	6	0.29
(2,47)	2:B:101:9F0:H19	1:B:21:DA:H2	6	0.29
(2,184)	2:A:102:9F0:H37	1:A:6:DG:H2'	3	0.29
(2,184)	2:A:102:9F0:H37	1:B:6:DG:H2'	3	0.29
(2,184)	2:B:102:9F0:H37	1:A:6:DG:H2'	3	0.29
(2,184)	2:B:102:9F0:H37	1:B:6:DG:H2'	3	0.29
(2,178)	2:A:102:9F0:H16	1:A:13:DT:H6	9	0.29
(2,178)	2:A:102:9F0:H16	1:B:13:DT:H6	9	0.29
(2,178)	2:B:102:9F0:H16	1:A:13:DT:H6	9	0.29
(2,178)	2:B:102:9F0:H16	1:B:13:DT:H6	9	0.29
(2,104)	2:A:101:9F0:H27	1:A:8:DT:H2'	10	0.29
(2,104)	2:A:101:9F0:H27	1:B:8:DT:H2'	10	0.29
(2,104)	2:B:101:9F0:H27	1:A:8:DT:H2'	10	0.29
(2,104)	2:B:101:9F0:H27	1:B:8:DT:H2'	10	0.29
(2,1)	2:A:101:9F0:H14	1:A:3:DA:H2	4	0.29
(2,1)	2:A:101:9F0:H14	1:B:3:DA:H2	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	2:B:101:9F0:H14	1:A:3:DA:H2	4	0.29
(2,1)	2:B:101:9F0:H14	1:B:3:DA:H2	4	0.29
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	2	0.29
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	2	0.29
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	2	0.29
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	2	0.29
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	4	0.29
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	4	0.29
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	4	0.29
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	4	0.29
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	2	0.29
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	2	0.29
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	2	0.29
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	2	0.29
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	10	0.29
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	10	0.29
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	10	0.29
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	10	0.29
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	10	0.29
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	10	0.29
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	10	0.29
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	10	0.29
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	7	0.29
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	7	0.29
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	7	0.29
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	7	0.29
(6,39)	2:A:102:9F0:H41	2:A:102:9F0:H34	9	0.28
(6,39)	2:A:102:9F0:H41	2:B:102:9F0:H34	9	0.28
(6,39)	2:B:102:9F0:H41	2:A:102:9F0:H34	9	0.28
(6,39)	2:B:102:9F0:H41	2:B:102:9F0:H34	9	0.28
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	1	0.28
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	1	0.28
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	1	0.28
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	1	0.28
(5,15)	1:A:3:DA:H2'	1:A:3:DA:H8	2	0.28
(5,15)	1:A:3:DA:H2'	1:B:3:DA:H8	2	0.28
(5,15)	1:B:3:DA:H2'	1:A:3:DA:H8	2	0.28
(5,15)	1:B:3:DA:H2'	1:B:3:DA:H8	2	0.28
(5,15)	1:A:3:DA:H2'	1:A:3:DA:H8	4	0.28
(5,15)	1:A:3:DA:H2'	1:B:3:DA:H8	4	0.28
(5,15)	1:B:3:DA:H2'	1:A:3:DA:H8	4	0.28
(5,15)	1:B:3:DA:H2'	1:B:3:DA:H8	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,12)	1:A:2:DA:H5"	1:A:2:DA:H8	4	0.28
(5,12)	1:A:2:DA:H5"	1:B:2:DA:H8	4	0.28
(5,12)	1:B:2:DA:H5"	1:A:2:DA:H8	4	0.28
(5,12)	1:B:2:DA:H5"	1:B:2:DA:H8	4	0.28
(4,97)	1:A:26:DA:H8	1:A:14:DT:H3'	4	0.28
(4,97)	1:A:26:DA:H8	1:B:14:DT:H3'	4	0.28
(4,97)	1:B:26:DA:H8	1:A:14:DT:H3'	4	0.28
(4,97)	1:B:26:DA:H8	1:B:14:DT:H3'	4	0.28
(4,23)	1:A:19:DT:H3'	1:A:21:DA:H8	3	0.28
(4,23)	1:A:19:DT:H3'	1:B:21:DA:H8	3	0.28
(4,23)	1:B:19:DT:H3'	1:A:21:DA:H8	3	0.28
(4,23)	1:B:19:DT:H3'	1:B:21:DA:H8	3	0.28
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	10	0.28
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	10	0.28
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	10	0.28
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	10	0.28
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	2	0.28
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	2	0.28
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	2	0.28
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	2	0.28
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	4	0.28
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	4	0.28
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	4	0.28
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	4	0.28
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	10	0.28
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	10	0.28
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	10	0.28
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	10	0.28
(2,58)	2:A:101:9F0:H37	1:A:3:DA:H2'	7	0.28
(2,58)	2:A:101:9F0:H37	1:B:3:DA:H2'	7	0.28
(2,58)	2:B:101:9F0:H37	1:A:3:DA:H2'	7	0.28
(2,58)	2:B:101:9F0:H37	1:B:3:DA:H2'	7	0.28
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	2	0.28
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	2	0.28
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	2	0.28
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	2	0.28
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	3	0.28
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	3	0.28
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	3	0.28
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	3	0.28
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	5	0.28
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	5	0.28
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	5	0.28
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	6	0.28
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	6	0.28
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	6	0.28
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	6	0.28
(2,145)	2:A:102:9F0:H28	1:A:14:DT:H6	8	0.28
(2,145)	2:A:102:9F0:H28	1:B:14:DT:H6	8	0.28
(2,145)	2:B:102:9F0:H28	1:A:14:DT:H6	8	0.28
(2,145)	2:B:102:9F0:H28	1:B:14:DT:H6	8	0.28
(2,104)	2:A:101:9F0:H27	1:A:8:DT:H2'	7	0.28
(2,104)	2:A:101:9F0:H27	1:B:8:DT:H2'	7	0.28
(2,104)	2:B:101:9F0:H27	1:A:8:DT:H2'	7	0.28
(2,104)	2:B:101:9F0:H27	1:B:8:DT:H2'	7	0.28
(2,1)	2:A:101:9F0:H14	1:A:3:DA:H2	3	0.28
(2,1)	2:A:101:9F0:H14	1:B:3:DA:H2	3	0.28
(2,1)	2:B:101:9F0:H14	1:A:3:DA:H2	3	0.28
(2,1)	2:B:101:9F0:H14	1:B:3:DA:H2	3	0.28
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	10	0.28
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	10	0.28
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	10	0.28
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	10	0.28
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	3	0.28
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	3	0.28
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	3	0.28
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	3	0.28
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	9	0.28
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	9	0.28
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	9	0.28
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	9	0.28
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	2	0.28
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	2	0.28
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	2	0.28
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	2	0.28
(5,83)	1:A:15:DA:H3'	1:A:15:DA:H8	5	0.27
(5,83)	1:A:15:DA:H3'	1:B:15:DA:H8	5	0.27
(5,83)	1:B:15:DA:H3'	1:A:15:DA:H8	5	0.27
(5,83)	1:B:15:DA:H3'	1:B:15:DA:H8	5	0.27
(4,82)	1:A:26:DA:H8	1:A:14:DT:H2"	4	0.27
(4,82)	1:A:26:DA:H8	1:B:14:DT:H2"	4	0.27
(4,82)	1:B:26:DA:H8	1:A:14:DT:H2"	4	0.27
(4,82)	1:B:26:DA:H8	1:B:14:DT:H2"	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	6	0.27
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	6	0.27
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	6	0.27
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	6	0.27
(4,60)	1:A:15:DA:H2"	1:A:16:DG:H1	3	0.27
(4,60)	1:A:15:DA:H2"	1:B:16:DG:H1	3	0.27
(4,60)	1:B:15:DA:H2"	1:A:16:DG:H1	3	0.27
(4,60)	1:B:15:DA:H2"	1:B:16:DG:H1	3	0.27
(4,24)	1:A:20:DT:H6	1:A:21:DA:H8	7	0.27
(4,24)	1:A:20:DT:H6	1:B:21:DA:H8	7	0.27
(4,24)	1:B:20:DT:H6	1:A:21:DA:H8	7	0.27
(4,24)	1:B:20:DT:H6	1:B:21:DA:H8	7	0.27
(4,24)	1:A:20:DT:H6	1:A:21:DA:H8	8	0.27
(4,24)	1:A:20:DT:H6	1:B:21:DA:H8	8	0.27
(4,24)	1:B:20:DT:H6	1:A:21:DA:H8	8	0.27
(4,24)	1:B:20:DT:H6	1:B:21:DA:H8	8	0.27
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	6	0.27
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	6	0.27
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	6	0.27
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	6	0.27
(3,1)	2:A:102:9F0:H33	1:A:15:DA:N6	1	0.27
(3,1)	2:A:102:9F0:H33	1:B:15:DA:N6	1	0.27
(3,1)	2:B:102:9F0:H33	1:A:15:DA:N6	1	0.27
(3,1)	2:B:102:9F0:H33	1:B:15:DA:N6	1	0.27
(2,58)	2:A:101:9F0:H37	1:A:3:DA:H2'	6	0.27
(2,58)	2:A:101:9F0:H37	1:B:3:DA:H2'	6	0.27
(2,58)	2:B:101:9F0:H37	1:A:3:DA:H2'	6	0.27
(2,58)	2:B:101:9F0:H37	1:B:3:DA:H2'	6	0.27
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	4	0.27
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	4	0.27
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	4	0.27
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	4	0.27
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	7	0.27
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	7	0.27
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	7	0.27
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	7	0.27
(2,108)	2:A:101:9F0:H27	1:A:9:DA:H2'	1	0.27
(2,108)	2:A:101:9F0:H27	1:B:9:DA:H2'	1	0.27
(2,108)	2:B:101:9F0:H27	1:A:9:DA:H2'	1	0.27
(2,108)	2:B:101:9F0:H27	1:B:9:DA:H2'	1	0.27
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	8	0.27
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	8	0.27
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	8	0.27
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	5	0.27
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	5	0.27
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	5	0.27
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	5	0.27
(1,42)	1:A:12:DG:N7	1:A:6:DG:N2	8	0.27
(1,42)	1:A:12:DG:N7	1:B:6:DG:N2	8	0.27
(1,42)	1:B:12:DG:N7	1:A:6:DG:N2	8	0.27
(1,42)	1:B:12:DG:N7	1:B:6:DG:N2	8	0.27
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	6	0.27
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	6	0.27
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	6	0.27
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	6	0.27
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	4	0.27
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	4	0.27
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	4	0.27
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	4	0.27
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	6	0.27
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	6	0.27
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	6	0.27
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	6	0.27
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	7	0.27
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	7	0.27
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	7	0.27
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	7	0.27
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	8	0.27
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	8	0.27
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	8	0.27
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	8	0.27
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	1	0.27
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	1	0.27
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	1	0.27
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	1	0.27
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	5	0.27
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	5	0.27
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	5	0.27
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	5	0.27
(6,15)	2:A:101:9F0:H41	2:A:101:9F0:H36	4	0.26
(6,15)	2:A:101:9F0:H41	2:B:101:9F0:H36	4	0.26
(6,15)	2:B:101:9F0:H41	2:A:101:9F0:H36	4	0.26
(6,15)	2:B:101:9F0:H41	2:B:101:9F0:H36	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,71)	1:A:14:DT:H2'	1:A:14:DT:H6	4	0.26
(5,71)	1:A:14:DT:H2'	1:B:14:DT:H6	4	0.26
(5,71)	1:B:14:DT:H2'	1:A:14:DT:H6	4	0.26
(5,71)	1:B:14:DT:H2'	1:B:14:DT:H6	4	0.26
(4,60)	1:A:15:DA:H2"	1:A:16:DG:H1	6	0.26
(4,60)	1:A:15:DA:H2"	1:B:16:DG:H1	6	0.26
(4,60)	1:B:15:DA:H2"	1:A:16:DG:H1	6	0.26
(4,60)	1:B:15:DA:H2"	1:B:16:DG:H1	6	0.26
(4,53)	1:A:14:DT:H4'	1:A:15:DA:H8	8	0.26
(4,53)	1:A:14:DT:H4'	1:B:15:DA:H8	8	0.26
(4,53)	1:B:14:DT:H4'	1:A:15:DA:H8	8	0.26
(4,53)	1:B:14:DT:H4'	1:B:15:DA:H8	8	0.26
(4,13)	1:A:3:DA:H2	1:A:9:DA:H2	7	0.26
(4,13)	1:A:3:DA:H2	1:B:9:DA:H2	7	0.26
(4,13)	1:B:3:DA:H2	1:A:9:DA:H2	7	0.26
(4,13)	1:B:3:DA:H2	1:B:9:DA:H2	7	0.26
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	8	0.26
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	8	0.26
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	8	0.26
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	8	0.26
(3,1)	2:A:102:9F0:H33	1:A:15:DA:N6	10	0.26
(3,1)	2:A:102:9F0:H33	1:B:15:DA:N6	10	0.26
(3,1)	2:B:102:9F0:H33	1:A:15:DA:N6	10	0.26
(3,1)	2:B:102:9F0:H33	1:B:15:DA:N6	10	0.26
(2,92)	2:A:101:9F0:H6	1:A:4:DG:H8	7	0.26
(2,92)	2:A:101:9F0:H6	1:B:4:DG:H8	7	0.26
(2,92)	2:B:101:9F0:H6	1:A:4:DG:H8	7	0.26
(2,92)	2:B:101:9F0:H6	1:B:4:DG:H8	7	0.26
(2,3)	2:A:101:9F0:H14	1:A:9:DA:H1'	3	0.26
(2,3)	2:A:101:9F0:H14	1:B:9:DA:H1'	3	0.26
(2,3)	2:B:101:9F0:H14	1:A:9:DA:H1'	3	0.26
(2,3)	2:B:101:9F0:H14	1:B:9:DA:H1'	3	0.26
(2,3)	2:A:101:9F0:H14	1:A:9:DA:H1'	4	0.26
(2,3)	2:A:101:9F0:H14	1:B:9:DA:H1'	4	0.26
(2,3)	2:B:101:9F0:H14	1:A:9:DA:H1'	4	0.26
(2,3)	2:B:101:9F0:H14	1:B:9:DA:H1'	4	0.26
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	9	0.26
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	9	0.26
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	9	0.26
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	9	0.26
(2,184)	2:A:102:9F0:H37	1:A:6:DG:H2'	1	0.26
(2,184)	2:A:102:9F0:H37	1:B:6:DG:H2'	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	2:B:102:9F0:H37	1:A:6:DG:H2'	1	0.26
(2,184)	2:B:102:9F0:H37	1:B:6:DG:H2'	1	0.26
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	5	0.26
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	5	0.26
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	5	0.26
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	5	0.26
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	9	0.26
