



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:47 PM UTC

PDB ID : 2LGM / pdb_00002lgm
BMRB ID : 17814
Title : Structure of DNA Containing an Aristolactam II-dA Lesion
Authors : Lukin, M.; Zaliznyak, T.; Johnson, F.; de los Santos, C.
Deposited on : 2011-07-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

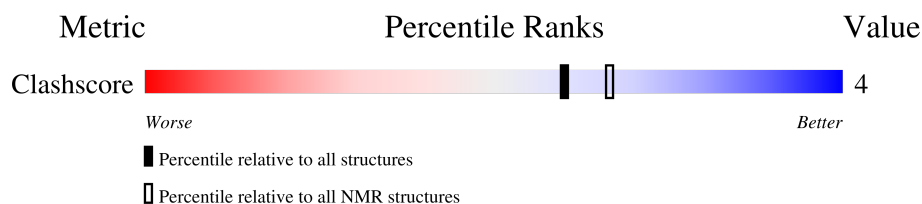
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 17%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424

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

Mol	Chain	Length	Quality of chain
1	1	11	 64% 36%
2	2	11	 91% 9%

2 Ensemble composition and analysis ⓘ

This entry contains 26 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 723 atoms, of which 258 are hydrogens and 0 are deuteriums.

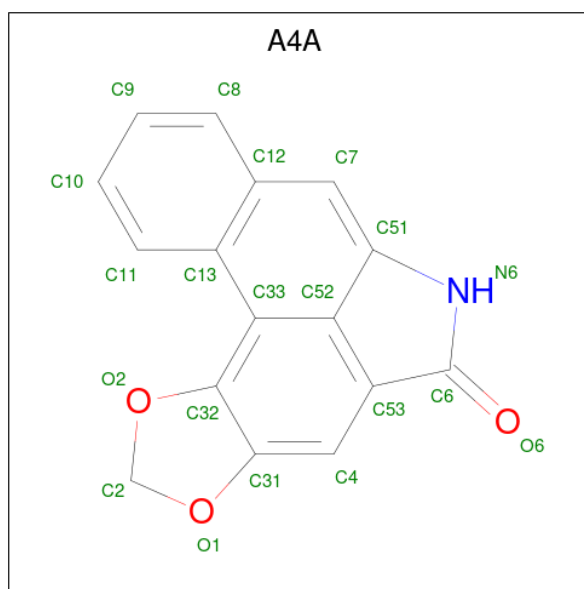
- Molecule 1 is a DNA chain called DNA (5'-D(*CP*GP*TP*AP*CP*AP*CP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms						Trace
1	1	11	Total	C	H	N	O	P	0
			344	106	124	41	63	10	

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

Mol	Chain	Residues	Atoms						Trace
2	2	11	Total	C	H	N	O	P	0
			351	108	126	42	65	10	

- Molecule 3 is [1,3]benzodioxolo[6,5,4-cd]benzo[f]indol-5(6H)-one (CCD ID: A4A) (formula: C₁₆H₉NO₃).



Mol	Chain	Residues	Atoms				
3	1	1	Total	C	H	N	O
			28	16	8	1	3

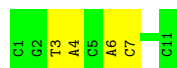
4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

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

Chain 1: 



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

Chain 2: 



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

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

Chain 1: 



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

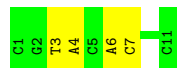
Chain 2: 



4.2.2 Score per residue for model 2

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

Chain 1:  64% 36%



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

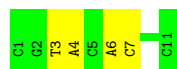
Chain 2:  91% 9%



4.2.3 Score per residue for model 3

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

Chain 1:  64% 36%



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

Chain 2:  91% 9%



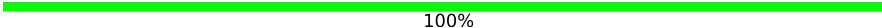
4.2.4 Score per residue for model 4

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

Chain 1:  64% 36%



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

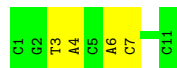
Chain 2:  100%

There are no outlier residues in this chain.

4.2.5 Score per residue for model 5

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

Chain 1:  64% 36%



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

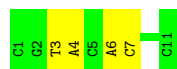
Chain 2:  91% 9%



4.2.6 Score per residue for model 6

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

Chain 1:  64% 36%



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

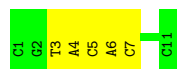
Chain 2:  100%

There are no outlier residues in this chain.