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	9	0.26
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	9	0.26
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	9	0.26
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	10	0.26
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	10	0.26
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	10	0.26
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	10	0.26
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	3	0.26
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	3	0.26
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	3	0.26
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	3	0.26
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	5	0.26
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	5	0.26
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	5	0.26
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	5	0.26
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	8	0.26
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	8	0.26
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	8	0.26
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	8	0.26
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	9	0.26
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	9	0.26
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	9	0.26
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	9	0.26
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	10	0.26
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	10	0.26
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	10	0.26
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	10	0.26
(6,39)	2:A:102:9F0:H41	2:A:102:9F0:H34	4	0.25
(6,39)	2:A:102:9F0:H41	2:B:102:9F0:H34	4	0.25
(6,39)	2:B:102:9F0:H41	2:A:102:9F0:H34	4	0.25
(6,39)	2:B:102:9F0:H41	2:B:102:9F0:H34	4	0.25
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	4	0.25
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	4	0.25
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	4	0.25
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	7	0.25
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	7	0.25
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	7	0.25
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	7	0.25
(5,12)	1:A:2:DA:H5"	1:A:2:DA:H8	5	0.25
(5,12)	1:A:2:DA:H5"	1:B:2:DA:H8	5	0.25
(5,12)	1:B:2:DA:H5"	1:A:2:DA:H8	5	0.25
(5,12)	1:B:2:DA:H5"	1:B:2:DA:H8	5	0.25
(4,64)	1:A:15:DA:H4'	1:A:16:DG:H1'	4	0.25
(4,64)	1:A:15:DA:H4'	1:B:16:DG:H1'	4	0.25
(4,64)	1:B:15:DA:H4'	1:A:16:DG:H1'	4	0.25
(4,64)	1:B:15:DA:H4'	1:B:16:DG:H1'	4	0.25
(4,24)	1:A:20:DT:H6	1:A:21:DA:H8	3	0.25
(4,24)	1:A:20:DT:H6	1:B:21:DA:H8	3	0.25
(4,24)	1:B:20:DT:H6	1:A:21:DA:H8	3	0.25
(4,24)	1:B:20:DT:H6	1:B:21:DA:H8	3	0.25
(4,23)	1:A:19:DT:H3'	1:A:21:DA:H8	1	0.25
(4,23)	1:A:19:DT:H3'	1:B:21:DA:H8	1	0.25
(4,23)	1:B:19:DT:H3'	1:A:21:DA:H8	1	0.25
(4,23)	1:B:19:DT:H3'	1:B:21:DA:H8	1	0.25
(4,169)	1:A:17:DG:H2'	1:A:18:DG:H1'	7	0.25
(4,169)	1:A:17:DG:H2'	1:B:18:DG:H1'	7	0.25
(4,169)	1:B:17:DG:H2'	1:A:18:DG:H1'	7	0.25
(4,169)	1:B:17:DG:H2'	1:B:18:DG:H1'	7	0.25
(2,96)	2:A:101:9F0:H6	1:A:9:DA:H3'	8	0.25
(2,96)	2:A:101:9F0:H6	1:B:9:DA:H3'	8	0.25
(2,96)	2:B:101:9F0:H6	1:A:9:DA:H3'	8	0.25
(2,96)	2:B:101:9F0:H6	1:B:9:DA:H3'	8	0.25
(2,79)	2:A:101:9F0:H9	1:A:9:DA:H2	3	0.25
(2,79)	2:A:101:9F0:H9	1:B:9:DA:H2	3	0.25
(2,79)	2:B:101:9F0:H9	1:A:9:DA:H2	3	0.25
(2,79)	2:B:101:9F0:H9	1:B:9:DA:H2	3	0.25
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	1	0.25
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	1	0.25
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	1	0.25
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	1	0.25
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	10	0.25
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	10	0.25
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	10	0.25
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	10	0.25
(2,12)	2:A:101:9F0:H13	1:A:9:DA:H2"	4	0.25
(2,12)	2:A:101:9F0:H13	1:B:9:DA:H2"	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	2:B:101:9F0:H13	1:A:9:DA:H2"	4	0.25
(2,12)	2:B:101:9F0:H13	1:B:9:DA:H2"	4	0.25
(2,112)	2:A:101:9F0:H26	1:A:8:DT:H1'	5	0.25
(2,112)	2:A:101:9F0:H26	1:B:8:DT:H1'	5	0.25
(2,112)	2:B:101:9F0:H26	1:A:8:DT:H1'	5	0.25
(2,112)	2:B:101:9F0:H26	1:B:8:DT:H1'	5	0.25
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	1	0.25
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	1	0.25
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	1	0.25
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	1	0.25
(1,8)	1:A:14:DT:O2	1:A:25:DA:N6	3	0.25
(1,8)	1:A:14:DT:O2	1:B:25:DA:N6	3	0.25
(1,8)	1:B:14:DT:O2	1:A:25:DA:N6	3	0.25
(1,8)	1:B:14:DT:O2	1:B:25:DA:N6	3	0.25
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	6	0.25
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	6	0.25
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	6	0.25
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	6	0.25
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	2	0.25
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	2	0.25
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	2	0.25
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	2	0.25
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	3	0.25
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	3	0.25
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	3	0.25
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	3	0.25
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	5	0.25
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	5	0.25
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	5	0.25
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	5	0.25
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	1	0.25
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	1	0.25
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	1	0.25
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	1	0.25
(6,39)	2:A:102:9F0:H41	2:A:102:9F0:H34	7	0.24
(6,39)	2:A:102:9F0:H41	2:B:102:9F0:H34	7	0.24
(6,39)	2:B:102:9F0:H41	2:A:102:9F0:H34	7	0.24
(6,39)	2:B:102:9F0:H41	2:B:102:9F0:H34	7	0.24
(6,16)	2:A:101:9F0:H42	2:A:101:9F0:H34	2	0.24
(6,16)	2:A:101:9F0:H42	2:B:101:9F0:H34	2	0.24
(6,16)	2:B:101:9F0:H42	2:A:101:9F0:H34	2	0.24
(6,16)	2:B:101:9F0:H42	2:B:101:9F0:H34	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,83)	1:A:15:DA:H3'	1:A:15:DA:H8	1	0.24
(5,83)	1:A:15:DA:H3'	1:B:15:DA:H8	1	0.24
(5,83)	1:B:15:DA:H3'	1:A:15:DA:H8	1	0.24
(5,83)	1:B:15:DA:H3'	1:B:15:DA:H8	1	0.24
(5,15)	1:A:3:DA:H2'	1:A:3:DA:H8	3	0.24
(5,15)	1:A:3:DA:H2'	1:B:3:DA:H8	3	0.24
(5,15)	1:B:3:DA:H2'	1:A:3:DA:H8	3	0.24
(5,15)	1:B:3:DA:H2'	1:B:3:DA:H8	3	0.24
(5,12)	1:A:2:DA:H5"	1:A:2:DA:H8	2	0.24
(5,12)	1:A:2:DA:H5"	1:B:2:DA:H8	2	0.24
(5,12)	1:B:2:DA:H5"	1:A:2:DA:H8	2	0.24
(5,12)	1:B:2:DA:H5"	1:B:2:DA:H8	2	0.24
(4,97)	1:A:26:DA:H8	1:A:14:DT:H3'	2	0.24
(4,97)	1:A:26:DA:H8	1:B:14:DT:H3'	2	0.24
(4,97)	1:B:26:DA:H8	1:A:14:DT:H3'	2	0.24
(4,97)	1:B:26:DA:H8	1:B:14:DT:H3'	2	0.24
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	7	0.24
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	7	0.24
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	7	0.24
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	7	0.24
(4,61)	1:A:15:DA:H2"	1:A:16:DG:H8	5	0.24
(4,61)	1:A:15:DA:H2"	1:B:16:DG:H8	5	0.24
(4,61)	1:B:15:DA:H2"	1:A:16:DG:H8	5	0.24
(4,61)	1:B:15:DA:H2"	1:B:16:DG:H8	5	0.24
(4,60)	1:A:15:DA:H2"	1:A:16:DG:H1	7	0.24
(4,60)	1:A:15:DA:H2"	1:B:16:DG:H1	7	0.24
(4,60)	1:B:15:DA:H2"	1:A:16:DG:H1	7	0.24
(4,60)	1:B:15:DA:H2"	1:B:16:DG:H1	7	0.24
(4,34)	1:A:21:DA:H2	1:A:10:DG:H1	7	0.24
(4,34)	1:A:21:DA:H2	1:B:10:DG:H1	7	0.24
(4,34)	1:B:21:DA:H2	1:A:10:DG:H1	7	0.24
(4,34)	1:B:21:DA:H2	1:B:10:DG:H1	7	0.24
(4,34)	1:A:21:DA:H2	1:A:10:DG:H1	10	0.24
(4,34)	1:A:21:DA:H2	1:B:10:DG:H1	10	0.24
(4,34)	1:B:21:DA:H2	1:A:10:DG:H1	10	0.24
(4,34)	1:B:21:DA:H2	1:B:10:DG:H1	10	0.24
(4,169)	1:A:17:DG:H2'	1:A:18:DG:H1'	8	0.24
(4,169)	1:A:17:DG:H2'	1:B:18:DG:H1'	8	0.24
(4,169)	1:B:17:DG:H2'	1:A:18:DG:H1'	8	0.24
(4,169)	1:B:17:DG:H2'	1:B:18:DG:H1'	8	0.24
(4,169)	1:A:17:DG:H2'	1:A:18:DG:H1'	10	0.24
(4,169)	1:A:17:DG:H2'	1:B:18:DG:H1'	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,169)	1:B:17:DG:H2'	1:A:18:DG:H1'	10	0.24
(4,169)	1:B:17:DG:H2'	1:B:18:DG:H1'	10	0.24
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	3	0.24
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	3	0.24
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	3	0.24
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	3	0.24
(4,13)	1:A:3:DA:H2	1:A:9:DA:H2	8	0.24
(4,13)	1:A:3:DA:H2	1:B:9:DA:H2	8	0.24
(4,13)	1:B:3:DA:H2	1:A:9:DA:H2	8	0.24
(4,13)	1:B:3:DA:H2	1:B:9:DA:H2	8	0.24
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	6	0.24
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	6	0.24
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	6	0.24
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	6	0.24
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	7	0.24
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	7	0.24
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	7	0.24
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	7	0.24
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	9	0.24
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	9	0.24
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	9	0.24
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	9	0.24
(3,1)	2:A:102:9F0:H33	1:A:15:DA:N6	6	0.24
(3,1)	2:A:102:9F0:H33	1:B:15:DA:N6	6	0.24
(3,1)	2:B:102:9F0:H33	1:A:15:DA:N6	6	0.24
(3,1)	2:B:102:9F0:H33	1:B:15:DA:N6	6	0.24
(2,200)	2:A:102:9F0:H9	1:A:6:DG:H8	2	0.24
(2,200)	2:A:102:9F0:H9	1:B:6:DG:H8	2	0.24
(2,200)	2:B:102:9F0:H9	1:A:6:DG:H8	2	0.24
(2,200)	2:B:102:9F0:H9	1:B:6:DG:H8	2	0.24
(2,192)	2:A:102:9F0:H34	1:A:12:DG:H3'	4	0.24
(2,192)	2:A:102:9F0:H34	1:B:12:DG:H3'	4	0.24
(2,192)	2:B:102:9F0:H34	1:A:12:DG:H3'	4	0.24
(2,192)	2:B:102:9F0:H34	1:B:12:DG:H3'	4	0.24
(2,191)	2:A:102:9F0:H34	1:A:12:DG:H2'	2	0.24
(2,191)	2:A:102:9F0:H34	1:B:12:DG:H2'	2	0.24
(2,191)	2:B:102:9F0:H34	1:A:12:DG:H2'	2	0.24
(2,191)	2:B:102:9F0:H34	1:B:12:DG:H2'	2	0.24
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	7	0.24
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	7	0.24
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	7	0.24
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,190)	2:A:102:9F0:H34	1:A:12:DG:H8	8	0.24
(2,190)	2:A:102:9F0:H34	1:B:12:DG:H8	8	0.24
(2,190)	2:B:102:9F0:H34	1:A:12:DG:H8	8	0.24
(2,190)	2:B:102:9F0:H34	1:B:12:DG:H8	8	0.24
(2,184)	2:A:102:9F0:H37	1:A:6:DG:H2'	4	0.24
(2,184)	2:A:102:9F0:H37	1:B:6:DG:H2'	4	0.24
(2,184)	2:B:102:9F0:H37	1:A:6:DG:H2'	4	0.24
(2,184)	2:B:102:9F0:H37	1:B:6:DG:H2'	4	0.24
(2,13)	2:A:101:9F0:H13	1:A:9:DA:H3'	6	0.24
(2,13)	2:A:101:9F0:H13	1:B:9:DA:H3'	6	0.24
(2,13)	2:B:101:9F0:H13	1:A:9:DA:H3'	6	0.24
(2,13)	2:B:101:9F0:H13	1:B:9:DA:H3'	6	0.24
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	7	0.24
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	7	0.24
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	7	0.24
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	7	0.24
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	1	0.24
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	1	0.24
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	1	0.24
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	1	0.24
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	6	0.24
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	6	0.24
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	6	0.24
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	6	0.24
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	7	0.24
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	7	0.24
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	7	0.24
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	7	0.24
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	3	0.24
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	3	0.24
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	3	0.24
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	3	0.24
(6,39)	2:A:102:9F0:H41	2:A:102:9F0:H34	2	0.23
(6,39)	2:A:102:9F0:H41	2:B:102:9F0:H34	2	0.23
(6,39)	2:B:102:9F0:H41	2:A:102:9F0:H34	2	0.23
(6,39)	2:B:102:9F0:H41	2:B:102:9F0:H34	2	0.23
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	6	0.23
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	6	0.23
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	6	0.23
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	6	0.23
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	9	0.23
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	9	0.23
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	9	0.23
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	9	0.23
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	9	0.23
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	9	0.23
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	9	0.23
(4,21)	1:A:19:DT:H3'	1:A:20:DT:H6	9	0.23
(4,21)	1:A:19:DT:H3'	1:B:20:DT:H6	9	0.23
(4,21)	1:B:19:DT:H3'	1:A:20:DT:H6	9	0.23
(4,21)	1:B:19:DT:H3'	1:B:20:DT:H6	9	0.23
(4,169)	1:A:17:DG:H2'	1:A:18:DG:H1'	3	0.23
(4,169)	1:A:17:DG:H2'	1:B:18:DG:H1'	3	0.23
(4,169)	1:B:17:DG:H2'	1:A:18:DG:H1'	3	0.23
(4,169)	1:B:17:DG:H2'	1:B:18:DG:H1'	3	0.23
(4,1)	1:A:1:DA:H2	1:A:2:DA:H8	8	0.23
(4,1)	1:A:1:DA:H2	1:B:2:DA:H8	8	0.23
(4,1)	1:B:1:DA:H2	1:A:2:DA:H8	8	0.23
(4,1)	1:B:1:DA:H2	1:B:2:DA:H8	8	0.23
(2,96)	2:A:101:9F0:H6	1:A:9:DA:H3'	10	0.23
(2,96)	2:A:101:9F0:H6	1:B:9:DA:H3'	10	0.23
(2,96)	2:B:101:9F0:H6	1:A:9:DA:H3'	10	0.23
(2,96)	2:B:101:9F0:H6	1:B:9:DA:H3'	10	0.23
(2,4)	2:A:101:9F0:H14	1:A:9:DA:H2'	2	0.23
(2,4)	2:A:101:9F0:H14	1:B:9:DA:H2'	2	0.23
(2,4)	2:B:101:9F0:H14	1:A:9:DA:H2'	2	0.23
(2,4)	2:B:101:9F0:H14	1:B:9:DA:H2'	2	0.23
(2,3)	2:A:101:9F0:H14	1:A:9:DA:H1'	2	0.23
(2,3)	2:A:101:9F0:H14	1:B:9:DA:H1'	2	0.23
(2,3)	2:B:101:9F0:H14	1:A:9:DA:H1'	2	0.23
(2,3)	2:B:101:9F0:H14	1:B:9:DA:H1'	2	0.23
(2,192)	2:A:102:9F0:H34	1:A:12:DG:H3'	5	0.23
(2,192)	2:A:102:9F0:H34	1:B:12:DG:H3'	5	0.23
(2,192)	2:B:102:9F0:H34	1:A:12:DG:H3'	5	0.23
(2,192)	2:B:102:9F0:H34	1:B:12:DG:H3'	5	0.23
(2,184)	2:A:102:9F0:H37	1:A:6:DG:H2'	6	0.23
(2,184)	2:A:102:9F0:H37	1:B:6:DG:H2'	6	0.23
(2,184)	2:B:102:9F0:H37	1:A:6:DG:H2'	6	0.23
(2,184)	2:B:102:9F0:H37	1:B:6:DG:H2'	6	0.23