4.2.7 Score per residue for model 7

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

Chain 1:  55% 45%



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

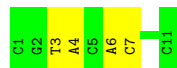
Chain 2:  91% 9%



4.2.8 Score per residue for model 8

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

Chain 1:  64% 36%



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

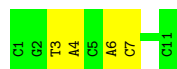
Chain 2:  91% 9%



4.2.9 Score per residue for model 9

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

Chain 1:  64% 36%



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

Chain 2:  91% 9%



4.2.10 Score per residue for model 10

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

Chain 1:  73% 27%



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

Chain 2:  91% 9%



4.2.11 Score per residue for model 11

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

Chain 1:  73% 27%



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

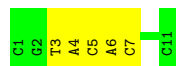
Chain 2:  100%

There are no outlier residues in this chain.

4.2.12 Score per residue for model 12

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

Chain 1:  55% 45%



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

Chain 2:  100%

There are no outlier residues in this chain.

4.2.13 Score per residue for model 13

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

Chain 1:  64% 36%



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

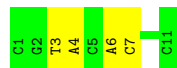
Chain 2:  100%

There are no outlier residues in this chain.

4.2.14 Score per residue for model 14

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

Chain 1:  64% 36%



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

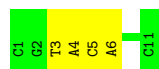
Chain 2:  91% 9%



4.2.15 Score per residue for model 15

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

Chain 1:  64% 36%



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

Chain 2:  91% 9%



4.2.16 Score per residue for model 16

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

Chain 1:  64% 36%



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

Chain 2:  91% 9%



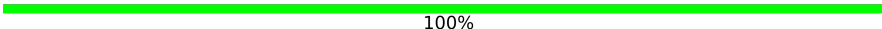
4.2.17 Score per residue for model 17

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

Chain 1:  73% 27%



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

Chain 2:  100%

There are no outlier residues in this chain.

4.2.18 Score per residue for model 18

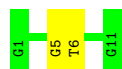
- Molecule 1: DNA (5'-D(*CP*GP*TP*AP*CP*AP*CP*AP*TP*GP*C)-3')

Chain 1:  73% 27%



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

Chain 2:  82% 18%



4.2.19 Score per residue for model 19

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

Chain 1:  64% 36%



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

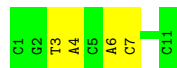
Chain 2:  91% 9%



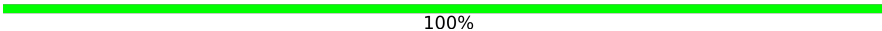
4.2.20 Score per residue for model 20

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

Chain 1:  64% 36%



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

Chain 2:  100%

There are no outlier residues in this chain.

4.2.21 Score per residue for model 21

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

Chain 1:  64% 36%



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

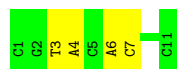
Chain 2:  91% 9%



4.2.22 Score per residue for model 22

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

Chain 1:  64% 36%



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

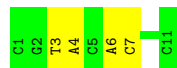
Chain 2:  91% 9%



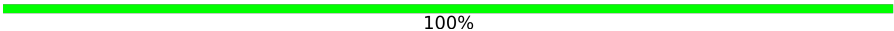
4.2.23 Score per residue for model 23

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

Chain 1:  64% 36%



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

Chain 2:  100%

There are no outlier residues in this chain.

4.2.24 Score per residue for model 24

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

Chain 1:  64% 36%



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

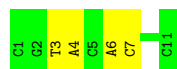
Chain 2:  91% 9%



4.2.25 Score per residue for model 25

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

Chain 1:  64% 36%



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

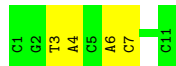
Chain 2:  91% 9%



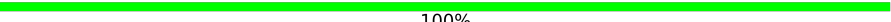
4.2.26 Score per residue for model 26

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

Chain 1:  64% 36%



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

Chain 2:  100%

There are no outlier residues in this chain.