(2,18)	2:A:101:9F0:H11	1:A:21:DA:H2	6	0.23
(2,18)	2:A:101:9F0:H11	1:B:21:DA:H2	6	0.23
(2,18)	2:B:101:9F0:H11	1:A:21:DA:H2	6	0.23
(2,18)	2:B:101:9F0:H11	1:B:21:DA:H2	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,159)	2:A:102:9F0:H48	1:A:14:DT:H6	10	0.23
(2,159)	2:A:102:9F0:H48	1:B:14:DT:H6	10	0.23
(2,159)	2:B:102:9F0:H48	1:A:14:DT:H6	10	0.23
(2,159)	2:B:102:9F0:H48	1:B:14:DT:H6	10	0.23
(2,12)	2:A:101:9F0:H13	1:A:9:DA:H2"	6	0.23
(2,12)	2:A:101:9F0:H13	1:B:9:DA:H2"	6	0.23
(2,12)	2:B:101:9F0:H13	1:A:9:DA:H2"	6	0.23
(2,12)	2:B:101:9F0:H13	1:B:9:DA:H2"	6	0.23
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	2	0.23
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	2	0.23
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	2	0.23
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	2	0.23
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	1	0.23
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	1	0.23
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	1	0.23
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	1	0.23
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	3	0.23
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	3	0.23
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	3	0.23
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	3	0.23
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	9	0.23
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	9	0.23
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	9	0.23
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	9	0.23
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	3	0.23
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	3	0.23
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	3	0.23
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	3	0.23
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	8	0.23
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	8	0.23
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	8	0.23
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	8	0.23
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	9	0.23
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	9	0.23
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	9	0.23
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	9	0.23
(1,21)	1:A:10:DG:N7	1:A:18:DG:H21	10	0.23
(1,21)	1:A:10:DG:N7	1:B:18:DG:H21	10	0.23
(1,21)	1:B:10:DG:N7	1:A:18:DG:H21	10	0.23
(1,21)	1:B:10:DG:N7	1:B:18:DG:H21	10	0.23
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	5	0.23
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	5	0.23
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	5	0.23
(5,71)	1:A:14:DT:H2'	1:A:14:DT:H6	2	0.22
(5,71)	1:A:14:DT:H2'	1:B:14:DT:H6	2	0.22
(5,71)	1:B:14:DT:H2'	1:A:14:DT:H6	2	0.22
(5,71)	1:B:14:DT:H2'	1:B:14:DT:H6	2	0.22
(4,97)	1:A:26:DA:H8	1:A:14:DT:H3'	7	0.22
(4,97)	1:A:26:DA:H8	1:B:14:DT:H3'	7	0.22
(4,97)	1:B:26:DA:H8	1:A:14:DT:H3'	7	0.22
(4,97)	1:B:26:DA:H8	1:B:14:DT:H3'	7	0.22
(4,28)	1:A:20:DT:H2'	1:A:21:DA:H8	7	0.22
(4,28)	1:A:20:DT:H2'	1:B:21:DA:H8	7	0.22
(4,28)	1:B:20:DT:H2'	1:A:21:DA:H8	7	0.22
(4,28)	1:B:20:DT:H2'	1:B:21:DA:H8	7	0.22
(4,21)	1:A:19:DT:H3'	1:A:20:DT:H6	3	0.22
(4,21)	1:A:19:DT:H3'	1:B:20:DT:H6	3	0.22
(4,21)	1:B:19:DT:H3'	1:A:20:DT:H6	3	0.22
(4,21)	1:B:19:DT:H3'	1:B:20:DT:H6	3	0.22
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	1	0.22
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	1	0.22
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	1	0.22
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	1	0.22
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	1	0.22
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	1	0.22
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	1	0.22
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	1	0.22
(2,79)	2:A:101:9F0:H9	1:A:9:DA:H2	5	0.22
(2,79)	2:A:101:9F0:H9	1:B:9:DA:H2	5	0.22
(2,79)	2:B:101:9F0:H9	1:A:9:DA:H2	5	0.22
(2,79)	2:B:101:9F0:H9	1:B:9:DA:H2	5	0.22
(2,79)	2:A:101:9F0:H9	1:A:9:DA:H2	6	0.22
(2,79)	2:A:101:9F0:H9	1:B:9:DA:H2	6	0.22
(2,79)	2:B:101:9F0:H9	1:A:9:DA:H2	6	0.22
(2,79)	2:B:101:9F0:H9	1:B:9:DA:H2	6	0.22
(2,79)	2:A:101:9F0:H9	1:A:9:DA:H2	9	0.22
(2,79)	2:A:101:9F0:H9	1:B:9:DA:H2	9	0.22
(2,79)	2:B:101:9F0:H9	1:A:9:DA:H2	9	0.22
(2,79)	2:B:101:9F0:H9	1:B:9:DA:H2	9	0.22
(2,79)	2:A:101:9F0:H9	1:A:9:DA:H2	10	0.22
(2,79)	2:A:101:9F0:H9	1:B:9:DA:H2	10	0.22
(2,79)	2:B:101:9F0:H9	1:A:9:DA:H2	10	0.22
(2,79)	2:B:101:9F0:H9	1:B:9:DA:H2	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,58)	2:A:101:9F0:H37	1:A:3:DA:H2'	4	0.22
(2,58)	2:A:101:9F0:H37	1:B:3:DA:H2'	4	0.22
(2,58)	2:B:101:9F0:H37	1:A:3:DA:H2'	4	0.22
(2,58)	2:B:101:9F0:H37	1:B:3:DA:H2'	4	0.22
(2,55)	2:A:101:9F0:H16	1:A:4:DG:H8	7	0.22
(2,55)	2:A:101:9F0:H16	1:B:4:DG:H8	7	0.22
(2,55)	2:B:101:9F0:H16	1:A:4:DG:H8	7	0.22
(2,55)	2:B:101:9F0:H16	1:B:4:DG:H8	7	0.22
(2,47)	2:A:101:9F0:H19	1:A:21:DA:H2	2	0.22
(2,47)	2:A:101:9F0:H19	1:B:21:DA:H2	2	0.22
(2,47)	2:B:101:9F0:H19	1:A:21:DA:H2	2	0.22
(2,47)	2:B:101:9F0:H19	1:B:21:DA:H2	2	0.22
(2,28)	2:A:101:9F0:H31	1:A:10:DG:H1'	3	0.22
(2,28)	2:A:101:9F0:H31	1:B:10:DG:H1'	3	0.22
(2,28)	2:B:101:9F0:H31	1:A:10:DG:H1'	3	0.22
(2,28)	2:B:101:9F0:H31	1:B:10:DG:H1'	3	0.22
(2,184)	2:A:102:9F0:H37	1:A:6:DG:H2'	5	0.22
(2,184)	2:A:102:9F0:H37	1:B:6:DG:H2'	5	0.22
(2,184)	2:B:102:9F0:H37	1:A:6:DG:H2'	5	0.22
(2,184)	2:B:102:9F0:H37	1:B:6:DG:H2'	5	0.22
(2,18)	2:A:101:9F0:H11	1:A:21:DA:H2	8	0.22
(2,18)	2:A:101:9F0:H11	1:B:21:DA:H2	8	0.22
(2,18)	2:B:101:9F0:H11	1:A:21:DA:H2	8	0.22
(2,18)	2:B:101:9F0:H11	1:B:21:DA:H2	8	0.22
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	2	0.22
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	2	0.22
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	2	0.22
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	2	0.22
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	4	0.22
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	4	0.22
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	4	0.22
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	4	0.22
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	6	0.22
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	6	0.22
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	6	0.22
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	6	0.22
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	9	0.22
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	9	0.22
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	9	0.22
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	9	0.22
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	7	0.22
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	7	0.22
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	7	0.22
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	9	0.22
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	9	0.22
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	9	0.22
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	9	0.22
(1,20)	1:A:18:DG:O6	1:A:22:DG:N1	9	0.22
(1,20)	1:A:18:DG:O6	1:B:22:DG:N1	9	0.22
(1,20)	1:B:18:DG:O6	1:A:22:DG:N1	9	0.22
(1,20)	1:B:18:DG:O6	1:B:22:DG:N1	9	0.22
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	4	0.22
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	4	0.22
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	4	0.22
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	4	0.22
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	6	0.22
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	6	0.22
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	6	0.22
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	6	0.22
(6,8)	2:A:101:9F0:H47	2:A:101:9F0:H31	2	0.21
(6,8)	2:A:101:9F0:H47	2:B:101:9F0:H31	2	0.21
(6,8)	2:B:101:9F0:H47	2:A:101:9F0:H31	2	0.21
(6,8)	2:B:101:9F0:H47	2:B:101:9F0:H31	2	0.21
(6,15)	2:A:101:9F0:H41	2:A:101:9F0:H36	2	0.21
(6,15)	2:A:101:9F0:H41	2:B:101:9F0:H36	2	0.21
(6,15)	2:B:101:9F0:H41	2:A:101:9F0:H36	2	0.21
(6,15)	2:B:101:9F0:H41	2:B:101:9F0:H36	2	0.21
(5,83)	1:A:15:DA:H3'	1:A:15:DA:H8	4	0.21
(5,83)	1:A:15:DA:H3'	1:B:15:DA:H8	4	0.21
(5,83)	1:B:15:DA:H3'	1:A:15:DA:H8	4	0.21
(5,83)	1:B:15:DA:H3'	1:B:15:DA:H8	4	0.21
(5,58)	1:A:21:DA:H5'	1:A:21:DA:H8	2	0.21
(5,58)	1:A:21:DA:H5'	1:B:21:DA:H8	2	0.21
(5,58)	1:B:21:DA:H5'	1:A:21:DA:H8	2	0.21
(5,58)	1:B:21:DA:H5'	1:B:21:DA:H8	2	0.21
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	10	0.21
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	10	0.21
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	10	0.21
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	10	0.21
(5,15)	1:A:3:DA:H2'	1:A:3:DA:H8	5	0.21
(5,15)	1:A:3:DA:H2'	1:B:3:DA:H8	5	0.21
(5,15)	1:B:3:DA:H2'	1:A:3:DA:H8	5	0.21
(5,15)	1:B:3:DA:H2'	1:B:3:DA:H8	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,12)	1:A:2:DA:H5"	1:A:2:DA:H8	3	0.21
(5,12)	1:A:2:DA:H5"	1:B:2:DA:H8	3	0.21
(5,12)	1:B:2:DA:H5"	1:A:2:DA:H8	3	0.21
(5,12)	1:B:2:DA:H5"	1:B:2:DA:H8	3	0.21
(4,97)	1:A:26:DA:H8	1:A:14:DT:H3'	6	0.21
(4,97)	1:A:26:DA:H8	1:B:14:DT:H3'	6	0.21
(4,97)	1:B:26:DA:H8	1:A:14:DT:H3'	6	0.21
(4,97)	1:B:26:DA:H8	1:B:14:DT:H3'	6	0.21
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	8	0.21
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	8	0.21
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	8	0.21
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	8	0.21
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	10	0.21
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	10	0.21
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	10	0.21
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	10	0.21
(2,96)	2:A:101:9F0:H6	1:A:9:DA:H3'	7	0.21
(2,96)	2:A:101:9F0:H6	1:B:9:DA:H3'	7	0.21
(2,96)	2:B:101:9F0:H6	1:A:9:DA:H3'	7	0.21
(2,96)	2:B:101:9F0:H6	1:B:9:DA:H3'	7	0.21
(2,79)	2:A:101:9F0:H9	1:A:9:DA:H2	7	0.21
(2,79)	2:A:101:9F0:H9	1:B:9:DA:H2	7	0.21
(2,79)	2:B:101:9F0:H9	1:A:9:DA:H2	7	0.21
(2,79)	2:B:101:9F0:H9	1:B:9:DA:H2	7	0.21
(2,58)	2:A:101:9F0:H37	1:A:3:DA:H2'	1	0.21
(2,58)	2:A:101:9F0:H37	1:B:3:DA:H2'	1	0.21
(2,58)	2:B:101:9F0:H37	1:A:3:DA:H2'	1	0.21
(2,58)	2:B:101:9F0:H37	1:B:3:DA:H2'	1	0.21
(2,35)	2:A:101:9F0:H60	1:A:10:DG:H8	6	0.21
(2,35)	2:A:101:9F0:H60	1:B:10:DG:H8	6	0.21
(2,35)	2:B:101:9F0:H60	1:A:10:DG:H8	6	0.21
(2,35)	2:B:101:9F0:H60	1:B:10:DG:H8	6	0.21
(2,18)	2:A:101:9F0:H11	1:A:21:DA:H2	7	0.21
(2,18)	2:A:101:9F0:H11	1:B:21:DA:H2	7	0.21
(2,18)	2:B:101:9F0:H11	1:A:21:DA:H2	7	0.21
(2,18)	2:B:101:9F0:H11	1:B:21:DA:H2	7	0.21
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	1	0.21
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	1	0.21
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	1	0.21
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	1	0.21
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	6	0.21
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	6	0.21
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	6	0.21
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	10	0.21
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	10	0.21
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	10	0.21
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	10	0.21
(2,157)	2:A:102:9F0:H29	1:A:15:DA:H8	4	0.21
(2,157)	2:A:102:9F0:H29	1:B:15:DA:H8	4	0.21
(2,157)	2:B:102:9F0:H29	1:A:15:DA:H8	4	0.21
(2,157)	2:B:102:9F0:H29	1:B:15:DA:H8	4	0.21
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	8	0.21
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	8	0.21
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	8	0.21
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	8	0.21
(2,105)	2:A:101:9F0:H27	1:A:8:DT:H2”	1	0.21
(2,105)	2:A:101:9F0:H27	1:B:8:DT:H2”	1	0.21
(2,105)	2:B:101:9F0:H27	1:A:8:DT:H2”	1	0.21
(2,105)	2:B:101:9F0:H27	1:B:8:DT:H2”	1	0.21
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	5	0.21
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	5	0.21
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	5	0.21
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	5	0.21
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	7	0.21
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	7	0.21
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	7	0.21
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	7	0.21
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	8	0.21
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	8	0.21
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	8	0.21
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	8	0.21
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	10	0.21
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	10	0.21
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	10	0.21
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	10	0.21
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	5	0.21
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	5	0.21
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	5	0.21
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	5	0.21
(1,29)	1:A:5:DG:N7	1:A:23:DG:H22	9	0.21
(1,29)	1:A:5:DG:N7	1:B:23:DG:H22	9	0.21
(1,29)	1:B:5:DG:N7	1:A:23:DG:H22	9	0.21
(1,29)	1:B:5:DG:N7	1:B:23:DG:H22	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:A:5:DG:N7	1:A:23:DG:H22	10	0.21
(1,29)	1:A:5:DG:N7	1:B:23:DG:H22	10	0.21
(1,29)	1:B:5:DG:N7	1:A:23:DG:H22	10	0.21
(1,29)	1:B:5:DG:N7	1:B:23:DG:H22	10	0.21
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	3	0.21
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	3	0.21
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	3	0.21
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	3	0.21
(1,12)	1:A:4:DG:O6	1:A:10:DG:N1	8	0.21
(1,12)	1:A:4:DG:O6	1:B:10:DG:N1	8	0.21
(1,12)	1:B:4:DG:O6	1:A:10:DG:N1	8	0.21
(1,12)	1:B:4:DG:O6	1:B:10:DG:N1	8	0.21
(6,16)	2:A:101:9F0:H42	2:A:101:9F0:H34	1	0.2
(6,16)	2:A:101:9F0:H42	2:B:101:9F0:H34	1	0.2
(6,16)	2:B:101:9F0:H42	2:A:101:9F0:H34	1	0.2
(6,16)	2:B:101:9F0:H42	2:B:101:9F0:H34	1	0.2
(6,16)	2:A:101:9F0:H42	2:A:101:9F0:H34	3	0.2
(6,16)	2:A:101:9F0:H42	2:B:101:9F0:H34	3	0.2
(6,16)	2:B:101:9F0:H42	2:A:101:9F0:H34	3	0.2
(6,16)	2:B:101:9F0:H42	2:B:101:9F0:H34	3	0.2
(5,2)	1:A:1:DA:H2'	1:A:1:DA:H8	8	0.2
(5,2)	1:A:1:DA:H2'	1:B:1:DA:H8	8	0.2
(5,2)	1:B:1:DA:H2'	1:A:1:DA:H8	8	0.2
(5,2)	1:B:1:DA:H2'	1:B:1:DA:H8	8	0.2
(4,96)	1:A:26:DA:H8	1:A:14:DT:H2"	4	0.2
(4,96)	1:A:26:DA:H8	1:B:14:DT:H2"	4	0.2
(4,96)	1:B:26:DA:H8	1:A:14:DT:H2"	4	0.2