5 Refinement protocol and experimental data overview

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

Of the 26 calculated structures, 26 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
HYPER	geometry optimization	
X-PLOR NIH	refinement	

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	82
Number of shifts mapped to atoms	82
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	17%

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: A4A

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	1	0.56±0.01	0±0/246 (0.0± 0.0%)	1.38±0.02	0±0/377 (0.0± 0.1%)
2	2	0.58±0.02	0±0/252 (0.0± 0.1%)	1.31±0.04	1±1/388 (0.2± 0.2%)
All	All	0.57	1/12948 (0.0%)	1.35	26/19890 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	2	1	DG	O5'-C5'	-5.08	1.27	1.42	1	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	2	6	DT	P-O3'-C3'	8.52	132.98	120.20	16	2
2	2	5	DG	C4'-C3'-O3'	6.54	119.82	110.00	9	4
2	2	5	DG	P-O3'-C3'	6.04	129.26	120.20	24	4
2	2	6	DT	N1-C1'-C2'	5.60	121.89	113.50	16	12
2	2	6	DT	C2'-C3'-O3'	-5.44	103.34	111.50	16	1
1	1	5	DC	N1-C1'-C2'	5.29	121.44	113.50	12	1
1	1	1	DC	P-O3'-C3'	5.18	127.97	120.20	4	1
2	2	1	DG	O5'-C5'-C4'	-5.17	103.05	110.80	1	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	1	220	124	124	3±1
2	2	225	126	126	0±0
3	1	20	8	8	1±0
All	All	12090	6708	6708	84

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
1:1:6:DA:N1	3:1:12:A4A:N6	0.57	2.53	8	26
1:1:5:DC:OP2	1:1:5:DC:H2'	0.49	2.07	15	2
1:1:3:DT:H2''	1:1:4:DA:O5'	0.47	2.09	18	26
1:1:6:DA:H2''	1:1:7:DC:O5'	0.47	2.10	26	20
2:2:6:DT:OP2	2:2:6:DT:H6	0.47	1.93	16	3
1:1:4:DA:H2''	1:1:5:DC:OP2	0.45	2.11	7	2
1:1:6:DA:H1'	1:1:7:DC:O4'	0.44	2.13	5	5

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	A4A	1	12	1	22,24,24	1.91±0.01	4±0 (18±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	A4A	1	12	1	32,37,37	1.70±0.02	7±1 (20±1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A4A	1	12	1	-	-	0±0,5,5,5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	1	12	A4A	C53-C6	5.64	1.40	1.48	17	26
3	1	12	A4A	C7-C51	4.62	1.44	1.36	5	26
3	1	12	A4A	C4-C31	2.96	1.43	1.38	3	26
3	1	12	A4A	C4-C53	2.55	1.42	1.38	10	26

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

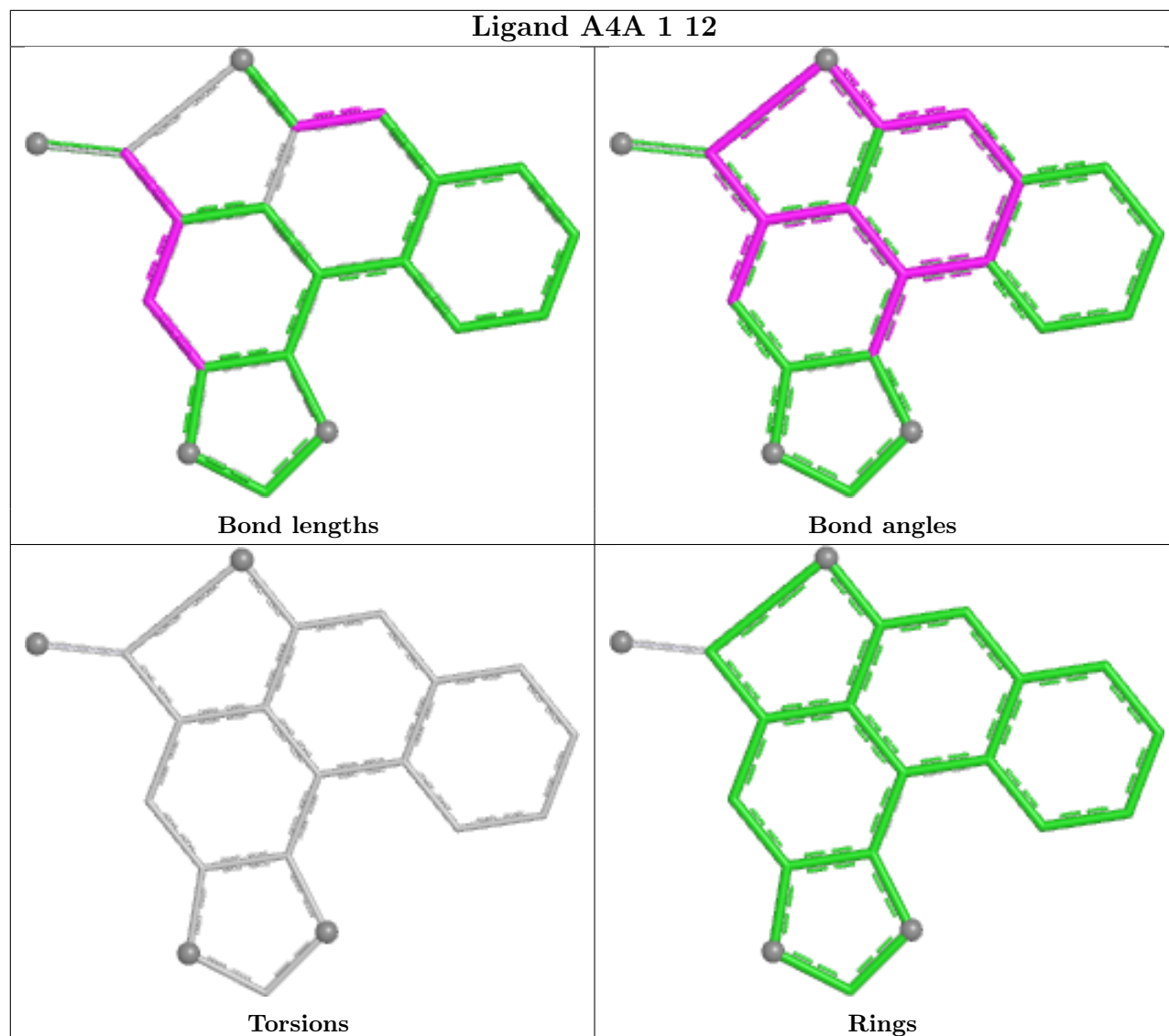
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	1	12	A4A	C32-C33-C13	5.03	130.26	124.04	10	26
3	1	12	A4A	C51-N6-C6	3.72	108.94	111.34	10	26
3	1	12	A4A	C51-C7-C12	3.54	117.50	121.25	10	26
3	1	12	A4A	C4-C53-C6	3.36	134.14	129.81	5	26
3	1	12	A4A	C7-C51-N6	2.95	133.75	128.97	20	26
3	1	12	A4A	C33-C13-C12	2.37	121.02	118.83	10	18
3	1	12	A4A	C53-C52-C33	2.30	126.11	122.81	15	23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 17% for the well-defined parts and 17% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	82
Number of shifts mapped to atoms	82
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 17%, i.e. 73 atoms were assigned a chemical shift out of a possible 436. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	58/264 (22%)	58/154 (38%)	0/110 (0%)	0/0 (—%)
Base	15/172 (9%)	15/106 (14%)	0/38 (0%)	0/28 (0%)
Overall	73/436 (17%)	73/260 (28%)	0/148 (0%)	0/28 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 17%, i.e. 73 atoms were assigned a chemical shift out of a possible 436. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Sugar	58/264 (22%)	58/154 (38%)	0/110 (0%)	0/0 (—%)
Base	15/172 (9%)	15/106 (14%)	0/38 (0%)	0/28 (0%)
Overall	73/436 (17%)	73/260 (28%)	0/148 (0%)	0/28 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	398
Intra-residue ($ i-j =0$)	265
Sequential ($ i-j =1$)	113
Medium range ($ i-j >1$ and $ i-j <5$)	1
Long range ($ i-j \geq 5$)	3
Inter-chain	16
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	17.3
Number of long range restraints per residue ¹	0.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	29.9	0.2
0.2-0.5 (Medium)	45.6	0.5
>0.5 (Large)	58.1	20.91