(4,96)	1:B:26:DA:H8	1:B:14:DT:H2"	4	0.2
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	1	0.2
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	1	0.2
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	1	0.2
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	1	0.2
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	3	0.2
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	3	0.2
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	3	0.2
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	3	0.2
(4,64)	1:A:15:DA:H4'	1:A:16:DG:H1'	9	0.2
(4,64)	1:A:15:DA:H4'	1:B:16:DG:H1'	9	0.2
(4,64)	1:B:15:DA:H4'	1:A:16:DG:H1'	9	0.2
(4,64)	1:B:15:DA:H4'	1:B:16:DG:H1'	9	0.2
(4,170)	1:A:17:DG:H2"	1:A:18:DG:H1'	6	0.2
(4,170)	1:A:17:DG:H2"	1:B:18:DG:H1'	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,170)	1:B:17:DG:H2"	1:A:18:DG:H1'	6	0.2
(4,170)	1:B:17:DG:H2"	1:B:18:DG:H1'	6	0.2
(4,16)	1:A:8:DT:H1'	1:A:9:DA:H8	9	0.2
(4,16)	1:A:8:DT:H1'	1:B:9:DA:H8	9	0.2
(4,16)	1:B:8:DT:H1'	1:A:9:DA:H8	9	0.2
(4,16)	1:B:8:DT:H1'	1:B:9:DA:H8	9	0.2
(4,120)	1:A:4:DG:H1	1:A:22:DG:H8	8	0.2
(4,120)	1:A:4:DG:H1	1:B:22:DG:H8	8	0.2
(4,120)	1:B:4:DG:H1	1:A:22:DG:H8	8	0.2
(4,120)	1:B:4:DG:H1	1:B:22:DG:H8	8	0.2
(2,96)	2:A:101:9F0:H6	1:A:9:DA:H3'	9	0.2
(2,96)	2:A:101:9F0:H6	1:B:9:DA:H3'	9	0.2
(2,96)	2:B:101:9F0:H6	1:A:9:DA:H3'	9	0.2
(2,96)	2:B:101:9F0:H6	1:B:9:DA:H3'	9	0.2
(2,184)	2:A:102:9F0:H37	1:A:6:DG:H2'	7	0.2
(2,184)	2:A:102:9F0:H37	1:B:6:DG:H2'	7	0.2
(2,184)	2:B:102:9F0:H37	1:A:6:DG:H2'	7	0.2
(2,184)	2:B:102:9F0:H37	1:B:6:DG:H2'	7	0.2
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	4	0.2
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	4	0.2
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	4	0.2
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	4	0.2
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	7	0.2
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	7	0.2
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	7	0.2
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	7	0.2
(2,142)	2:A:102:9F0:H32	1:A:24:DG:H3'	9	0.2
(2,142)	2:A:102:9F0:H32	1:B:24:DG:H3'	9	0.2
(2,142)	2:B:102:9F0:H32	1:A:24:DG:H3'	9	0.2
(2,142)	2:B:102:9F0:H32	1:B:24:DG:H3'	9	0.2
(2,142)	2:A:102:9F0:H32	1:A:24:DG:H3'	10	0.2
(2,142)	2:A:102:9F0:H32	1:B:24:DG:H3'	10	0.2
(2,142)	2:B:102:9F0:H32	1:A:24:DG:H3'	10	0.2
(2,142)	2:B:102:9F0:H32	1:B:24:DG:H3'	10	0.2
(2,129)	2:A:102:9F0:H10	1:A:25:DA:H2	10	0.2
(2,129)	2:A:102:9F0:H10	1:B:25:DA:H2	10	0.2
(2,129)	2:B:102:9F0:H10	1:A:25:DA:H2	10	0.2
(2,129)	2:B:102:9F0:H10	1:B:25:DA:H2	10	0.2
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	3	0.2
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	3	0.2
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	3	0.2
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:A:24:DG:N7	1:A:16:DG:N2	1	0.2
(1,50)	1:A:24:DG:N7	1:B:16:DG:N2	1	0.2
(1,50)	1:B:24:DG:N7	1:A:16:DG:N2	1	0.2
(1,50)	1:B:24:DG:N7	1:B:16:DG:N2	1	0.2
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	7	0.2
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	7	0.2
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	7	0.2
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	7	0.2
(1,29)	1:A:5:DG:N7	1:A:23:DG:H22	2	0.2
(1,29)	1:A:5:DG:N7	1:B:23:DG:H22	2	0.2
(1,29)	1:B:5:DG:N7	1:A:23:DG:H22	2	0.2
(1,29)	1:B:5:DG:N7	1:B:23:DG:H22	2	0.2
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	1	0.2
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	1	0.2
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	1	0.2
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	1	0.2
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	4	0.2
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	4	0.2
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	4	0.2
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	4	0.2
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	5	0.2
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	5	0.2
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	5	0.2
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	5	0.2
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	6	0.2
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	6	0.2
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	6	0.2
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	6	0.2
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	10	0.2
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	10	0.2
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	10	0.2
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	10	0.2
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	2	0.2
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	2	0.2
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	2	0.2
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	2	0.2
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	6	0.2
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	6	0.2
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	6	0.2
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	6	0.2
(5,71)	1:A:14:DT:H2'	1:A:14:DT:H6	6	0.19
(5,71)	1:A:14:DT:H2'	1:B:14:DT:H6	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,71)	1:B:14:DT:H2'	1:A:14:DT:H6	6	0.19
(5,71)	1:B:14:DT:H2'	1:B:14:DT:H6	6	0.19
(5,58)	1:A:21:DA:H5'	1:A:21:DA:H8	4	0.19
(5,58)	1:A:21:DA:H5'	1:B:21:DA:H8	4	0.19
(5,58)	1:B:21:DA:H5'	1:A:21:DA:H8	4	0.19
(5,58)	1:B:21:DA:H5'	1:B:21:DA:H8	4	0.19
(5,12)	1:A:2:DA:H5"	1:A:2:DA:H8	6	0.19
(5,12)	1:A:2:DA:H5"	1:B:2:DA:H8	6	0.19
(5,12)	1:B:2:DA:H5"	1:A:2:DA:H8	6	0.19
(5,12)	1:B:2:DA:H5"	1:B:2:DA:H8	6	0.19
(4,169)	1:A:17:DG:H2'	1:A:18:DG:H1'	1	0.19
(4,169)	1:A:17:DG:H2'	1:B:18:DG:H1'	1	0.19
(4,169)	1:B:17:DG:H2'	1:A:18:DG:H1'	1	0.19
(4,169)	1:B:17:DG:H2'	1:B:18:DG:H1'	1	0.19
(4,169)	1:A:17:DG:H2'	1:A:18:DG:H1'	5	0.19
(4,169)	1:A:17:DG:H2'	1:B:18:DG:H1'	5	0.19
(4,169)	1:B:17:DG:H2'	1:A:18:DG:H1'	5	0.19
(4,169)	1:B:17:DG:H2'	1:B:18:DG:H1'	5	0.19
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	8	0.19
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	8	0.19
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	8	0.19
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	8	0.19
(4,13)	1:A:3:DA:H2	1:A:9:DA:H2	1	0.19
(4,13)	1:A:3:DA:H2	1:B:9:DA:H2	1	0.19
(4,13)	1:B:3:DA:H2	1:A:9:DA:H2	1	0.19
(4,13)	1:B:3:DA:H2	1:B:9:DA:H2	1	0.19
(4,13)	1:A:3:DA:H2	1:A:9:DA:H2	3	0.19
(4,13)	1:A:3:DA:H2	1:B:9:DA:H2	3	0.19
(4,13)	1:B:3:DA:H2	1:A:9:DA:H2	3	0.19
(4,13)	1:B:3:DA:H2	1:B:9:DA:H2	3	0.19
(2,79)	2:A:101:9F0:H9	1:A:9:DA:H2	4	0.19
(2,79)	2:A:101:9F0:H9	1:B:9:DA:H2	4	0.19
(2,79)	2:B:101:9F0:H9	1:A:9:DA:H2	4	0.19
(2,79)	2:B:101:9F0:H9	1:B:9:DA:H2	4	0.19
(2,77)	2:A:101:9F0:H9	1:A:3:DA:H2	3	0.19
(2,77)	2:A:101:9F0:H9	1:B:3:DA:H2	3	0.19
(2,77)	2:B:101:9F0:H9	1:A:3:DA:H2	3	0.19
(2,77)	2:B:101:9F0:H9	1:B:3:DA:H2	3	0.19
(2,55)	2:A:101:9F0:H16	1:A:4:DG:H8	10	0.19
(2,55)	2:A:101:9F0:H16	1:B:4:DG:H8	10	0.19
(2,55)	2:B:101:9F0:H16	1:A:4:DG:H8	10	0.19
(2,55)	2:B:101:9F0:H16	1:B:4:DG:H8	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,40)	2:A:101:9F0:H19	1:A:3:DA:H2	9	0.19
(2,40)	2:A:101:9F0:H19	1:B:3:DA:H2	9	0.19
(2,40)	2:B:101:9F0:H19	1:A:3:DA:H2	9	0.19
(2,40)	2:B:101:9F0:H19	1:B:3:DA:H2	9	0.19
(2,28)	2:A:101:9F0:H31	1:A:10:DG:H1'	4	0.19
(2,28)	2:A:101:9F0:H31	1:B:10:DG:H1'	4	0.19
(2,28)	2:B:101:9F0:H31	1:A:10:DG:H1'	4	0.19
(2,28)	2:B:101:9F0:H31	1:B:10:DG:H1'	4	0.19
(2,211)	2:A:102:9F0:H6	1:A:25:DA:H1'	2	0.19
(2,211)	2:A:102:9F0:H6	1:B:25:DA:H1'	2	0.19
(2,211)	2:B:102:9F0:H6	1:A:25:DA:H1'	2	0.19
(2,211)	2:B:102:9F0:H6	1:B:25:DA:H1'	2	0.19
(2,191)	2:A:102:9F0:H34	1:A:12:DG:H2'	4	0.19
(2,191)	2:A:102:9F0:H34	1:B:12:DG:H2'	4	0.19
(2,191)	2:B:102:9F0:H34	1:A:12:DG:H2'	4	0.19
(2,191)	2:B:102:9F0:H34	1:B:12:DG:H2'	4	0.19
(2,180)	2:A:102:9F0:H18	1:A:13:DT:H1'	2	0.19
(2,180)	2:A:102:9F0:H18	1:B:13:DT:H1'	2	0.19
(2,180)	2:B:102:9F0:H18	1:A:13:DT:H1'	2	0.19
(2,180)	2:B:102:9F0:H18	1:B:13:DT:H1'	2	0.19
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	9	0.19
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	9	0.19
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	9	0.19
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	9	0.19
(2,164)	2:A:102:9F0:H19	1:A:6:DG:H1	2	0.19
(2,164)	2:A:102:9F0:H19	1:B:6:DG:H1	2	0.19
(2,164)	2:B:102:9F0:H19	1:A:6:DG:H1	2	0.19
(2,164)	2:B:102:9F0:H19	1:B:6:DG:H1	2	0.19
(2,164)	2:A:102:9F0:H19	1:A:6:DG:H1	9	0.19
(2,164)	2:A:102:9F0:H19	1:B:6:DG:H1	9	0.19
(2,164)	2:B:102:9F0:H19	1:A:6:DG:H1	9	0.19
(2,164)	2:B:102:9F0:H19	1:B:6:DG:H1	9	0.19
(2,159)	2:A:102:9F0:H48	1:A:14:DT:H6	1	0.19
(2,159)	2:A:102:9F0:H48	1:B:14:DT:H6	1	0.19
(2,159)	2:B:102:9F0:H48	1:A:14:DT:H6	1	0.19
(2,159)	2:B:102:9F0:H48	1:B:14:DT:H6	1	0.19
(2,144)	2:A:102:9F0:H28	1:A:14:DT:H3	4	0.19
(2,144)	2:A:102:9F0:H28	1:B:14:DT:H3	4	0.19
(2,144)	2:B:102:9F0:H28	1:A:14:DT:H3	4	0.19
(2,144)	2:B:102:9F0:H28	1:B:14:DT:H3	4	0.19
(2,117)	2:A:101:9F0:H45	1:A:8:DT:H2'	8	0.19
(2,117)	2:A:101:9F0:H45	1:B:8:DT:H2'	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,117)	2:B:101:9F0:H45	1:A:8:DT:H2'	8	0.19
(2,117)	2:B:101:9F0:H45	1:B:8:DT:H2'	8	0.19
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	7	0.19
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	7	0.19
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	7	0.19
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	7	0.19
(1,5)	1:A:14:DT:N3	1:A:25:DA:N7	2	0.19
(1,5)	1:A:14:DT:N3	1:B:25:DA:N7	2	0.19
(1,5)	1:B:14:DT:N3	1:A:25:DA:N7	2	0.19
(1,5)	1:B:14:DT:N3	1:B:25:DA:N7	2	0.19
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	1	0.19
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	1	0.19
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	1	0.19
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	1	0.19
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	4	0.19
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	4	0.19
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	4	0.19
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	4	0.19
(1,29)	1:A:5:DG:N7	1:A:23:DG:H22	6	0.19
(1,29)	1:A:5:DG:N7	1:B:23:DG:H22	6	0.19
(1,29)	1:B:5:DG:N7	1:A:23:DG:H22	6	0.19
(1,29)	1:B:5:DG:N7	1:B:23:DG:H22	6	0.19
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	2	0.19
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	2	0.19
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	2	0.19
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	2	0.19
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	4	0.19
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	4	0.19
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	4	0.19
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	4	0.19
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	10	0.19
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	10	0.19
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	10	0.19
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	10	0.19
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	9	0.19
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	9	0.19
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	9	0.19
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	9	0.19
(6,16)	2:A:101:9F0:H42	2:A:101:9F0:H34	5	0.18
(6,16)	2:A:101:9F0:H42	2:B:101:9F0:H34	5	0.18
(6,16)	2:B:101:9F0:H42	2:A:101:9F0:H34	5	0.18
(6,16)	2:B:101:9F0:H42	2:B:101:9F0:H34	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,15)	2:A:101:9F0:H41	2:A:101:9F0:H36	3	0.18
(6,15)	2:A:101:9F0:H41	2:B:101:9F0:H36	3	0.18
(6,15)	2:B:101:9F0:H41	2:A:101:9F0:H36	3	0.18
(6,15)	2:B:101:9F0:H41	2:B:101:9F0:H36	3	0.18
(5,71)	1:A:14:DT:H2'	1:A:14:DT:H6	7	0.18
(5,71)	1:A:14:DT:H2'	1:B:14:DT:H6	7	0.18
(5,71)	1:B:14:DT:H2'	1:A:14:DT:H6	7	0.18
(5,71)	1:B:14:DT:H2'	1:B:14:DT:H6	7	0.18
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	9	0.18
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	9	0.18
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	9	0.18
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	9	0.18
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	10	0.18
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	10	0.18
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	10	0.18
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	10	0.18
(5,37)	1:A:19:DT:H2"	1:A:19:DT:H6	9	0.18
(5,37)	1:A:19:DT:H2"	1:B:19:DT:H6	9	0.18
(5,37)	1:B:19:DT:H2"	1:A:19:DT:H6	9	0.18
(5,37)	1:B:19:DT:H2"	1:B:19:DT:H6	9	0.18
(4,61)	1:A:15:DA:H2"	1:A:16:DG:H8	8	0.18
(4,61)	1:A:15:DA:H2"	1:B:16:DG:H8	8	0.18
(4,61)	1:B:15:DA:H2"	1:A:16:DG:H8	8	0.18
(4,61)	1:B:15:DA:H2"	1:B:16:DG:H8	8	0.18
(4,24)	1:A:20:DT:H6	1:A:21:DA:H8	1	0.18
(4,24)	1:A:20:DT:H6	1:B:21:DA:H8	1	0.18
(4,24)	1:B:20:DT:H6	1:A:21:DA:H8	1	0.18
(4,24)	1:B:20:DT:H6	1:B:21:DA:H8	1	0.18
(4,19)	1:A:8:DT:H3'	1:A:9:DA:H8	6	0.18
(4,19)	1:A:8:DT:H3'	1:B:9:DA:H8	6	0.18
(4,19)	1:B:8:DT:H3'	1:A:9:DA:H8	6	0.18
(4,19)	1:B:8:DT:H3'	1:B:9:DA:H8	6	0.18
(4,187)	1:A:18:DG:H4'	1:A:19:DT:C5	7	0.18
(4,187)	1:A:18:DG:H4'	1:B:19:DT:C5	7	0.18
(4,187)	1:B:18:DG:H4'	1:A:19:DT:C5	7	0.18
(4,187)	1:B:18:DG:H4'	1:B:19:DT:C5	7	0.18
(2,86)	2:A:101:9F0:H8	1:A:3:DA:H1'	3	0.18
(2,86)	2:A:101:9F0:H8	1:B:3:DA:H1'	3	0.18
(2,86)	2:B:101:9F0:H8	1:A:3:DA:H1'	3	0.18
(2,86)	2:B:101:9F0:H8	1:B:3:DA:H1'	3	0.18
(2,55)	2:A:101:9F0:H16	1:A:4:DG:H8	9	0.18
(2,55)	2:A:101:9F0:H16	1:B:4:DG:H8	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,55)	2:B:101:9F0:H16	1:A:4:DG:H8	9	0.18
(2,55)	2:B:101:9F0:H16	1:B:4:DG:H8	9	0.18
(2,47)	2:A:101:9F0:H19	1:A:21:DA:H2	8	0.18
(2,47)	2:A:101:9F0:H19	1:B:21:DA:H2	8	0.18
(2,47)	2:B:101:9F0:H19	1:A:21:DA:H2	8	0.18
(2,47)	2:B:101:9F0:H19	1:B:21:DA:H2	8	0.18
(2,18)	2:A:101:9F0:H11	1:A:21:DA:H2	2	0.18
(2,18)	2:A:101:9F0:H11	1:B:21:DA:H2	2	0.18
(2,18)	2:B:101:9F0:H11	1:A:21:DA:H2	2	0.18
(2,18)	2:B:101:9F0:H11	1:B:21:DA:H2	2	0.18
(2,18)	2:A:101:9F0:H11	1:A:21:DA:H2	10	0.18
(2,18)	2:A:101:9F0:H11	1:B:21:DA:H2	10	0.18
(2,18)	2:B:101:9F0:H11	1:A:21:DA:H2	10	0.18
(2,18)	2:B:101:9F0:H11	1:B:21:DA:H2	10	0.18
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	3	0.18
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	3	0.18
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	3	0.18
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	3	0.18
(2,164)	2:A:102:9F0:H19	1:A:6:DG:H1	1	0.18
(2,164)	2:A:102:9F0:H19	1:B:6:DG:H1	1	0.18
(2,164)	2:B:102:9F0:H19	1:A:6:DG:H1	1	0.18
(2,164)	2:B:102:9F0:H19	1:B:6:DG:H1	1	0.18