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

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

9 Distance violation analysis ⓘ

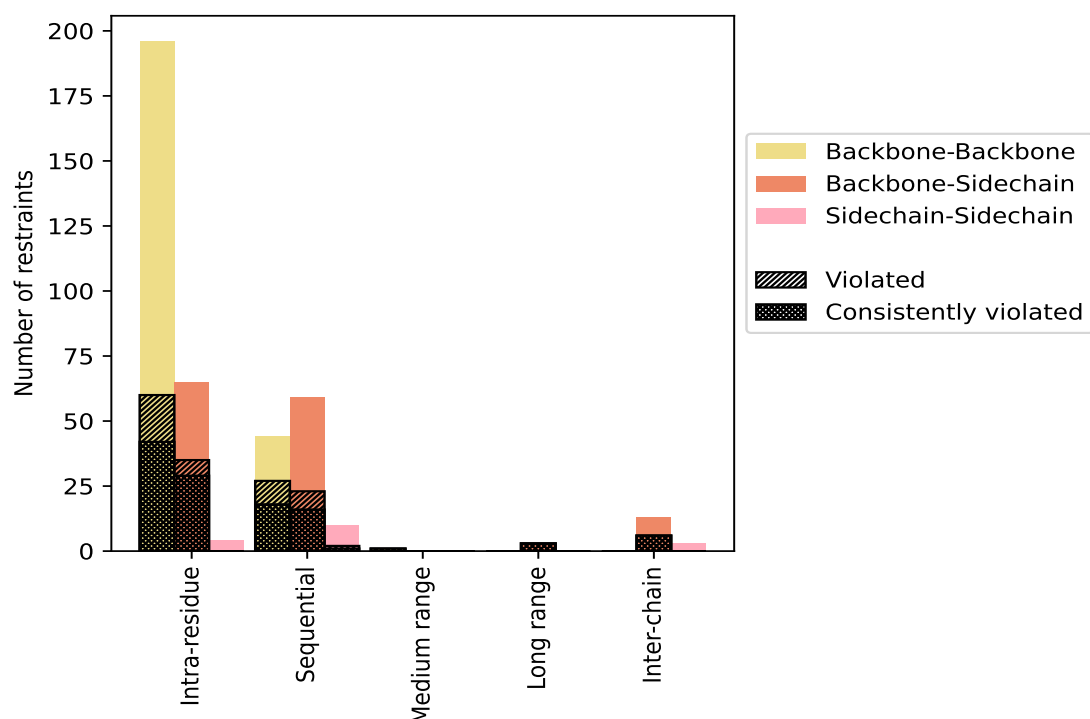
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	265	66.6	95	35.8	23.9	71	26.8	17.8
Backbone-Backbone	196	49.2	60	30.6	15.1	42	21.4	10.6
Backbone-Sidechain	65	16.3	35	53.8	8.8	29	44.6	7.3
Sidechain-Sidechain	4	1.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	113	28.4	52	46.0	13.1	35	31.0	8.8
Backbone-Backbone	44	11.1	27	61.4	6.8	18	40.9	4.5
Backbone-Sidechain	59	14.8	23	39.0	5.8	16	27.1	4.0
Sidechain-Sidechain	10	2.5	2	20.0	0.5	1	10.0	0.3
Medium range (i-j >1 & i-j <5)	1	0.3	1	100.0	0.3	1	100.0	0.3
Backbone-Backbone	1	0.3	1	100.0	0.3	1	100.0	0.3
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	3	0.8	3	100.0	0.8	3	100.0	0.8
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3	0.8	3	100.0	0.8	3	100.0	0.8
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	16	4.0	6	37.5	1.5	6	37.5	1.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	13	3.3	6	46.2	1.5	6	46.2	1.5
Sidechain-Sidechain	3	0.8	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	398	100.0	157	39.4	39.4	116	29.1	29.1
Backbone-Backbone	241	60.6	88	36.5	22.1	61	25.3	15.3
Backbone-Sidechain	140	35.2	67	47.9	16.8	54	38.6	13.6
Sidechain-Sidechain	17	4.3	2	11.8	0.5	1	5.9	0.3

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	82	43	1	3	6	135	1.36	20.65	2.82	0.41
2	82	44	1	3	6	136	1.37	20.3	2.77	0.42
3	80	45	1	3	6	135	1.35	20.6	2.81	0.41
4	82	44	1	3	6	136	1.34	20.73	2.81	0.4
5	80	44	1	3	6	134	1.36	20.6	2.83	0.42
6	81	43	1	3	6	134	1.37	20.46	2.8	0.44
7	81	44	1	3	6	135	1.35	20.53	2.8	0.41
8	80	44	1	3	6	134	1.39	20.54	2.82	0.43
9	83	40	1	3	6	133	1.38	20.73	2.84	0.42
10	82	44	1	3	6	136	1.34	20.77	2.82	0.42

Continued on next page...

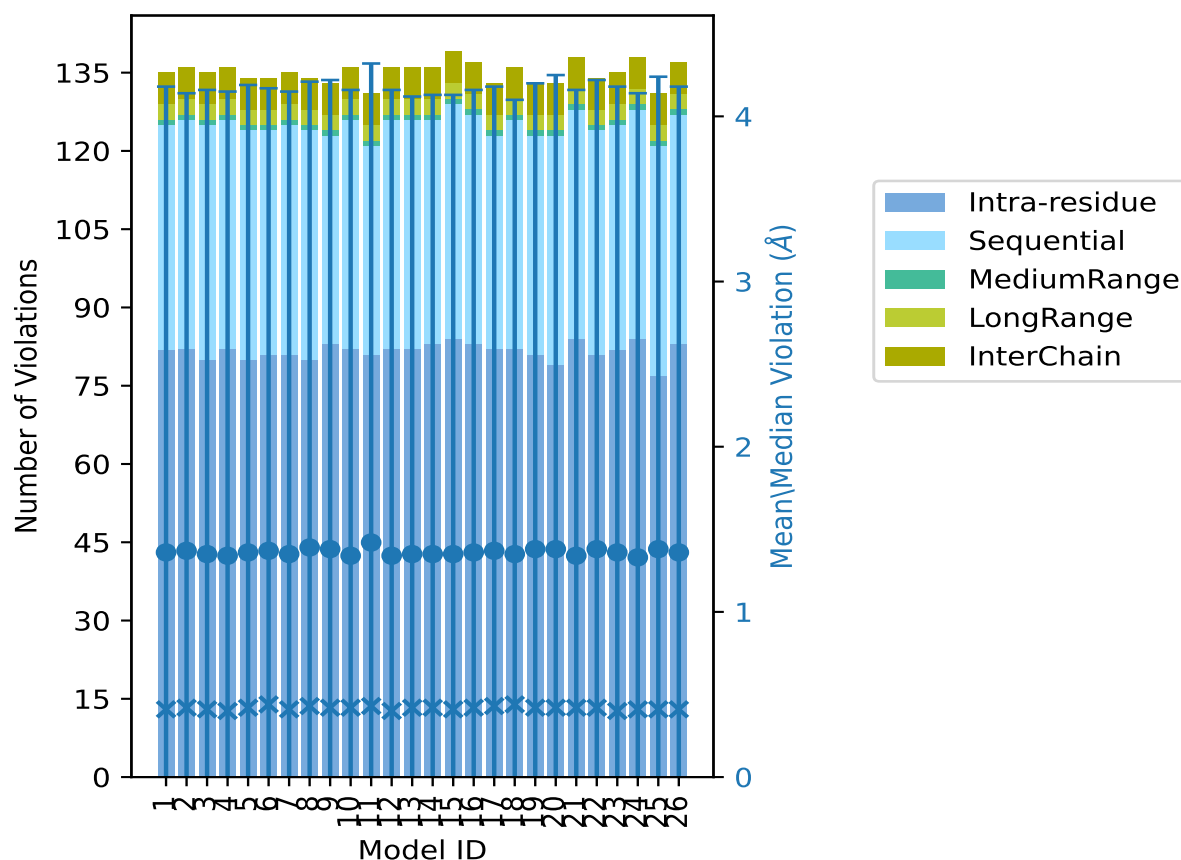
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	81	40	1	3	6	131	1.42	20.9	2.9	0.43
12	82	44	1	3	6	136	1.34	20.75	2.82	0.4
13	82	44	1	3	6	136	1.35	20.36	2.77	0.42
14	83	43	1	3	6	136	1.35	20.46	2.78	0.42
15	84	45	1	3	6	139	1.35	20.53	2.78	0.41
16	83	44	1	3	6	137	1.36	20.52	2.8	0.42
17	82	41	1	3	6	133	1.37	20.59	2.81	0.43
18	82	44	1	3	6	136	1.35	20.2	2.75	0.44
19	81	42	1	3	6	133	1.38	20.51	2.82	0.42
20	79	44	1	3	6	133	1.38	20.91	2.87	0.42
21	84	44	1	3	6	138	1.34	20.78	2.82	0.42
22	81	43	1	3	6	134	1.38	20.67	2.84	0.42
23	82	43	1	3	6	135	1.36	20.63	2.82	0.4
24	84	44	1	3	6	138	1.33	20.76	2.81	0.41
25	77	44	1	3	6	131	1.38	20.69	2.86	0.41
26	83	44	1	3	6	137	1.36	20.68	2.82	0.41