(2,152)	2:A:102:9F0:H31	1:A:24:DG:H3’	1	0.18
(2,152)	2:A:102:9F0:H31	1:B:24:DG:H3’	1	0.18
(2,152)	2:B:102:9F0:H31	1:A:24:DG:H3’	1	0.18
(2,152)	2:B:102:9F0:H31	1:B:24:DG:H3’	1	0.18
(2,152)	2:A:102:9F0:H31	1:A:24:DG:H3’	10	0.18
(2,152)	2:A:102:9F0:H31	1:B:24:DG:H3’	10	0.18
(2,152)	2:B:102:9F0:H31	1:A:24:DG:H3’	10	0.18
(2,152)	2:B:102:9F0:H31	1:B:24:DG:H3’	10	0.18
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	10	0.18
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	10	0.18
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	10	0.18
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	10	0.18
(1,54)	1:A:16:DG:N7	1:A:12:DG:N2	9	0.18
(1,54)	1:A:16:DG:N7	1:B:12:DG:N2	9	0.18
(1,54)	1:B:16:DG:N7	1:A:12:DG:N2	9	0.18
(1,54)	1:B:16:DG:N7	1:B:12:DG:N2	9	0.18
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	1	0.18
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	1	0.18
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	1	0.18
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	8	0.18
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	8	0.18
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	8	0.18
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	8	0.18
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	9	0.18
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	9	0.18
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	9	0.18
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	9	0.18
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	10	0.18
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	10	0.18
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	10	0.18
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	10	0.18
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	5	0.18
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	5	0.18
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	5	0.18
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	5	0.18
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	10	0.18
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	10	0.18
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	10	0.18
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	10	0.18
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	7	0.18
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	7	0.18
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	7	0.18
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	7	0.18
(1,28)	1:A:11:DG:O6	1:A:5:DG:N1	8	0.18
(1,28)	1:A:11:DG:O6	1:B:5:DG:N1	8	0.18
(1,28)	1:B:11:DG:O6	1:A:5:DG:N1	8	0.18
(1,28)	1:B:11:DG:O6	1:B:5:DG:N1	8	0.18
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	3	0.18
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	3	0.18
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	3	0.18
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	3	0.18
(1,11)	1:A:4:DG:O6	1:A:10:DG:H1	2	0.18
(1,11)	1:A:4:DG:O6	1:B:10:DG:H1	2	0.18
(1,11)	1:B:4:DG:O6	1:A:10:DG:H1	2	0.18
(1,11)	1:B:4:DG:O6	1:B:10:DG:H1	2	0.18
(6,39)	2:A:102:9F0:H41	2:A:102:9F0:H34	6	0.17
(6,39)	2:A:102:9F0:H41	2:B:102:9F0:H34	6	0.17
(6,39)	2:B:102:9F0:H41	2:A:102:9F0:H34	6	0.17
(6,39)	2:B:102:9F0:H41	2:B:102:9F0:H34	6	0.17
(6,15)	2:A:101:9F0:H41	2:A:101:9F0:H36	1	0.17
(6,15)	2:A:101:9F0:H41	2:B:101:9F0:H36	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,15)	2:B:101:9F0:H41	2:A:101:9F0:H36	1	0.17
(6,15)	2:B:101:9F0:H41	2:B:101:9F0:H36	1	0.17
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	2	0.17
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	2	0.17
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	2	0.17
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	2	0.17
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	8	0.17
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	8	0.17
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	8	0.17
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	8	0.17
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	4	0.17
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	4	0.17
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	4	0.17
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	4	0.17
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	6	0.17
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	6	0.17
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	6	0.17
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	6	0.17
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	7	0.17
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	7	0.17
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	7	0.17
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	7	0.17
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	8	0.17
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	8	0.17
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	8	0.17
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	8	0.17
(5,131)	1:A:6:DG:H2'	1:A:6:DG:H8	7	0.17
(5,131)	1:A:6:DG:H2'	1:B:6:DG:H8	7	0.17
(5,131)	1:B:6:DG:H2'	1:A:6:DG:H8	7	0.17
(5,131)	1:B:6:DG:H2'	1:B:6:DG:H8	7	0.17
(5,12)	1:A:2:DA:H5"	1:A:2:DA:H8	1	0.17
(5,12)	1:A:2:DA:H5"	1:B:2:DA:H8	1	0.17
(5,12)	1:B:2:DA:H5"	1:A:2:DA:H8	1	0.17
(5,12)	1:B:2:DA:H5"	1:B:2:DA:H8	1	0.17
(5,12)	1:A:2:DA:H5"	1:A:2:DA:H8	7	0.17
(5,12)	1:A:2:DA:H5"	1:B:2:DA:H8	7	0.17
(5,12)	1:B:2:DA:H5"	1:A:2:DA:H8	7	0.17
(5,12)	1:B:2:DA:H5"	1:B:2:DA:H8	7	0.17
(4,45)	1:A:21:DA:H2"	1:A:22:DG:H1	2	0.17
(4,45)	1:A:21:DA:H2"	1:B:22:DG:H1	2	0.17
(4,45)	1:B:21:DA:H2"	1:A:22:DG:H1	2	0.17
(4,45)	1:B:21:DA:H2"	1:B:22:DG:H1	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,18)	1:A:8:DT:H2"	1:A:9:DA:H8	2	0.17
(4,18)	1:A:8:DT:H2"	1:B:9:DA:H8	2	0.17
(4,18)	1:B:8:DT:H2"	1:A:9:DA:H8	2	0.17
(4,18)	1:B:8:DT:H2"	1:B:9:DA:H8	2	0.17
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	5	0.17
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	5	0.17
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	5	0.17
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	5	0.17
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	7	0.17
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	7	0.17
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	7	0.17
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	7	0.17
(4,120)	1:A:4:DG:H1	1:A:22:DG:H8	3	0.17
(4,120)	1:A:4:DG:H1	1:B:22:DG:H8	3	0.17
(4,120)	1:B:4:DG:H1	1:A:22:DG:H8	3	0.17
(4,120)	1:B:4:DG:H1	1:B:22:DG:H8	3	0.17
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	3	0.17
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	3	0.17
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	3	0.17
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	3	0.17
(2,79)	2:A:101:9F0:H9	1:A:9:DA:H2	8	0.17
(2,79)	2:A:101:9F0:H9	1:B:9:DA:H2	8	0.17
(2,79)	2:B:101:9F0:H9	1:A:9:DA:H2	8	0.17
(2,79)	2:B:101:9F0:H9	1:B:9:DA:H2	8	0.17
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	5	0.17
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	5	0.17
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	5	0.17
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	5	0.17
(2,172)	2:A:102:9F0:H15	1:A:25:DA:H2	8	0.17
(2,172)	2:A:102:9F0:H15	1:B:25:DA:H2	8	0.17
(2,172)	2:B:102:9F0:H15	1:A:25:DA:H2	8	0.17
(2,172)	2:B:102:9F0:H15	1:B:25:DA:H2	8	0.17
(2,164)	2:A:102:9F0:H19	1:A:6:DG:H1	8	0.17
(2,164)	2:A:102:9F0:H19	1:B:6:DG:H1	8	0.17
(2,164)	2:B:102:9F0:H19	1:A:6:DG:H1	8	0.17
(2,164)	2:B:102:9F0:H19	1:B:6:DG:H1	8	0.17
(2,164)	2:A:102:9F0:H19	1:A:6:DG:H1	10	0.17
(2,164)	2:A:102:9F0:H19	1:B:6:DG:H1	10	0.17
(2,164)	2:B:102:9F0:H19	1:A:6:DG:H1	10	0.17
(2,164)	2:B:102:9F0:H19	1:B:6:DG:H1	10	0.17
(2,159)	2:A:102:9F0:H48	1:A:14:DT:H6	3	0.17
(2,159)	2:A:102:9F0:H48	1:B:14:DT:H6	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,159)	2:B:102:9F0:H48	1:A:14:DT:H6	3	0.17
(2,159)	2:B:102:9F0:H48	1:B:14:DT:H6	3	0.17
(2,159)	2:A:102:9F0:H48	1:A:14:DT:H6	9	0.17
(2,159)	2:A:102:9F0:H48	1:B:14:DT:H6	9	0.17
(2,159)	2:B:102:9F0:H48	1:A:14:DT:H6	9	0.17
(2,159)	2:B:102:9F0:H48	1:B:14:DT:H6	9	0.17
(2,154)	2:A:102:9F0:H29	1:A:14:DT:H6	8	0.17
(2,154)	2:A:102:9F0:H29	1:B:14:DT:H6	8	0.17
(2,154)	2:B:102:9F0:H29	1:A:14:DT:H6	8	0.17
(2,154)	2:B:102:9F0:H29	1:B:14:DT:H6	8	0.17
(2,152)	2:A:102:9F0:H31	1:A:24:DG:H3'	2	0.17
(2,152)	2:A:102:9F0:H31	1:B:24:DG:H3'	2	0.17
(2,152)	2:B:102:9F0:H31	1:A:24:DG:H3'	2	0.17
(2,152)	2:B:102:9F0:H31	1:B:24:DG:H3'	2	0.17
(2,15)	2:A:101:9F0:H11	1:A:10:DG:H1	3	0.17
(2,15)	2:A:101:9F0:H11	1:B:10:DG:H1	3	0.17
(2,15)	2:B:101:9F0:H11	1:A:10:DG:H1	3	0.17
(2,15)	2:B:101:9F0:H11	1:B:10:DG:H1	3	0.17
(2,142)	2:A:102:9F0:H32	1:A:24:DG:H3'	1	0.17
(2,142)	2:A:102:9F0:H32	1:B:24:DG:H3'	1	0.17
(2,142)	2:B:102:9F0:H32	1:A:24:DG:H3'	1	0.17
(2,142)	2:B:102:9F0:H32	1:B:24:DG:H3'	1	0.17
(2,142)	2:A:102:9F0:H32	1:A:24:DG:H3'	2	0.17
(2,142)	2:A:102:9F0:H32	1:B:24:DG:H3'	2	0.17
(2,142)	2:B:102:9F0:H32	1:A:24:DG:H3'	2	0.17
(2,142)	2:B:102:9F0:H32	1:B:24:DG:H3'	2	0.17
(2,129)	2:A:102:9F0:H10	1:A:25:DA:H2	1	0.17
(2,129)	2:A:102:9F0:H10	1:B:25:DA:H2	1	0.17
(2,129)	2:B:102:9F0:H10	1:A:25:DA:H2	1	0.17
(2,129)	2:B:102:9F0:H10	1:B:25:DA:H2	1	0.17
(2,12)	2:A:101:9F0:H13	1:A:9:DA:H2"	3	0.17
(2,12)	2:A:101:9F0:H13	1:B:9:DA:H2"	3	0.17
(2,12)	2:B:101:9F0:H13	1:A:9:DA:H2"	3	0.17
(2,12)	2:B:101:9F0:H13	1:B:9:DA:H2"	3	0.17
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	1	0.17
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	1	0.17
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	1	0.17
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	1	0.17
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	1	0.17
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	1	0.17
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	1	0.17
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	6	0.17
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	6	0.17
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	6	0.17
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	6	0.17
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	6	0.17
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	6	0.17
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	6	0.17
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	6	0.17
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	10	0.17
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	10	0.17
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	10	0.17
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	10	0.17
(1,14)	1:A:22:DG:N7	1:A:4:DG:N2	2	0.17
(1,14)	1:A:22:DG:N7	1:B:4:DG:N2	2	0.17
(1,14)	1:B:22:DG:N7	1:A:4:DG:N2	2	0.17
(1,14)	1:B:22:DG:N7	1:B:4:DG:N2	2	0.17
(1,11)	1:A:4:DG:O6	1:A:10:DG:H1	7	0.17
(1,11)	1:A:4:DG:O6	1:B:10:DG:H1	7	0.17
(1,11)	1:B:4:DG:O6	1:A:10:DG:H1	7	0.17
(1,11)	1:B:4:DG:O6	1:B:10:DG:H1	7	0.17
(5,58)	1:A:21:DA:H5'	1:A:21:DA:H8	9	0.16
(5,58)	1:A:21:DA:H5'	1:B:21:DA:H8	9	0.16
(5,58)	1:B:21:DA:H5'	1:A:21:DA:H8	9	0.16
(5,58)	1:B:21:DA:H5'	1:B:21:DA:H8	9	0.16
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	1	0.16
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	1	0.16
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	1	0.16
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	1	0.16
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	2	0.16
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	2	0.16
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	2	0.16
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	2	0.16
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	3	0.16
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	3	0.16
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	3	0.16
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	3	0.16
(5,41)	1:A:20:DT:H2'	1:A:20:DT:H1'	5	0.16
(5,41)	1:A:20:DT:H2'	1:B:20:DT:H1'	5	0.16
(5,41)	1:B:20:DT:H2'	1:A:20:DT:H1'	5	0.16
(5,41)	1:B:20:DT:H2'	1:B:20:DT:H1'	5	0.16
(5,142)	1:A:6:DG:H5'	1:A:6:DG:H8	8	0.16
(5,142)	1:A:6:DG:H5'	1:B:6:DG:H8	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,142)	1:B:6:DG:H5'	1:A:6:DG:H8	8	0.16
(5,142)	1:B:6:DG:H5'	1:B:6:DG:H8	8	0.16
(5,131)	1:A:6:DG:H2'	1:A:6:DG:H8	10	0.16
(5,131)	1:A:6:DG:H2'	1:B:6:DG:H8	10	0.16
(5,131)	1:B:6:DG:H2'	1:A:6:DG:H8	10	0.16
(5,131)	1:B:6:DG:H2'	1:B:6:DG:H8	10	0.16
(4,45)	1:A:21:DA:H2"	1:A:22:DG:H1	6	0.16
(4,45)	1:A:21:DA:H2"	1:B:22:DG:H1	6	0.16
(4,45)	1:B:21:DA:H2"	1:A:22:DG:H1	6	0.16
(4,45)	1:B:21:DA:H2"	1:B:22:DG:H1	6	0.16
(4,179)	1:A:18:DG:H1'	1:A:17:DG:H8	9	0.16
(4,179)	1:A:18:DG:H1'	1:B:17:DG:H8	9	0.16
(4,179)	1:B:18:DG:H1'	1:A:17:DG:H8	9	0.16
(4,179)	1:B:18:DG:H1'	1:B:17:DG:H8	9	0.16
(4,170)	1:A:17:DG:H2"	1:A:18:DG:H1'	7	0.16
(4,170)	1:A:17:DG:H2"	1:B:18:DG:H1'	7	0.16
(4,170)	1:B:17:DG:H2"	1:A:18:DG:H1'	7	0.16
(4,170)	1:B:17:DG:H2"	1:B:18:DG:H1'	7	0.16
(4,170)	1:A:17:DG:H2"	1:A:18:DG:H1'	10	0.16
(4,170)	1:A:17:DG:H2"	1:B:18:DG:H1'	10	0.16
(4,170)	1:B:17:DG:H2"	1:A:18:DG:H1'	10	0.16
(4,170)	1:B:17:DG:H2"	1:B:18:DG:H1'	10	0.16
(4,16)	1:A:8:DT:H1'	1:A:9:DA:H8	4	0.16
(4,16)	1:A:8:DT:H1'	1:B:9:DA:H8	4	0.16
(4,16)	1:B:8:DT:H1'	1:A:9:DA:H8	4	0.16
(4,16)	1:B:8:DT:H1'	1:B:9:DA:H8	4	0.16
(4,16)	1:A:8:DT:H1'	1:A:9:DA:H8	10	0.16
(4,16)	1:A:8:DT:H1'	1:B:9:DA:H8	10	0.16
(4,16)	1:B:8:DT:H1'	1:A:9:DA:H8	10	0.16
(4,16)	1:B:8:DT:H1'	1:B:9:DA:H8	10	0.16
(4,13)	1:A:3:DA:H2	1:A:9:DA:H2	2	0.16
(4,13)	1:A:3:DA:H2	1:B:9:DA:H2	2	0.16
(4,13)	1:B:3:DA:H2	1:A:9:DA:H2	2	0.16
(4,13)	1:B:3:DA:H2	1:B:9:DA:H2	2	0.16
(4,13)	1:A:3:DA:H2	1:A:9:DA:H2	5	0.16
(4,13)	1:A:3:DA:H2	1:B:9:DA:H2	5	0.16
(4,13)	1:B:3:DA:H2	1:A:9:DA:H2	5	0.16
(4,13)	1:B:3:DA:H2	1:B:9:DA:H2	5	0.16
(4,13)	1:A:3:DA:H2	1:A:9:DA:H2	9	0.16
(4,13)	1:A:3:DA:H2	1:B:9:DA:H2	9	0.16
(4,13)	1:B:3:DA:H2	1:A:9:DA:H2	9	0.16
(4,13)	1:B:3:DA:H2	1:B:9:DA:H2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,120)	1:A:4:DG:H1	1:A:22:DG:H8	6	0.16
(4,120)	1:A:4:DG:H1	1:B:22:DG:H8	6	0.16
(4,120)	1:B:4:DG:H1	1:A:22:DG:H8	6	0.16
(4,120)	1:B:4:DG:H1	1:B:22:DG:H8	6	0.16
(4,120)	1:A:4:DG:H1	1:A:22:DG:H8	10	0.16
(4,120)	1:A:4:DG:H1	1:B:22:DG:H8	10	0.16
(4,120)	1:B:4:DG:H1	1:A:22:DG:H8	10	0.16
(4,120)	1:B:4:DG:H1	1:B:22:DG:H8	10	0.16
(4,11)	1:A:2:DA:H3'	1:A:3:DA:H8	5	0.16
(4,11)	1:A:2:DA:H3'	1:B:3:DA:H8	5	0.16
(4,11)	1:B:2:DA:H3'	1:A:3:DA:H8	5	0.16
(4,11)	1:B:2:DA:H3'	1:B:3:DA:H8	5	0.16
(3,1)	2:A:102:9F0:H33	1:A:15:DA:N6	2	0.16
(3,1)	2:A:102:9F0:H33	1:B:15:DA:N6	2	0.16
(3,1)	2:B:102:9F0:H33	1:A:15:DA:N6	2	0.16
(3,1)	2:B:102:9F0:H33	1:B:15:DA:N6	2	0.16
(2,79)	2:A:101:9F0:H9	1:A:9:DA:H2	1	0.16
(2,79)	2:A:101:9F0:H9	1:B:9:DA:H2	1	0.16
(2,79)	2:B:101:9F0:H9	1:A:9:DA:H2	1	0.16
(2,79)	2:B:101:9F0:H9	1:B:9:DA:H2	1	0.16
(2,55)	2:A:101:9F0:H16	1:A:4:DG:H8	5	0.16
(2,55)	2:A:101:9F0:H16	1:B:4:DG:H8	5	0.16
(2,55)	2:B:101:9F0:H16	1:A:4:DG:H8	5	0.16
(2,55)	2:B:101:9F0:H16	1:B:4:DG:H8	5	0.16
(2,35)	2:A:101:9F0:H60	1:A:10:DG:H8	8	0.16
(2,35)	2:A:101:9F0:H60	1:B:10:DG:H8	8	0.16
(2,35)	2:B:101:9F0:H60	1:A:10:DG:H8	8	0.16
(2,35)	2:B:101:9F0:H60	1:B:10:DG:H8	8	0.16
(2,159)	2:A:102:9F0:H48	1:A:14:DT:H6	2	0.16
(2,159)	2:A:102:9F0:H48	1:B:14:DT:H6	2	0.16
(2,159)	2:B:102:9F0:H48	1:A:14:DT:H6	2	0.16
(2,159)	2:B:102:9F0:H48	1:B:14:DT:H6	2	0.16
(2,137)	2:A:102:9F0:H28	1:A:16:DG:H1	1	0.16
(2,137)	2:A:102:9F0:H28	1:B:16:DG:H1	1	0.16
(2,137)	2:B:102:9F0:H28	1:A:16:DG:H1	1	0.16
(2,137)	2:B:102:9F0:H28	1:B:16:DG:H1	1	0.16
(2,117)	2:A:101:9F0:H45	1:A:8:DT:H2'	7	0.16
(2,117)	2:A:101:9F0:H45	1:B:8:DT:H2'	7	0.16
(2,117)	2:B:101:9F0:H45	1:A:8:DT:H2'	7	0.16
(2,117)	2:B:101:9F0:H45	1:B:8:DT:H2'	7	0.16
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	9	0.16
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	9	0.16
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	9	0.16
(1,54)	1:A:16:DG:N7	1:A:12:DG:N2	1	0.16
(1,54)	1:A:16:DG:N7	1:B:12:DG:N2	1	0.16
(1,54)	1:B:16:DG:N7	1:A:12:DG:N2	1	0.16
(1,54)	1:B:16:DG:N7	1:B:12:DG:N2	1	0.16
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	6	0.16
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	6	0.16
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	6	0.16
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	6	0.16
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	7	0.16
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	7	0.16
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	7	0.16
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	7	0.16
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	2	0.16
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	2	0.16
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	2	0.16
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	2	0.16
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	9	0.16
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	9	0.16
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	9	0.16
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	9	0.16
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	7	0.16
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	7	0.16
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	7	0.16
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	7	0.16
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	8	0.16
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	8	0.16
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	8	0.16
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	8	0.16
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	5	0.16
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	5	0.16
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	5	0.16
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	5	0.16
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	7	0.16
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	7	0.16
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	7	0.16
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	7	0.16
(6,15)	2:A:101:9F0:H41	2:A:101:9F0:H36	5	0.15
(6,15)	2:A:101:9F0:H41	2:B:101:9F0:H36	5	0.15
(6,15)	2:B:101:9F0:H41	2:A:101:9F0:H36	5	0.15
(6,15)	2:B:101:9F0:H41	2:B:101:9F0:H36	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	9	0.15
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	9	0.15
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	9	0.15
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	9	0.15
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	10	0.15
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	10	0.15
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	10	0.15
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	10	0.15
(5,83)	1:A:15:DA:H3'	1:A:15:DA:H8	10	0.15
(5,83)	1:A:15:DA:H3'	1:B:15:DA:H8	10	0.15
(5,83)	1:B:15:DA:H3'	1:A:15:DA:H8	10	0.15
(5,83)	1:B:15:DA:H3'	1:B:15:DA:H8	10	0.15
(4,83)	1:A:26:DA:H8	1:A:14:DT:H3'	3	0.15
(4,83)	1:A:26:DA:H8	1:B:14:DT:H3'	3	0.15
(4,83)	1:B:26:DA:H8	1:A:14:DT:H3'	3	0.15
(4,83)	1:B:26:DA:H8	1:B:14:DT:H3'	3	0.15
(4,42)	1:A:21:DA:H2'	1:A:18:DG:H8	3	0.15
(4,42)	1:A:21:DA:H2'	1:B:18:DG:H8	3	0.15
(4,42)	1:B:21:DA:H2'	1:A:18:DG:H8	3	0.15
(4,42)	1:B:21:DA:H2'	1:B:18:DG:H8	3	0.15
(4,170)	1:A:17:DG:H2"	1:A:18:DG:H1'	5	0.15
(4,170)	1:A:17:DG:H2"	1:B:18:DG:H1'	5	0.15
(4,170)	1:B:17:DG:H2"	1:A:18:DG:H1'	5	0.15
(4,170)	1:B:17:DG:H2"	1:B:18:DG:H1'	5	0.15
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	6	0.15
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	6	0.15
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	6	0.15
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	6	0.15
(4,16)	1:A:8:DT:H1'	1:A:9:DA:H8	8	0.15
(4,16)	1:A:8:DT:H1'	1:B:9:DA:H8	8	0.15
(4,16)	1:B:8:DT:H1'	1:A:9:DA:H8	8	0.15
(4,16)	1:B:8:DT:H1'	1:B:9:DA:H8	8	0.15
(4,144)	1:A:5:DG:H2"	1:A:6:DG:H8	8	0.15
(4,144)	1:A:5:DG:H2"	1:B:6:DG:H8	8	0.15
(4,144)	1:B:5:DG:H2"	1:A:6:DG:H8	8	0.15
(4,144)	1:B:5:DG:H2"	1:B:6:DG:H8	8	0.15
(2,5)	2:A:101:9F0:H14	1:A:9:DA:H2"	2	0.15
(2,5)	2:A:101:9F0:H14	1:B:9:DA:H2"	2	0.15
(2,5)	2:B:101:9F0:H14	1:A:9:DA:H2"	2	0.15
(2,5)	2:B:101:9F0:H14	1:B:9:DA:H2"	2	0.15
(2,164)	2:A:102:9F0:H19	1:A:6:DG:H1	6	0.15
(2,164)	2:A:102:9F0:H19	1:B:6:DG:H1	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,164)	2:B:102:9F0:H19	1:A:6:DG:H1	6	0.15
(2,164)	2:B:102:9F0:H19	1:B:6:DG:H1	6	0.15
(2,164)	2:A:102:9F0:H19	1:A:6:DG:H1	7	0.15
(2,164)	2:A:102:9F0:H19	1:B:6:DG:H1	7	0.15
(2,164)	2:B:102:9F0:H19	1:A:6:DG:H1	7	0.15
(2,164)	2:B:102:9F0:H19	1:B:6:DG:H1	7	0.15
(2,152)	2:A:102:9F0:H31	1:A:24:DG:H3'	9	0.15
(2,152)	2:A:102:9F0:H31	1:B:24:DG:H3'	9	0.15
(2,152)	2:B:102:9F0:H31	1:A:24:DG:H3'	9	0.15
(2,152)	2:B:102:9F0:H31	1:B:24:DG:H3'	9	0.15
(2,12)	2:A:101:9F0:H13	1:A:9:DA:H2"	9	0.15
(2,12)	2:A:101:9F0:H13	1:B:9:DA:H2"	9	0.15
(2,12)	2:B:101:9F0:H13	1:A:9:DA:H2"	9	0.15
(2,12)	2:B:101:9F0:H13	1:B:9:DA:H2"	9	0.15
(2,117)	2:A:101:9F0:H45	1:A:8:DT:H2'	10	0.15
(2,117)	2:A:101:9F0:H45	1:B:8:DT:H2'	10	0.15
(2,117)	2:B:101:9F0:H45	1:A:8:DT:H2'	10	0.15
(2,117)	2:B:101:9F0:H45	1:B:8:DT:H2'	10	0.15
(1,6)	1:A:14:DT:H3	1:A:25:DA:N7	4	0.15
(1,6)	1:A:14:DT:H3	1:B:25:DA:N7	4	0.15
(1,6)	1:B:14:DT:H3	1:A:25:DA:N7	4	0.15
(1,6)	1:B:14:DT:H3	1:B:25:DA:N7	4	0.15
(1,6)	1:A:14:DT:H3	1:A:25:DA:N7	5	0.15
(1,6)	1:A:14:DT:H3	1:B:25:DA:N7	5	0.15
(1,6)	1:B:14:DT:H3	1:A:25:DA:N7	5	0.15
(1,6)	1:B:14:DT:H3	1:B:25:DA:N7	5	0.15
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	6	0.15
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	6	0.15
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	6	0.15
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	6	0.15
(1,54)	1:A:16:DG:N7	1:A:12:DG:N2	8	0.15
(1,54)	1:A:16:DG:N7	1:B:12:DG:N2	8	0.15
(1,54)	1:B:16:DG:N7	1:A:12:DG:N2	8	0.15
(1,54)	1:B:16:DG:N7	1:B:12:DG:N2	8	0.15
(1,54)	1:A:16:DG:N7	1:A:12:DG:N2	10	0.15
(1,54)	1:A:16:DG:N7	1:B:12:DG:N2	10	0.15
(1,54)	1:B:16:DG:N7	1:A:12:DG:N2	10	0.15
(1,54)	1:B:16:DG:N7	1:B:12:DG:N2	10	0.15
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	4	0.15
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	4	0.15
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	4	0.15
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	8	0.15
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	8	0.15
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	8	0.15
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	8	0.15
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	2	0.15
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	2	0.15
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	2	0.15
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	2	0.15
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	8	0.15
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	8	0.15
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	8	0.15
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	8	0.15
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	4	0.15
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	4	0.15
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	4	0.15
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	4	0.15
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	8	0.15
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	8	0.15
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	8	0.15
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	8	0.15
(1,11)	1:A:4:DG:O6	1:A:10:DG:H1	1	0.15
(1,11)	1:A:4:DG:O6	1:B:10:DG:H1	1	0.15
(1,11)	1:B:4:DG:O6	1:A:10:DG:H1	1	0.15
(1,11)	1:B:4:DG:O6	1:B:10:DG:H1	1	0.15
(1,11)	1:A:4:DG:O6	1:A:10:DG:H1	5	0.15
(1,11)	1:A:4:DG:O6	1:B:10:DG:H1	5	0.15
(1,11)	1:B:4:DG:O6	1:A:10:DG:H1	5	0.15
(1,11)	1:B:4:DG:O6	1:B:10:DG:H1	5	0.15
(1,11)	1:A:4:DG:O6	1:A:10:DG:H1	9	0.15
(1,11)	1:A:4:DG:O6	1:B:10:DG:H1	9	0.15
(1,11)	1:B:4:DG:O6	1:A:10:DG:H1	9	0.15
(1,11)	1:B:4:DG:O6	1:B:10:DG:H1	9	0.15
(1,11)	1:A:4:DG:O6	1:A:10:DG:H1	10	0.15
(1,11)	1:A:4:DG:O6	1:B:10:DG:H1	10	0.15
(1,11)	1:B:4:DG:O6	1:A:10:DG:H1	10	0.15
(1,11)	1:B:4:DG:O6	1:B:10:DG:H1	10	0.15
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	1	0.14
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	1	0.14
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	1	0.14
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	1	0.14
(5,131)	1:A:6:DG:H2'	1:A:6:DG:H8	9	0.14
(5,131)	1:A:6:DG:H2'	1:B:6:DG:H8	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,131)	1:B:6:DG:H2'	1:A:6:DG:H8	9	0.14
(5,131)	1:B:6:DG:H2'	1:B:6:DG:H8	9	0.14
(4,42)	1:A:21:DA:H2'	1:A:18:DG:H8	4	0.14
(4,42)	1:A:21:DA:H2'	1:B:18:DG:H8	4	0.14
(4,42)	1:B:21:DA:H2'	1:A:18:DG:H8	4	0.14
(4,42)	1:B:21:DA:H2'	1:B:18:DG:H8	4	0.14
(4,184)	1:A:18:DG:H3'	1:A:19:DT:H6	9	0.14
(4,184)	1:A:18:DG:H3'	1:B:19:DT:H6	9	0.14
(4,184)	1:B:18:DG:H3'	1:A:19:DT:H6	9	0.14
(4,184)	1:B:18:DG:H3'	1:B:19:DT:H6	9	0.14
(4,170)	1:A:17:DG:H2"	1:A:18:DG:H1'	8	0.14
(4,170)	1:A:17:DG:H2"	1:B:18:DG:H1'	8	0.14
(4,170)	1:B:17:DG:H2"	1:A:18:DG:H1'	8	0.14
(4,170)	1:B:17:DG:H2"	1:B:18:DG:H1'	8	0.14
(2,55)	2:A:101:9F0:H16	1:A:4:DG:H8	6	0.14
(2,55)	2:A:101:9F0:H16	1:B:4:DG:H8	6	0.14
(2,55)	2:B:101:9F0:H16	1:A:4:DG:H8	6	0.14
(2,55)	2:B:101:9F0:H16	1:B:4:DG:H8	6	0.14
(2,40)	2:A:101:9F0:H19	1:A:3:DA:H2	10	0.14
(2,40)	2:A:101:9F0:H19	1:B:3:DA:H2	10	0.14
(2,40)	2:B:101:9F0:H19	1:A:3:DA:H2	10	0.14
(2,40)	2:B:101:9F0:H19	1:B:3:DA:H2	10	0.14
(2,35)	2:A:101:9F0:H60	1:A:10:DG:H8	9	0.14
(2,35)	2:A:101:9F0:H60	1:B:10:DG:H8	9	0.14
(2,35)	2:B:101:9F0:H60	1:A:10:DG:H8	9	0.14
(2,35)	2:B:101:9F0:H60	1:B:10:DG:H8	9	0.14
(2,159)	2:A:102:9F0:H48	1:A:14:DT:H6	5	0.14
(2,159)	2:A:102:9F0:H48	1:B:14:DT:H6	5	0.14
(2,159)	2:B:102:9F0:H48	1:A:14:DT:H6	5	0.14
(2,159)	2:B:102:9F0:H48	1:B:14:DT:H6	5	0.14
(2,129)	2:A:102:9F0:H10	1:A:25:DA:H2	9	0.14
(2,129)	2:A:102:9F0:H10	1:B:25:DA:H2	9	0.14
(2,129)	2:B:102:9F0:H10	1:A:25:DA:H2	9	0.14
(2,129)	2:B:102:9F0:H10	1:B:25:DA:H2	9	0.14
(2,117)	2:A:101:9F0:H45	1:A:8:DT:H2'	9	0.14
(2,117)	2:A:101:9F0:H45	1:B:8:DT:H2'	9	0.14
(2,117)	2:B:101:9F0:H45	1:A:8:DT:H2'	9	0.14
(2,117)	2:B:101:9F0:H45	1:B:8:DT:H2'	9	0.14
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	3	0.14
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	3	0.14
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	3	0.14
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	5	0.14
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	5	0.14
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	5	0.14
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	5	0.14
(1,48)	1:A:6:DG:O6	1:A:24:DG:N1	3	0.14
(1,48)	1:A:6:DG:O6	1:B:24:DG:N1	3	0.14
(1,48)	1:B:6:DG:O6	1:A:24:DG:N1	3	0.14
(1,48)	1:B:6:DG:O6	1:B:24:DG:N1	3	0.14
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	1	0.14
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	1	0.14
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	1	0.14
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	1	0.14
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	3	0.14
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	3	0.14
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	3	0.14
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	3	0.14
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	5	0.14
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	5	0.14
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	5	0.14
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	5	0.14
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	8	0.14
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	8	0.14
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	8	0.14
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	8	0.14
(1,34)	1:A:23:DG:N7	1:A:17:DG:N2	3	0.14
(1,34)	1:A:23:DG:N7	1:B:17:DG:N2	3	0.14
(1,34)	1:B:23:DG:N7	1:A:17:DG:N2	3	0.14
(1,34)	1:B:23:DG:N7	1:B:17:DG:N2	3	0.14
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	1	0.14
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	1	0.14
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	1	0.14
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	1	0.14
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	5	0.14
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	5	0.14
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	5	0.14
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	5	0.14
(1,30)	1:A:5:DG:N7	1:A:23:DG:N2	3	0.14
(1,30)	1:A:5:DG:N7	1:B:23:DG:N2	3	0.14
(1,30)	1:B:5:DG:N7	1:A:23:DG:N2	3	0.14
(1,30)	1:B:5:DG:N7	1:B:23:DG:N2	3	0.14
(1,29)	1:A:5:DG:N7	1:A:23:DG:H22	7	0.14
(1,29)	1:A:5:DG:N7	1:B:23:DG:H22	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:B:5:DG:N7	1:A:23:DG:H22	7	0.14
(1,29)	1:B:5:DG:N7	1:B:23:DG:H22	7	0.14
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	1	0.14
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	1	0.14
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	1	0.14
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	1	0.14
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	1	0.14
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	1	0.14
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	1	0.14
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	1	0.14
(1,14)	1:A:22:DG:N7	1:A:4:DG:N2	4	0.14
(1,14)	1:A:22:DG:N7	1:B:4:DG:N2	4	0.14
(1,14)	1:B:22:DG:N7	1:A:4:DG:N2	4	0.14
(1,14)	1:B:22:DG:N7	1:B:4:DG:N2	4	0.14
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	5	0.13
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	5	0.13
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	5	0.13
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	5	0.13
(5,83)	1:A:15:DA:H3'	1:A:15:DA:H8	3	0.13
(5,83)	1:A:15:DA:H3'	1:B:15:DA:H8	3	0.13
(5,83)	1:B:15:DA:H3'	1:A:15:DA:H8	3	0.13
(5,83)	1:B:15:DA:H3'	1:B:15:DA:H8	3	0.13
(5,20)	1:A:3:DA:H4'	1:A:3:DA:H1'	7	0.13
(5,20)	1:A:3:DA:H4'	1:B:3:DA:H1'	7	0.13
(5,20)	1:B:3:DA:H4'	1:A:3:DA:H1'	7	0.13
(5,20)	1:B:3:DA:H4'	1:B:3:DA:H1'	7	0.13
(5,142)	1:A:6:DG:H5'	1:A:6:DG:H8	3	0.13
(5,142)	1:A:6:DG:H5'	1:B:6:DG:H8	3	0.13
(5,142)	1:B:6:DG:H5'	1:A:6:DG:H8	3	0.13
(5,142)	1:B:6:DG:H5'	1:B:6:DG:H8	3	0.13
(5,142)	1:A:6:DG:H5'	1:A:6:DG:H8	5	0.13
(5,142)	1:A:6:DG:H5'	1:B:6:DG:H8	5	0.13
(5,142)	1:B:6:DG:H5'	1:A:6:DG:H8	5	0.13
(5,142)	1:B:6:DG:H5'	1:B:6:DG:H8	5	0.13
(4,97)	1:A:26:DA:H8	1:A:14:DT:H3'	5	0.13
(4,97)	1:A:26:DA:H8	1:B:14:DT:H3'	5	0.13
(4,97)	1:B:26:DA:H8	1:A:14:DT:H3'	5	0.13
(4,97)	1:B:26:DA:H8	1:B:14:DT:H3'	5	0.13
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	4	0.13
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	4	0.13
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	4	0.13
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,50)	1:A:14:DT:H1'	1:A:15:DA:H2'	4	0.13
(4,50)	1:A:14:DT:H1'	1:B:15:DA:H2'	4	0.13
(4,50)	1:B:14:DT:H1'	1:A:15:DA:H2'	4	0.13
(4,50)	1:B:14:DT:H1'	1:B:15:DA:H2'	4	0.13
(4,24)	1:A:20:DT:H6	1:A:21:DA:H8	5	0.13
(4,24)	1:A:20:DT:H6	1:B:21:DA:H8	5	0.13
(4,24)	1:B:20:DT:H6	1:A:21:DA:H8	5	0.13
(4,24)	1:B:20:DT:H6	1:B:21:DA:H8	5	0.13
(4,21)	1:A:19:DT:H3'	1:A:20:DT:H6	10	0.13
(4,21)	1:A:19:DT:H3'	1:B:20:DT:H6	10	0.13
(4,21)	1:B:19:DT:H3'	1:A:20:DT:H6	10	0.13
(4,21)	1:B:19:DT:H3'	1:B:20:DT:H6	10	0.13
(4,170)	1:A:17:DG:H2"	1:A:18:DG:H1'	3	0.13
(4,170)	1:A:17:DG:H2"	1:B:18:DG:H1'	3	0.13
(4,170)	1:B:17:DG:H2"	1:A:18:DG:H1'	3	0.13
(4,170)	1:B:17:DG:H2"	1:B:18:DG:H1'	3	0.13
(4,144)	1:A:5:DG:H2"	1:A:6:DG:H8	2	0.13
(4,144)	1:A:5:DG:H2"	1:B:6:DG:H8	2	0.13
(4,144)	1:B:5:DG:H2"	1:A:6:DG:H8	2	0.13
(4,144)	1:B:5:DG:H2"	1:B:6:DG:H8	2	0.13
(4,120)	1:A:4:DG:H1	1:A:22:DG:H8	5	0.13
(4,120)	1:A:4:DG:H1	1:B:22:DG:H8	5	0.13
(4,120)	1:B:4:DG:H1	1:A:22:DG:H8	5	0.13
(4,120)	1:B:4:DG:H1	1:B:22:DG:H8	5	0.13
(2,5)	2:A:101:9F0:H14	1:A:9:DA:H2"	4	0.13
(2,5)	2:A:101:9F0:H14	1:B:9:DA:H2"	4	0.13
(2,5)	2:B:101:9F0:H14	1:A:9:DA:H2"	4	0.13
(2,5)	2:B:101:9F0:H14	1:B:9:DA:H2"	4	0.13
(2,47)	2:A:101:9F0:H19	1:A:21:DA:H2	1	0.13
(2,47)	2:A:101:9F0:H19	1:B:21:DA:H2	1	0.13
(2,47)	2:B:101:9F0:H19	1:A:21:DA:H2	1	0.13
(2,47)	2:B:101:9F0:H19	1:B:21:DA:H2	1	0.13
(2,211)	2:A:102:9F0:H6	1:A:25:DA:H1'	1	0.13
(2,211)	2:A:102:9F0:H6	1:B:25:DA:H1'	1	0.13
(2,211)	2:B:102:9F0:H6	1:A:25:DA:H1'	1	0.13
(2,211)	2:B:102:9F0:H6	1:B:25:DA:H1'	1	0.13
(2,211)	2:A:102:9F0:H6	1:A:25:DA:H1'	8	0.13
(2,211)	2:A:102:9F0:H6	1:B:25:DA:H1'	8	0.13
(2,211)	2:B:102:9F0:H6	1:A:25:DA:H1'	8	0.13
(2,211)	2:B:102:9F0:H6	1:B:25:DA:H1'	8	0.13
(2,195)	2:A:102:9F0:H34	1:A:13:DT:H1'	4	0.13
(2,195)	2:A:102:9F0:H34	1:B:13:DT:H1'	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,195)	2:B:102:9F0:H34	1:A:13:DT:H1'	4	0.13
(2,195)	2:B:102:9F0:H34	1:B:13:DT:H1'	4	0.13
(2,191)	2:A:102:9F0:H34	1:A:12:DG:H2'	5	0.13
(2,191)	2:A:102:9F0:H34	1:B:12:DG:H2'	5	0.13
(2,191)	2:B:102:9F0:H34	1:A:12:DG:H2'	5	0.13
(2,191)	2:B:102:9F0:H34	1:B:12:DG:H2'	5	0.13
(2,164)	2:A:102:9F0:H19	1:A:6:DG:H1	4	0.13
(2,164)	2:A:102:9F0:H19	1:B:6:DG:H1	4	0.13
(2,164)	2:B:102:9F0:H19	1:A:6:DG:H1	4	0.13
(2,164)	2:B:102:9F0:H19	1:B:6:DG:H1	4	0.13
(2,150)	2:A:102:9F0:H31	1:A:24:DG:H8	8	0.13
(2,150)	2:A:102:9F0:H31	1:B:24:DG:H8	8	0.13
(2,150)	2:B:102:9F0:H31	1:A:24:DG:H8	8	0.13
(2,150)	2:B:102:9F0:H31	1:B:24:DG:H8	8	0.13
(2,147)	2:A:102:9F0:H28	1:A:14:DT:H1'	5	0.13
(2,147)	2:A:102:9F0:H28	1:B:14:DT:H1'	5	0.13
(2,147)	2:B:102:9F0:H28	1:A:14:DT:H1'	5	0.13
(2,147)	2:B:102:9F0:H28	1:B:14:DT:H1'	5	0.13
(2,129)	2:A:102:9F0:H10	1:A:25:DA:H2	3	0.13
(2,129)	2:A:102:9F0:H10	1:B:25:DA:H2	3	0.13
(2,129)	2:B:102:9F0:H10	1:A:25:DA:H2	3	0.13
(2,129)	2:B:102:9F0:H10	1:B:25:DA:H2	3	0.13
(2,122)	2:A:102:9F0:H14	1:A:24:DG:H2'	9	0.13
(2,122)	2:A:102:9F0:H14	1:B:24:DG:H2'	9	0.13
(2,122)	2:B:102:9F0:H14	1:A:24:DG:H2'	9	0.13
(2,122)	2:B:102:9F0:H14	1:B:24:DG:H2'	9	0.13
(2,12)	2:A:101:9F0:H13	1:A:9:DA:H2"	7	0.13
(2,12)	2:A:101:9F0:H13	1:B:9:DA:H2"	7	0.13
(2,12)	2:B:101:9F0:H13	1:A:9:DA:H2"	7	0.13
(2,12)	2:B:101:9F0:H13	1:B:9:DA:H2"	7	0.13
(1,6)	1:A:14:DT:H3	1:A:25:DA:N7	6	0.13
(1,6)	1:A:14:DT:H3	1:B:25:DA:N7	6	0.13
(1,6)	1:B:14:DT:H3	1:A:25:DA:N7	6	0.13
(1,6)	1:B:14:DT:H3	1:B:25:DA:N7	6	0.13
(1,6)	1:A:14:DT:H3	1:A:25:DA:N7	8	0.13
(1,6)	1:A:14:DT:H3	1:B:25:DA:N7	8	0.13
(1,6)	1:B:14:DT:H3	1:A:25:DA:N7	8	0.13
(1,6)	1:B:14:DT:H3	1:B:25:DA:N7	8	0.13
(1,56)	1:A:16:DG:O6	1:A:12:DG:N1	8	0.13
(1,56)	1:A:16:DG:O6	1:B:12:DG:N1	8	0.13
(1,56)	1:B:16:DG:O6	1:A:12:DG:N1	8	0.13
(1,56)	1:B:16:DG:O6	1:B:12:DG:N1	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	2	0.13
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	2	0.13
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	2	0.13
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	2	0.13
(1,46)	1:A:6:DG:N7	1:A:24:DG:N2	8	0.13
(1,46)	1:A:6:DG:N7	1:B:24:DG:N2	8	0.13
(1,46)	1:B:6:DG:N7	1:A:24:DG:N2	8	0.13
(1,46)	1:B:6:DG:N7	1:B:24:DG:N2	8	0.13
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	2	0.13
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	2	0.13
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	2	0.13
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	2	0.13
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	6	0.13
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	6	0.13
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	6	0.13
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	6	0.13
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	7	0.13
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	7	0.13
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	7	0.13
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	7	0.13
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	9	0.13
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	9	0.13
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	9	0.13
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	9	0.13
(1,34)	1:A:23:DG:N7	1:A:17:DG:N2	6	0.13
(1,34)	1:A:23:DG:N7	1:B:17:DG:N2	6	0.13
(1,34)	1:B:23:DG:N7	1:A:17:DG:N2	6	0.13
(1,34)	1:B:23:DG:N7	1:B:17:DG:N2	6	0.13
(1,34)	1:A:23:DG:N7	1:A:17:DG:N2	7	0.13
(1,34)	1:A:23:DG:N7	1:B:17:DG:N2	7	0.13
(1,34)	1:B:23:DG:N7	1:A:17:DG:N2	7	0.13
(1,34)	1:B:23:DG:N7	1:B:17:DG:N2	7	0.13
(1,34)	1:A:23:DG:N7	1:A:17:DG:N2	10	0.13
(1,34)	1:A:23:DG:N7	1:B:17:DG:N2	10	0.13
(1,34)	1:B:23:DG:N7	1:A:17:DG:N2	10	0.13
(1,34)	1:B:23:DG:N7	1:B:17:DG:N2	10	0.13
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	3	0.13
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	3	0.13
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	3	0.13
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	3	0.13
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	4	0.13
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	4	0.13
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	4	0.13
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	8	0.13
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	8	0.13
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	8	0.13
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	8	0.13
(1,29)	1:A:5:DG:N7	1:A:23:DG:H22	5	0.13
(1,29)	1:A:5:DG:N7	1:B:23:DG:H22	5	0.13
(1,29)	1:B:5:DG:N7	1:A:23:DG:H22	5	0.13
(1,29)	1:B:5:DG:N7	1:B:23:DG:H22	5	0.13
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	3	0.13
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	3	0.13
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	3	0.13
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	3	0.13
(1,16)	1:A:22:DG:O6	1:A:4:DG:N1	2	0.13
(1,16)	1:A:22:DG:O6	1:B:4:DG:N1	2	0.13
(1,16)	1:B:22:DG:O6	1:A:4:DG:N1	2	0.13
(1,16)	1:B:22:DG:O6	1:B:4:DG:N1	2	0.13
(6,8)	2:A:101:9F0:H47	2:A:101:9F0:H31	4	0.12
(6,8)	2:A:101:9F0:H47	2:B:101:9F0:H31	4	0.12
(6,8)	2:B:101:9F0:H47	2:A:101:9F0:H31	4	0.12
(6,8)	2:B:101:9F0:H47	2:B:101:9F0:H31	4	0.12
(6,18)	2:A:101:9F0:H6	2:A:101:9F0:H27	6	0.12
(6,18)	2:A:101:9F0:H6	2:B:101:9F0:H27	6	0.12
(6,18)	2:B:101:9F0:H6	2:A:101:9F0:H27	6	0.12
(6,18)	2:B:101:9F0:H6	2:B:101:9F0:H27	6	0.12
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	3	0.12
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	3	0.12
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	3	0.12
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	3	0.12
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	4	0.12
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	4	0.12
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	4	0.12
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	4	0.12
(5,83)	1:A:15:DA:H3'	1:A:15:DA:H8	2	0.12
(5,83)	1:A:15:DA:H3'	1:B:15:DA:H8	2	0.12
(5,83)	1:B:15:DA:H3'	1:A:15:DA:H8	2	0.12
(5,83)	1:B:15:DA:H3'	1:B:15:DA:H8	2	0.12
(5,58)	1:A:21:DA:H5'	1:A:21:DA:H8	5	0.12
(5,58)	1:A:21:DA:H5'	1:B:21:DA:H8	5	0.12
(5,58)	1:B:21:DA:H5'	1:A:21:DA:H8	5	0.12
(5,58)	1:B:21:DA:H5'	1:B:21:DA:H8	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,58)	1:A:21:DA:H5'	1:A:21:DA:H8	7	0.12
(5,58)	1:A:21:DA:H5'	1:B:21:DA:H8	7	0.12
(5,58)	1:B:21:DA:H5'	1:A:21:DA:H8	7	0.12
(5,58)	1:B:21:DA:H5'	1:B:21:DA:H8	7	0.12
(5,58)	1:A:21:DA:H5'	1:A:21:DA:H8	10	0.12
(5,58)	1:A:21:DA:H5'	1:B:21:DA:H8	10	0.12
(5,58)	1:B:21:DA:H5'	1:A:21:DA:H8	10	0.12
(5,58)	1:B:21:DA:H5'	1:B:21:DA:H8	10	0.12
(5,37)	1:A:19:DT:H2"	1:A:19:DT:H6	10	0.12
(5,37)	1:A:19:DT:H2"	1:B:19:DT:H6	10	0.12
(5,37)	1:B:19:DT:H2"	1:A:19:DT:H6	10	0.12
(5,37)	1:B:19:DT:H2"	1:B:19:DT:H6	10	0.12
(5,20)	1:A:3:DA:H4'	1:A:3:DA:H1'	6	0.12
(5,20)	1:A:3:DA:H4'	1:B:3:DA:H1'	6	0.12
(5,20)	1:B:3:DA:H4'	1:A:3:DA:H1'	6	0.12
(5,20)	1:B:3:DA:H4'	1:B:3:DA:H1'	6	0.12
(5,20)	1:A:3:DA:H4'	1:A:3:DA:H1'	8	0.12
(5,20)	1:A:3:DA:H4'	1:B:3:DA:H1'	8	0.12
(5,20)	1:B:3:DA:H4'	1:A:3:DA:H1'	8	0.12
(5,20)	1:B:3:DA:H4'	1:B:3:DA:H1'	8	0.12
(5,20)	1:A:3:DA:H4'	1:A:3:DA:H1'	9	0.12
(5,20)	1:A:3:DA:H4'	1:B:3:DA:H1'	9	0.12
(5,20)	1:B:3:DA:H4'	1:A:3:DA:H1'	9	0.12
(5,20)	1:B:3:DA:H4'	1:B:3:DA:H1'	9	0.12
(4,96)	1:A:26:DA:H8	1:A:14:DT:H2"	5	0.12
(4,96)	1:A:26:DA:H8	1:B:14:DT:H2"	5	0.12
(4,96)	1:B:26:DA:H8	1:A:14:DT:H2"	5	0.12
(4,96)	1:B:26:DA:H8	1:B:14:DT:H2"	5	0.12
(4,73)	1:A:26:DA:H2	1:A:13:DT:H3	5	0.12
(4,73)	1:A:26:DA:H2	1:B:13:DT:H3	5	0.12
(4,73)	1:B:26:DA:H2	1:A:13:DT:H3	5	0.12
(4,73)	1:B:26:DA:H2	1:B:13:DT:H3	5	0.12
(4,50)	1:A:14:DT:H1'	1:A:15:DA:H2'	2	0.12
(4,50)	1:A:14:DT:H1'	1:B:15:DA:H2'	2	0.12
(4,50)	1:B:14:DT:H1'	1:A:15:DA:H2'	2	0.12
(4,50)	1:B:14:DT:H1'	1:B:15:DA:H2'	2	0.12
(4,42)	1:A:21:DA:H2'	1:A:18:DG:H8	1	0.12
(4,42)	1:A:21:DA:H2'	1:B:18:DG:H8	1	0.12
(4,42)	1:B:21:DA:H2'	1:A:18:DG:H8	1	0.12
(4,42)	1:B:21:DA:H2'	1:B:18:DG:H8	1	0.12
(4,169)	1:A:17:DG:H2'	1:A:18:DG:H1'	2	0.12
(4,169)	1:A:17:DG:H2'	1:B:18:DG:H1'	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,169)	1:B:17:DG:H2'	1:A:18:DG:H1'	2	0.12
(4,169)	1:B:17:DG:H2'	1:B:18:DG:H1'	2	0.12
(4,166)	1:A:17:DG:H1'	1:A:16:DG:H8	9	0.12
(4,166)	1:A:17:DG:H1'	1:B:16:DG:H8	9	0.12
(4,166)	1:B:17:DG:H1'	1:A:16:DG:H8	9	0.12
(4,166)	1:B:17:DG:H1'	1:B:16:DG:H8	9	0.12
(4,16)	1:A:8:DT:H1'	1:A:9:DA:H8	3	0.12
(4,16)	1:A:8:DT:H1'	1:B:9:DA:H8	3	0.12
(4,16)	1:B:8:DT:H1'	1:A:9:DA:H8	3	0.12
(4,16)	1:B:8:DT:H1'	1:B:9:DA:H8	3	0.12
(4,16)	1:A:8:DT:H1'	1:A:9:DA:H8	7	0.12
(4,16)	1:A:8:DT:H1'	1:B:9:DA:H8	7	0.12
(4,16)	1:B:8:DT:H1'	1:A:9:DA:H8	7	0.12
(4,16)	1:B:8:DT:H1'	1:B:9:DA:H8	7	0.12
(4,144)	1:A:5:DG:H2"	1:A:6:DG:H8	3	0.12
(4,144)	1:A:5:DG:H2"	1:B:6:DG:H8	3	0.12
(4,144)	1:B:5:DG:H2"	1:A:6:DG:H8	3	0.12
(4,144)	1:B:5:DG:H2"	1:B:6:DG:H8	3	0.12
(2,8)	2:A:101:9F0:H10	1:A:10:DG:H1	1	0.12
(2,8)	2:A:101:9F0:H10	1:B:10:DG:H1	1	0.12
(2,8)	2:B:101:9F0:H10	1:A:10:DG:H1	1	0.12
(2,8)	2:B:101:9F0:H10	1:B:10:DG:H1	1	0.12
(2,211)	2:A:102:9F0:H6	1:A:25:DA:H1'	4	0.12
(2,211)	2:A:102:9F0:H6	1:B:25:DA:H1'	4	0.12
(2,211)	2:B:102:9F0:H6	1:A:25:DA:H1'	4	0.12
(2,211)	2:B:102:9F0:H6	1:B:25:DA:H1'	4	0.12
(2,195)	2:A:102:9F0:H34	1:A:13:DT:H1'	5	0.12
(2,195)	2:A:102:9F0:H34	1:B:13:DT:H1'	5	0.12
(2,195)	2:B:102:9F0:H34	1:A:13:DT:H1'	5	0.12
(2,195)	2:B:102:9F0:H34	1:B:13:DT:H1'	5	0.12
(2,192)	2:A:102:9F0:H34	1:A:12:DG:H3'	3	0.12
(2,192)	2:A:102:9F0:H34	1:B:12:DG:H3'	3	0.12
(2,192)	2:B:102:9F0:H34	1:A:12:DG:H3'	3	0.12
(2,192)	2:B:102:9F0:H34	1:B:12:DG:H3'	3	0.12
(2,180)	2:A:102:9F0:H18	1:A:13:DT:H1'	5	0.12
(2,180)	2:A:102:9F0:H18	1:B:13:DT:H1'	5	0.12
(2,180)	2:B:102:9F0:H18	1:A:13:DT:H1'	5	0.12
(2,180)	2:B:102:9F0:H18	1:B:13:DT:H1'	5	0.12
(2,164)	2:A:102:9F0:H19	1:A:6:DG:H1	3	0.12
(2,164)	2:A:102:9F0:H19	1:B:6:DG:H1	3	0.12
(2,164)	2:B:102:9F0:H19	1:A:6:DG:H1	3	0.12
(2,164)	2:B:102:9F0:H19	1:B:6:DG:H1	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,159)	2:A:102:9F0:H48	1:A:14:DT:H6	7	0.12
(2,159)	2:A:102:9F0:H48	1:B:14:DT:H6	7	0.12
(2,159)	2:B:102:9F0:H48	1:A:14:DT:H6	7	0.12
(2,159)	2:B:102:9F0:H48	1:B:14:DT:H6	7	0.12
(2,12)	2:A:101:9F0:H13	1:A:9:DA:H2"	8	0.12
(2,12)	2:A:101:9F0:H13	1:B:9:DA:H2"	8	0.12
(2,12)	2:B:101:9F0:H13	1:A:9:DA:H2"	8	0.12
(2,12)	2:B:101:9F0:H13	1:B:9:DA:H2"	8	0.12
(2,12)	2:A:101:9F0:H13	1:A:9:DA:H2"	10	0.12
(2,12)	2:A:101:9F0:H13	1:B:9:DA:H2"	10	0.12
(2,12)	2:B:101:9F0:H13	1:A:9:DA:H2"	10	0.12
(2,12)	2:B:101:9F0:H13	1:B:9:DA:H2"	10	0.12
(2,108)	2:A:101:9F0:H27	1:A:9:DA:H2'	2	0.12
(2,108)	2:A:101:9F0:H27	1:B:9:DA:H2'	2	0.12
(2,108)	2:B:101:9F0:H27	1:A:9:DA:H2'	2	0.12
(2,108)	2:B:101:9F0:H27	1:B:9:DA:H2'	2	0.12
(1,6)	1:A:14:DT:H3	1:A:25:DA:N7	3	0.12
(1,6)	1:A:14:DT:H3	1:B:25:DA:N7	3	0.12
(1,6)	1:B:14:DT:H3	1:A:25:DA:N7	3	0.12
(1,6)	1:B:14:DT:H3	1:B:25:DA:N7	3	0.12
(1,6)	1:A:14:DT:H3	1:A:25:DA:N7	7	0.12
(1,6)	1:A:14:DT:H3	1:B:25:DA:N7	7	0.12
(1,6)	1:B:14:DT:H3	1:A:25:DA:N7	7	0.12
(1,6)	1:B:14:DT:H3	1:B:25:DA:N7	7	0.12
(1,54)	1:A:16:DG:N7	1:A:12:DG:N2	6	0.12
(1,54)	1:A:16:DG:N7	1:B:12:DG:N2	6	0.12
(1,54)	1:B:16:DG:N7	1:A:12:DG:N2	6	0.12
(1,54)	1:B:16:DG:N7	1:B:12:DG:N2	6	0.12
(1,54)	1:A:16:DG:N7	1:A:12:DG:N2	7	0.12
(1,54)	1:A:16:DG:N7	1:B:12:DG:N2	7	0.12
(1,54)	1:B:16:DG:N7	1:A:12:DG:N2	7	0.12
(1,54)	1:B:16:DG:N7	1:B:12:DG:N2	7	0.12
(1,52)	1:A:24:DG:O6	1:A:16:DG:N1	4	0.12
(1,52)	1:A:24:DG:O6	1:B:16:DG:N1	4	0.12
(1,52)	1:B:24:DG:O6	1:A:16:DG:N1	4	0.12
(1,52)	1:B:24:DG:O6	1:B:16:DG:N1	4	0.12
(1,46)	1:A:6:DG:N7	1:A:24:DG:N2	3	0.12
(1,46)	1:A:6:DG:N7	1:B:24:DG:N2	3	0.12
(1,46)	1:B:6:DG:N7	1:A:24:DG:N2	3	0.12
(1,46)	1:B:6:DG:N7	1:B:24:DG:N2	3	0.12
(1,46)	1:A:6:DG:N7	1:A:24:DG:N2	5	0.12
(1,46)	1:A:6:DG:N7	1:B:24:DG:N2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:B:6:DG:N7	1:A:24:DG:N2	5	0.12
(1,46)	1:B:6:DG:N7	1:B:24:DG:N2	5	0.12
(1,40)	1:A:17:DG:O6	1:A:11:DG:N1	8	0.12
(1,40)	1:A:17:DG:O6	1:B:11:DG:N1	8	0.12
(1,40)	1:B:17:DG:O6	1:A:11:DG:N1	8	0.12
(1,40)	1:B:17:DG:O6	1:B:11:DG:N1	8	0.12
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	4	0.12
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	4	0.12
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	4	0.12
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	4	0.12
(1,36)	1:A:23:DG:O6	1:A:17:DG:N1	10	0.12
(1,36)	1:A:23:DG:O6	1:B:17:DG:N1	10	0.12
(1,36)	1:B:23:DG:O6	1:A:17:DG:N1	10	0.12
(1,36)	1:B:23:DG:O6	1:B:17:DG:N1	10	0.12
(1,34)	1:A:23:DG:N7	1:A:17:DG:N2	4	0.12
(1,34)	1:A:23:DG:N7	1:B:17:DG:N2	4	0.12
(1,34)	1:B:23:DG:N7	1:A:17:DG:N2	4	0.12
(1,34)	1:B:23:DG:N7	1:B:17:DG:N2	4	0.12
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	6	0.12
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	6	0.12
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	6	0.12
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	6	0.12
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	7	0.12
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	7	0.12
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	7	0.12
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	7	0.12
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	5	0.12
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	5	0.12
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	5	0.12
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	5	0.12
(1,19)	1:A:18:DG:O6	1:A:22:DG:H1	9	0.12
(1,19)	1:A:18:DG:O6	1:B:22:DG:H1	9	0.12
(1,19)	1:B:18:DG:O6	1:A:22:DG:H1	9	0.12
(1,19)	1:B:18:DG:O6	1:B:22:DG:H1	9	0.12
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	6	0.11
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	6	0.11
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	6	0.11
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	6	0.11
(5,93)	1:A:25:DA:H4'	1:A:25:DA:H1'	7	0.11
(5,93)	1:A:25:DA:H4'	1:B:25:DA:H1'	7	0.11
(5,93)	1:B:25:DA:H4'	1:A:25:DA:H1'	7	0.11
(5,93)	1:B:25:DA:H4'	1:B:25:DA:H1'	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,58)	1:A:21:DA:H5'	1:A:21:DA:H8	3	0.11
(5,58)	1:A:21:DA:H5'	1:B:21:DA:H8	3	0.11
(5,58)	1:B:21:DA:H5'	1:A:21:DA:H8	3	0.11
(5,58)	1:B:21:DA:H5'	1:B:21:DA:H8	3	0.11
(5,37)	1:A:19:DT:H2"	1:A:19:DT:H6	6	0.11
(5,37)	1:A:19:DT:H2"	1:B:19:DT:H6	6	0.11
(5,37)	1:B:19:DT:H2"	1:A:19:DT:H6	6	0.11
(5,37)	1:B:19:DT:H2"	1:B:19:DT:H6	6	0.11
(5,37)	1:A:19:DT:H2"	1:A:19:DT:H6	8	0.11
(5,37)	1:A:19:DT:H2"	1:B:19:DT:H6	8	0.11
(5,37)	1:B:19:DT:H2"	1:A:19:DT:H6	8	0.11
(5,37)	1:B:19:DT:H2"	1:B:19:DT:H6	8	0.11
(5,142)	1:A:6:DG:H5'	1:A:6:DG:H8	6	0.11
(5,142)	1:A:6:DG:H5'	1:B:6:DG:H8	6	0.11
(5,142)	1:B:6:DG:H5'	1:A:6:DG:H8	6	0.11
(5,142)	1:B:6:DG:H5'	1:B:6:DG:H8	6	0.11
(5,131)	1:A:6:DG:H2'	1:A:6:DG:H8	6	0.11
(5,131)	1:A:6:DG:H2'	1:B:6:DG:H8	6	0.11
(5,131)	1:B:6:DG:H2'	1:A:6:DG:H8	6	0.11
(5,131)	1:B:6:DG:H2'	1:B:6:DG:H8	6	0.11
(5,12)	1:A:2:DA:H5"	1:A:2:DA:H8	10	0.11
(5,12)	1:A:2:DA:H5"	1:B:2:DA:H8	10	0.11
(5,12)	1:B:2:DA:H5"	1:A:2:DA:H8	10	0.11
(5,12)	1:B:2:DA:H5"	1:B:2:DA:H8	10	0.11
(4,64)	1:A:15:DA:H4'	1:A:16:DG:H1'	7	0.11
(4,64)	1:A:15:DA:H4'	1:B:16:DG:H1'	7	0.11
(4,64)	1:B:15:DA:H4'	1:A:16:DG:H1'	7	0.11
(4,64)	1:B:15:DA:H4'	1:B:16:DG:H1'	7	0.11
(4,42)	1:A:21:DA:H2'	1:A:18:DG:H8	2	0.11
(4,42)	1:A:21:DA:H2'	1:B:18:DG:H8	2	0.11
(4,42)	1:B:21:DA:H2'	1:A:18:DG:H8	2	0.11
(4,42)	1:B:21:DA:H2'	1:B:18:DG:H8	2	0.11
(4,42)	1:A:21:DA:H2'	1:A:18:DG:H8	6	0.11
(4,42)	1:A:21:DA:H2'	1:B:18:DG:H8	6	0.11
(4,42)	1:B:21:DA:H2'	1:A:18:DG:H8	6	0.11
(4,42)	1:B:21:DA:H2'	1:B:18:DG:H8	6	0.11
(4,42)	1:A:21:DA:H2'	1:A:18:DG:H8	8	0.11
(4,42)	1:A:21:DA:H2'	1:B:18:DG:H8	8	0.11
(4,42)	1:B:21:DA:H2'	1:A:18:DG:H8	8	0.11
(4,42)	1:B:21:DA:H2'	1:B:18:DG:H8	8	0.11
(4,37)	1:A:21:DA:H8	1:A:18:DG:H8	7	0.11
(4,37)	1:A:21:DA:H8	1:B:18:DG:H8	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:B:21:DA:H8	1:A:18:DG:H8	7	0.11
(4,37)	1:B:21:DA:H8	1:B:18:DG:H8	7	0.11
(4,170)	1:A:17:DG:H2"	1:A:18:DG:H1'	1	0.11
(4,170)	1:A:17:DG:H2"	1:B:18:DG:H1'	1	0.11
(4,170)	1:B:17:DG:H2"	1:A:18:DG:H1'	1	0.11
(4,170)	1:B:17:DG:H2"	1:B:18:DG:H1'	1	0.11
(4,153)	1:A:10:DG:H2"	1:A:11:DG:H8	2	0.11
(4,153)	1:A:10:DG:H2"	1:B:11:DG:H8	2	0.11
(4,153)	1:B:10:DG:H2"	1:A:11:DG:H8	2	0.11
(4,153)	1:B:10:DG:H2"	1:B:11:DG:H8	2	0.11
(4,10)	1:A:2:DA:H2"	1:A:3:DA:H8	2	0.11
(4,10)	1:A:2:DA:H2"	1:B:3:DA:H8	2	0.11
(4,10)	1:B:2:DA:H2"	1:A:3:DA:H8	2	0.11
(4,10)	1:B:2:DA:H2"	1:B:3:DA:H8	2	0.11
(4,10)	1:A:2:DA:H2"	1:A:3:DA:H8	3	0.11
(4,10)	1:A:2:DA:H2"	1:B:3:DA:H8	3	0.11
(4,10)	1:B:2:DA:H2"	1:A:3:DA:H8	3	0.11
(4,10)	1:B:2:DA:H2"	1:B:3:DA:H8	3	0.11
(2,55)	2:A:101:9F0:H16	1:A:4:DG:H8	1	0.11
(2,55)	2:A:101:9F0:H16	1:B:4:DG:H8	1	0.11
(2,55)	2:B:101:9F0:H16	1:A:4:DG:H8	1	0.11
(2,55)	2:B:101:9F0:H16	1:B:4:DG:H8	1	0.11
(2,43)	2:A:101:9F0:H15	1:A:4:DG:H1	2	0.11
(2,43)	2:A:101:9F0:H15	1:B:4:DG:H1	2	0.11
(2,43)	2:B:101:9F0:H15	1:A:4:DG:H1	2	0.11
(2,43)	2:B:101:9F0:H15	1:B:4:DG:H1	2	0.11
(2,40)	2:A:101:9F0:H19	1:A:3:DA:H2	7	0.11
(2,40)	2:A:101:9F0:H19	1:B:3:DA:H2	7	0.11
(2,40)	2:B:101:9F0:H19	1:A:3:DA:H2	7	0.11
(2,40)	2:B:101:9F0:H19	1:B:3:DA:H2	7	0.11
(2,35)	2:A:101:9F0:H60	1:A:10:DG:H8	4	0.11
(2,35)	2:A:101:9F0:H60	1:B:10:DG:H8	4	0.11
(2,35)	2:B:101:9F0:H60	1:A:10:DG:H8	4	0.11
(2,35)	2:B:101:9F0:H60	1:B:10:DG:H8	4	0.11
(2,211)	2:A:102:9F0:H6	1:A:25:DA:H1'	5	0.11
(2,211)	2:A:102:9F0:H6	1:B:25:DA:H1'	5	0.11
(2,211)	2:B:102:9F0:H6	1:A:25:DA:H1'	5	0.11
(2,211)	2:B:102:9F0:H6	1:B:25:DA:H1'	5	0.11
(2,184)	2:A:102:9F0:H37	1:A:6:DG:H2'	10	0.11
(2,184)	2:A:102:9F0:H37	1:B:6:DG:H2'	10	0.11
(2,184)	2:B:102:9F0:H37	1:A:6:DG:H2'	10	0.11
(2,184)	2:B:102:9F0:H37	1:B:6:DG:H2'	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,180)	2:A:102:9F0:H18	1:A:13:DT:H1'	3	0.11
(2,180)	2:A:102:9F0:H18	1:B:13:DT:H1'	3	0.11
(2,180)	2:B:102:9F0:H18	1:A:13:DT:H1'	3	0.11
(2,180)	2:B:102:9F0:H18	1:B:13:DT:H1'	3	0.11
(2,160)	2:A:102:9F0:H48	1:A:14:DT:C5	6	0.11
(2,160)	2:A:102:9F0:H48	1:B:14:DT:C5	6	0.11
(2,160)	2:B:102:9F0:H48	1:A:14:DT:C5	6	0.11
(2,160)	2:B:102:9F0:H48	1:B:14:DT:C5	6	0.11
(2,122)	2:A:102:9F0:H14	1:A:24:DG:H2'	10	0.11
(2,122)	2:A:102:9F0:H14	1:B:24:DG:H2'	10	0.11
(2,122)	2:B:102:9F0:H14	1:A:24:DG:H2'	10	0.11
(2,122)	2:B:102:9F0:H14	1:B:24:DG:H2'	10	0.11
(2,12)	2:A:101:9F0:H13	1:A:9:DA:H2"	2	0.11
(2,12)	2:A:101:9F0:H13	1:B:9:DA:H2"	2	0.11
(2,12)	2:B:101:9F0:H13	1:A:9:DA:H2"	2	0.11
(2,12)	2:B:101:9F0:H13	1:B:9:DA:H2"	2	0.11
(2,110)	2:A:101:9F0:H27	1:A:9:DA:H8	1	0.11
(2,110)	2:A:101:9F0:H27	1:B:9:DA:H8	1	0.11
(2,110)	2:B:101:9F0:H27	1:A:9:DA:H8	1	0.11
(2,110)	2:B:101:9F0:H27	1:B:9:DA:H8	1	0.11
(1,6)	1:A:14:DT:H3	1:A:25:DA:N7	1	0.11
(1,6)	1:A:14:DT:H3	1:B:25:DA:N7	1	0.11
(1,6)	1:B:14:DT:H3	1:A:25:DA:N7	1	0.11
(1,6)	1:B:14:DT:H3	1:B:25:DA:N7	1	0.11
(1,6)	1:A:14:DT:H3	1:A:25:DA:N7	9	0.11
(1,6)	1:A:14:DT:H3	1:B:25:DA:N7	9	0.11
(1,6)	1:B:14:DT:H3	1:A:25:DA:N7	9	0.11
(1,6)	1:B:14:DT:H3	1:B:25:DA:N7	9	0.11
(1,54)	1:A:16:DG:N7	1:A:12:DG:N2	2	0.11
(1,54)	1:A:16:DG:N7	1:B:12:DG:N2	2	0.11
(1,54)	1:B:16:DG:N7	1:A:12:DG:N2	2	0.11
(1,54)	1:B:16:DG:N7	1:B:12:DG:N2	2	0.11
(1,46)	1:A:6:DG:N7	1:A:24:DG:N2	1	0.11
(1,46)	1:A:6:DG:N7	1:B:24:DG:N2	1	0.11
(1,46)	1:B:6:DG:N7	1:A:24:DG:N2	1	0.11
(1,46)	1:B:6:DG:N7	1:B:24:DG:N2	1	0.11
(1,46)	1:A:6:DG:N7	1:A:24:DG:N2	4	0.11
(1,46)	1:A:6:DG:N7	1:B:24:DG:N2	4	0.11
(1,46)	1:B:6:DG:N7	1:A:24:DG:N2	4	0.11
(1,46)	1:B:6:DG:N7	1:B:24:DG:N2	4	0.11
(1,46)	1:A:6:DG:N7	1:A:24:DG:N2	6	0.11
(1,46)	1:A:6:DG:N7	1:B:24:DG:N2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:B:6:DG:N7	1:A:24:DG:N2	6	0.11
(1,46)	1:B:6:DG:N7	1:B:24:DG:N2	6	0.11
(1,46)	1:A:6:DG:N7	1:A:24:DG:N2	7	0.11
(1,46)	1:A:6:DG:N7	1:B:24:DG:N2	7	0.11
(1,46)	1:B:6:DG:N7	1:A:24:DG:N2	7	0.11
(1,46)	1:B:6:DG:N7	1:B:24:DG:N2	7	0.11
(1,40)	1:A:17:DG:O6	1:A:11:DG:N1	1	0.11
(1,40)	1:A:17:DG:O6	1:B:11:DG:N1	1	0.11
(1,40)	1:B:17:DG:O6	1:A:11:DG:N1	1	0.11
(1,40)	1:B:17:DG:O6	1:B:11:DG:N1	1	0.11
(1,40)	1:A:17:DG:O6	1:A:11:DG:N1	6	0.11
(1,40)	1:A:17:DG:O6	1:B:11:DG:N1	6	0.11
(1,40)	1:B:17:DG:O6	1:A:11:DG:N1	6	0.11
(1,40)	1:B:17:DG:O6	1:B:11:DG:N1	6	0.11
(1,40)	1:A:17:DG:O6	1:A:11:DG:N1	7	0.11
(1,40)	1:A:17:DG:O6	1:B:11:DG:N1	7	0.11
(1,40)	1:B:17:DG:O6	1:A:11:DG:N1	7	0.11
(1,40)	1:B:17:DG:O6	1:B:11:DG:N1	7	0.11
(1,40)	1:A:17:DG:O6	1:A:11:DG:N1	10	0.11
(1,40)	1:A:17:DG:O6	1:B:11:DG:N1	10	0.11
(1,40)	1:B:17:DG:O6	1:A:11:DG:N1	10	0.11
(1,40)	1:B:17:DG:O6	1:B:11:DG:N1	10	0.11
(1,34)	1:A:23:DG:N7	1:A:17:DG:N2	1	0.11
(1,34)	1:A:23:DG:N7	1:B:17:DG:N2	1	0.11
(1,34)	1:B:23:DG:N7	1:A:17:DG:N2	1	0.11
(1,34)	1:B:23:DG:N7	1:B:17:DG:N2	1	0.11
(1,34)	1:A:23:DG:N7	1:A:17:DG:N2	2	0.11
(1,34)	1:A:23:DG:N7	1:B:17:DG:N2	2	0.11
(1,34)	1:B:23:DG:N7	1:A:17:DG:N2	2	0.11
(1,34)	1:B:23:DG:N7	1:B:17:DG:N2	2	0.11
(1,34)	1:A:23:DG:N7	1:A:17:DG:N2	8	0.11
(1,34)	1:A:23:DG:N7	1:B:17:DG:N2	8	0.11
(1,34)	1:B:23:DG:N7	1:A:17:DG:N2	8	0.11
(1,34)	1:B:23:DG:N7	1:B:17:DG:N2	8	0.11
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	9	0.11
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	9	0.11
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	9	0.11
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	9	0.11
(1,32)	1:A:5:DG:O6	1:A:23:DG:N1	10	0.11
(1,32)	1:A:5:DG:O6	1:B:23:DG:N1	10	0.11
(1,32)	1:B:5:DG:O6	1:A:23:DG:N1	10	0.11
(1,32)	1:B:5:DG:O6	1:B:23:DG:N1	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:A:5:DG:N7	1:A:23:DG:H22	1	0.11
(1,29)	1:A:5:DG:N7	1:B:23:DG:H22	1	0.11
(1,29)	1:B:5:DG:N7	1:A:23:DG:H22	1	0.11
(1,29)	1:B:5:DG:N7	1:B:23:DG:H22	1	0.11
(1,27)	1:A:11:DG:O6	1:A:5:DG:H1	3	0.11
(1,27)	1:A:11:DG:O6	1:B:5:DG:H1	3	0.11
(1,27)	1:B:11:DG:O6	1:A:5:DG:H1	3	0.11
(1,27)	1:B:11:DG:O6	1:B:5:DG:H1	3	0.11
(1,17)	1:A:18:DG:N7	1:A:22:DG:H22	10	0.11
(1,17)	1:A:18:DG:N7	1:B:22:DG:H22	10	0.11
(1,17)	1:B:18:DG:N7	1:A:22:DG:H22	10	0.11
(1,17)	1:B:18:DG:N7	1:B:22:DG:H22	10	0.11
(1,14)	1:A:22:DG:N7	1:A:4:DG:N2	10	0.11
(1,14)	1:A:22:DG:N7	1:B:4:DG:N2	10	0.11
(1,14)	1:B:22:DG:N7	1:A:4:DG:N2	10	0.11
(1,14)	1:B:22:DG:N7	1:B:4:DG:N2	10	0.11
(1,11)	1:A:4:DG:O6	1:A:10:DG:H1	6	0.11
(1,11)	1:A:4:DG:O6	1:B:10:DG:H1	6	0.11
(1,11)	1:B:4:DG:O6	1:A:10:DG:H1	6	0.11
(1,11)	1:B:4:DG:O6	1:B:10:DG:H1	6	0.11

10 Dihedral-angle violation analysis

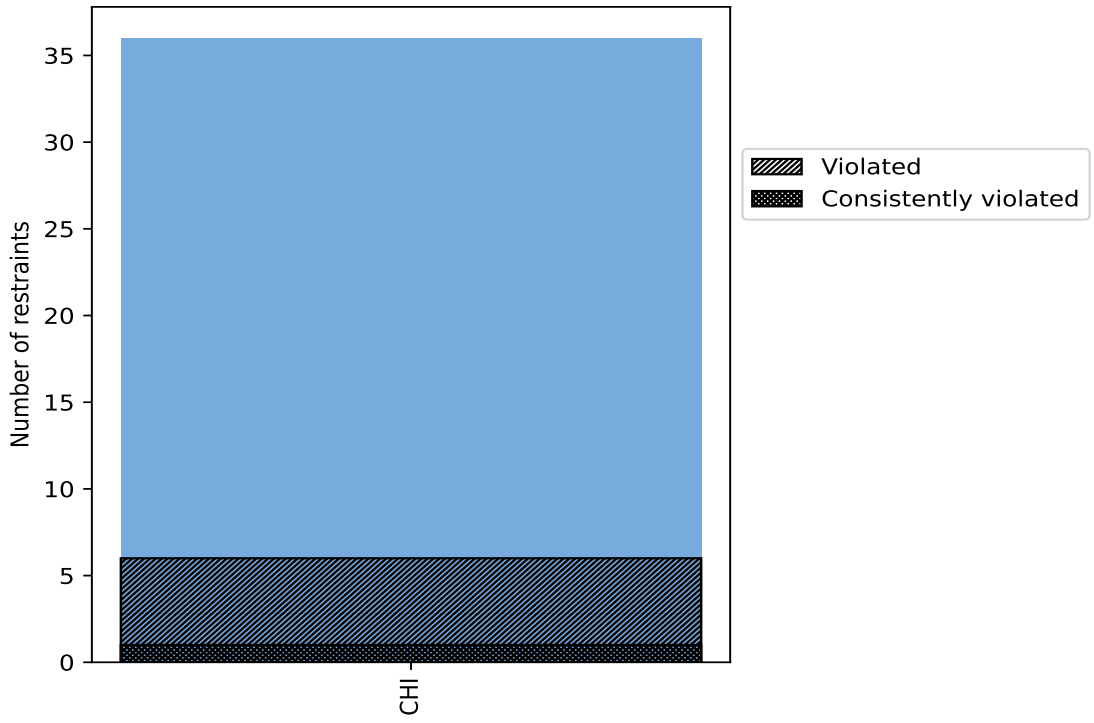
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
CHI	36	100.0	6	16.7	16.7	1	2.8	2.8
Total	36	100.0	6	16.7	16.7	1	2.8	2.8

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



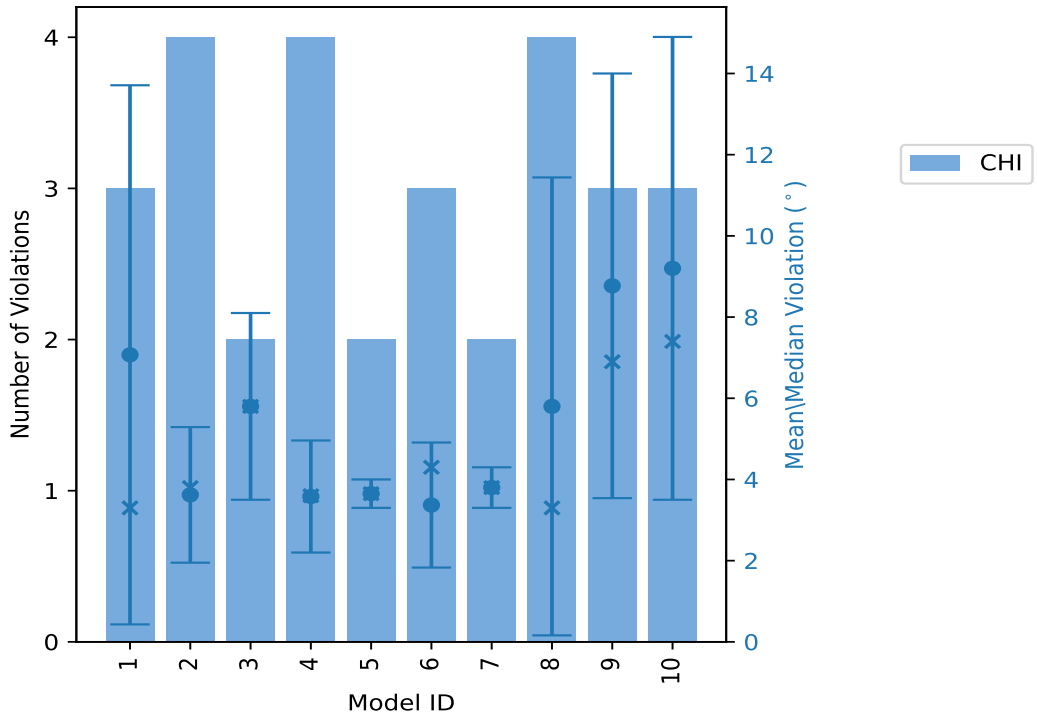
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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

Model ID	Number of violations		Mean (°)	Max (°)	SD (°)	Median (°)
	CHI	Total				
1	3	3	7.07	16.4	6.64	3.3
2	4	4	3.62	5.8	1.67	3.8
3	2	2	5.8	8.1	2.3	5.8
4	4	4	3.58	5.5	1.38	3.6
5	2	2	3.65	4.0	0.35	3.65
6	3	3	3.37	4.6	1.54	4.3
7	2	2	3.8	4.3	0.5	3.8
8	4	4	5.8	15.4	5.64	3.3
9	3	3	8.77	15.9	5.23	6.9
10	3	3	9.2	16.9	5.7	7.4

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



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

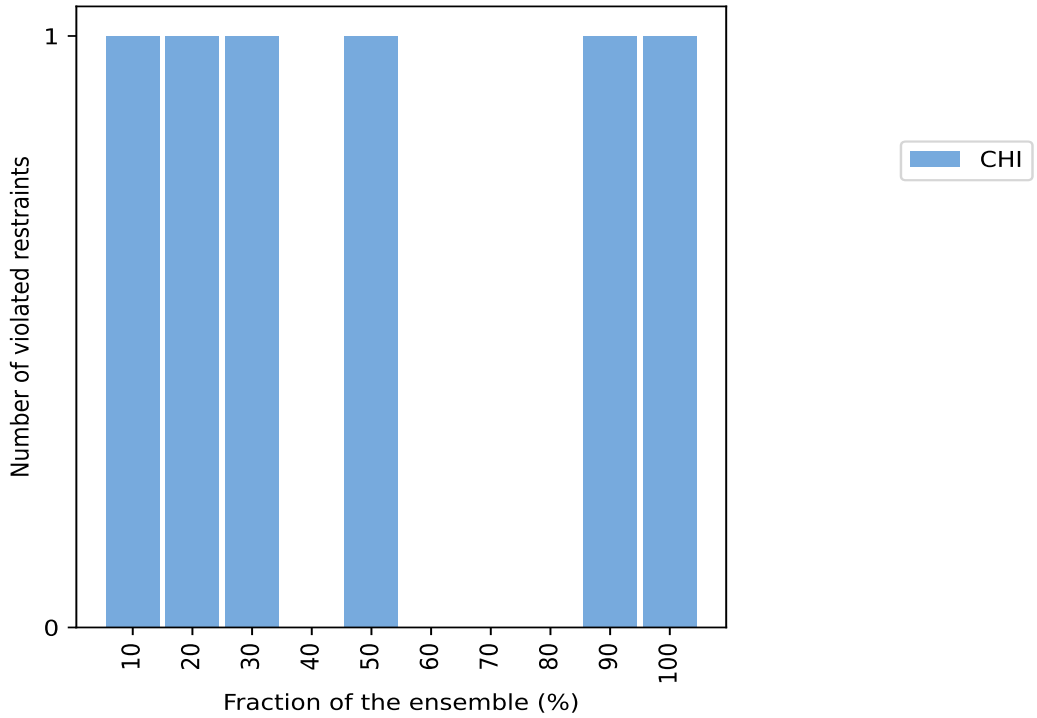
10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints		Fraction of the ensemble	
CHI	Total	Count[1]	%
1	1	1	10.0
1	1	2	20.0
1	1	3	30.0
0	0	4	40.0
1	1	5	50.0
0	0	6	60.0
0	0	7	70.0
0	0	8	80.0
1	1	9	90.0
1	1	10	100.0

[1] Number of models with violations

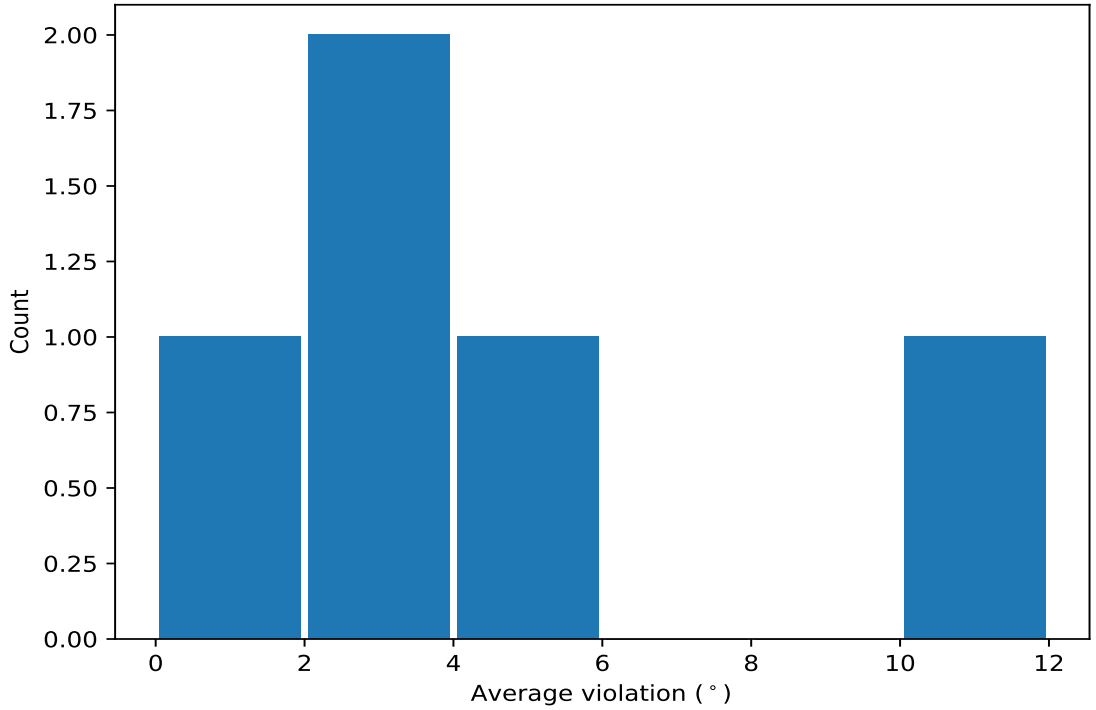
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

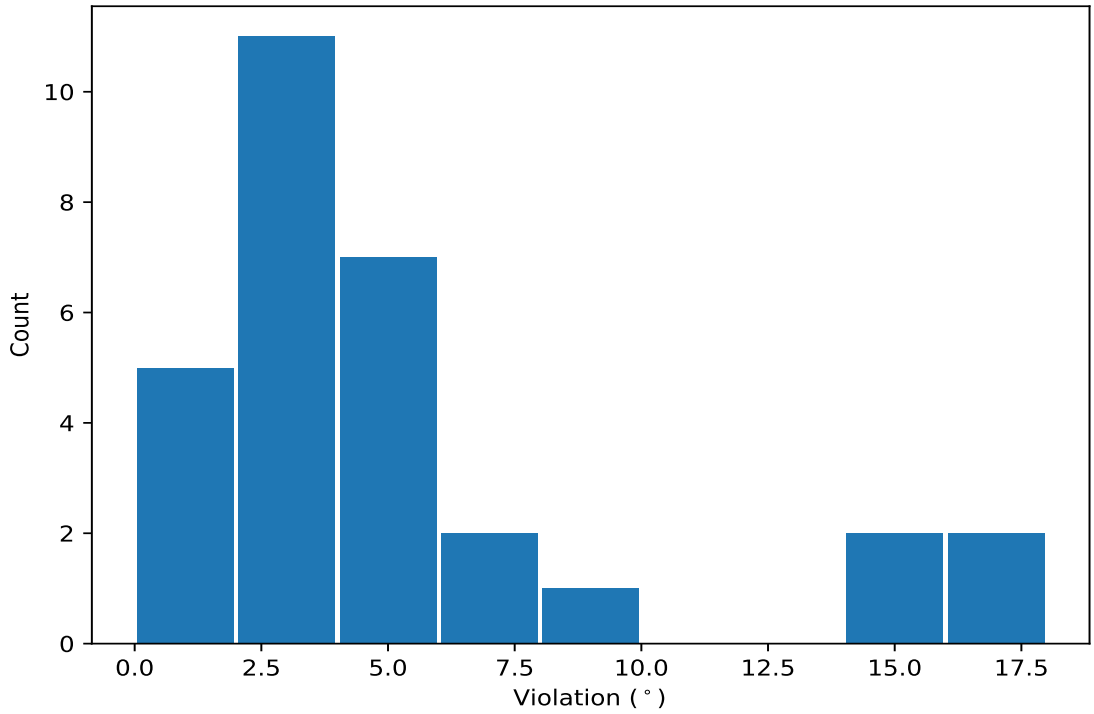
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	10	3.76	0.37	3.65
(1,26)	1:B:15:DA:O4'	1:B:15:DA:C1'	1:B:15:DA:N9	1:B:15:DA:C4	9	10.21	5.45	8.1
(1,8)	1:B:16:DG:O4'	1:B:16:DG:C1'	1:B:16:DG:N9	1:B:16:DG:C4	5	4.66	2.2	3.9
(1,7)	1:A:16:DG:O4'	1:A:16:DG:C1'	1:A:16:DG:N9	1:A:16:DG:C4	3	2.03	0.91	1.6
(1,25)	1:A:15:DA:O4'	1:A:15:DA:C1'	1:A:15:DA:N9	1:A:15:DA:C4	2	1.85	0.65	1.85

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,26)	1:B:15:DA:O4'	1:B:15:DA:C1'	1:B:15:DA:N9	1:B:15:DA:C4	10	16.9
(1,26)	1:B:15:DA:O4'	1:B:15:DA:C1'	1:B:15:DA:N9	1:B:15:DA:C4	1	16.4
(1,26)	1:B:15:DA:O4'	1:B:15:DA:C1'	1:B:15:DA:N9	1:B:15:DA:C4	9	15.9
(1,26)	1:B:15:DA:O4'	1:B:15:DA:C1'	1:B:15:DA:N9	1:B:15:DA:C4	8	15.4
(1,26)	1:B:15:DA:O4'	1:B:15:DA:C1'	1:B:15:DA:N9	1:B:15:DA:C4	3	8.1
(1,8)	1:B:16:DG:O4'	1:B:16:DG:C1'	1:B:16:DG:N9	1:B:16:DG:C4	10	7.4
(1,8)	1:B:16:DG:O4'	1:B:16:DG:C1'	1:B:16:DG:N9	1:B:16:DG:C4	9	6.9
(1,26)	1:B:15:DA:O4'	1:B:15:DA:C1'	1:B:15:DA:N9	1:B:15:DA:C4	2	5.8
(1,26)	1:B:15:DA:O4'	1:B:15:DA:C1'	1:B:15:DA:N9	1:B:15:DA:C4	4	5.5
(1,26)	1:B:15:DA:O4'	1:B:15:DA:C1'	1:B:15:DA:N9	1:B:15:DA:C4	6	4.6
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	6	4.3
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	7	4.3
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	8	4.1
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	5	4.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:B:16:DG:O4'	1:B:16:DG:C1'	1:B:16:DG:N9	1:B:16:DG:C4	2	3.9
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	2	3.7
(1,8)	1:B:16:DG:O4'	1:B:16:DG:C1'	1:B:16:DG:N9	1:B:16:DG:C4	4	3.6
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	4	3.6
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	3	3.5
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	9	3.5
(1,7)	1:A:16:DG:O4'	1:A:16:DG:C1'	1:A:16:DG:N9	1:A:16:DG:C4	5	3.3
(1,26)	1:B:15:DA:O4'	1:B:15:DA:C1'	1:B:15:DA:N9	1:B:15:DA:C4	7	3.3
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	1	3.3
(1,22)	1:B:12:DG:O4'	1:B:12:DG:C1'	1:B:12:DG:N9	1:B:12:DG:C4	10	3.3
(1,25)	1:A:15:DA:O4'	1:A:15:DA:C1'	1:A:15:DA:N9	1:A:15:DA:C4	8	2.5
(1,7)	1:A:16:DG:O4'	1:A:16:DG:C1'	1:A:16:DG:N9	1:A:16:DG:C4	4	1.6
(1,8)	1:B:16:DG:O4'	1:B:16:DG:C1'	1:B:16:DG:N9	1:B:16:DG:C4	1	1.5
(1,7)	1:A:16:DG:O4'	1:A:16:DG:C1'	1:A:16:DG:N9	1:A:16:DG:C4	8	1.2
(1,25)	1:A:15:DA:O4'	1:A:15:DA:C1'	1:A:15:DA:N9	1:A:15:DA:C4	6	1.2
(1,21)	1:A:12:DG:O4'	1:A:12:DG:C1'	1:A:12:DG:N9	1:A:12:DG:C4	2	1.1