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 241(IR:170, SQ:61, MR:0, LR:0, IC:10) 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	%
2	4	0	0	0	6	1	3.8
3	1	0	0	0	4	2	7.7
3	0	0	0	0	3	3	11.5
2	0	0	0	0	2	4	15.4
0	0	0	0	0	0	5	19.2
1	0	0	0	0	1	6	23.1

Continued on next page...

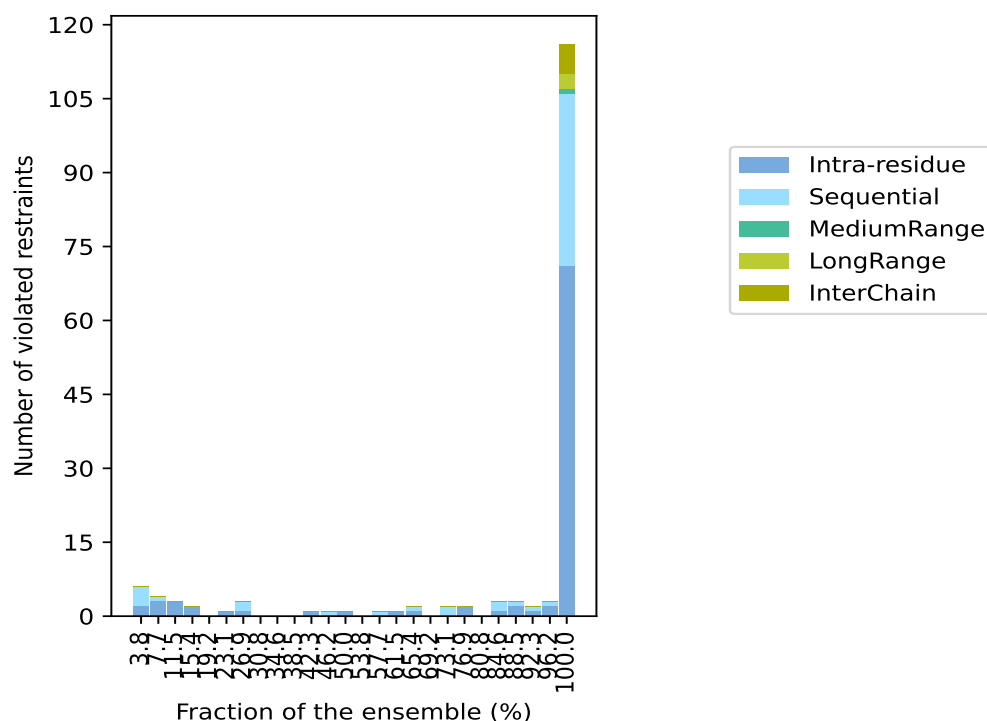
Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	2	0	0	0	3	7	26.9
0	0	0	0	0	0	8	30.8
0	0	0	0	0	0	9	34.6
0	0	0	0	0	0	10	38.5
1	0	0	0	0	1	11	42.3
0	1	0	0	0	1	12	46.2
1	0	0	0	0	1	13	50.0
0	0	0	0	0	0	14	53.8
0	1	0	0	0	1	15	57.7
1	0	0	0	0	1	16	61.5
1	1	0	0	0	2	17	65.4
0	0	0	0	0	0	18	69.2
0	2	0	0	0	2	19	73.1
2	0	0	0	0	2	20	76.9
0	0	0	0	0	0	21	80.8
1	2	0	0	0	3	22	84.6
2	1	0	0	0	3	23	88.5
1	1	0	0	0	2	24	92.3
2	1	0	0	0	3	25	96.2
71	35	1	3	6	116	26	100.0

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

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

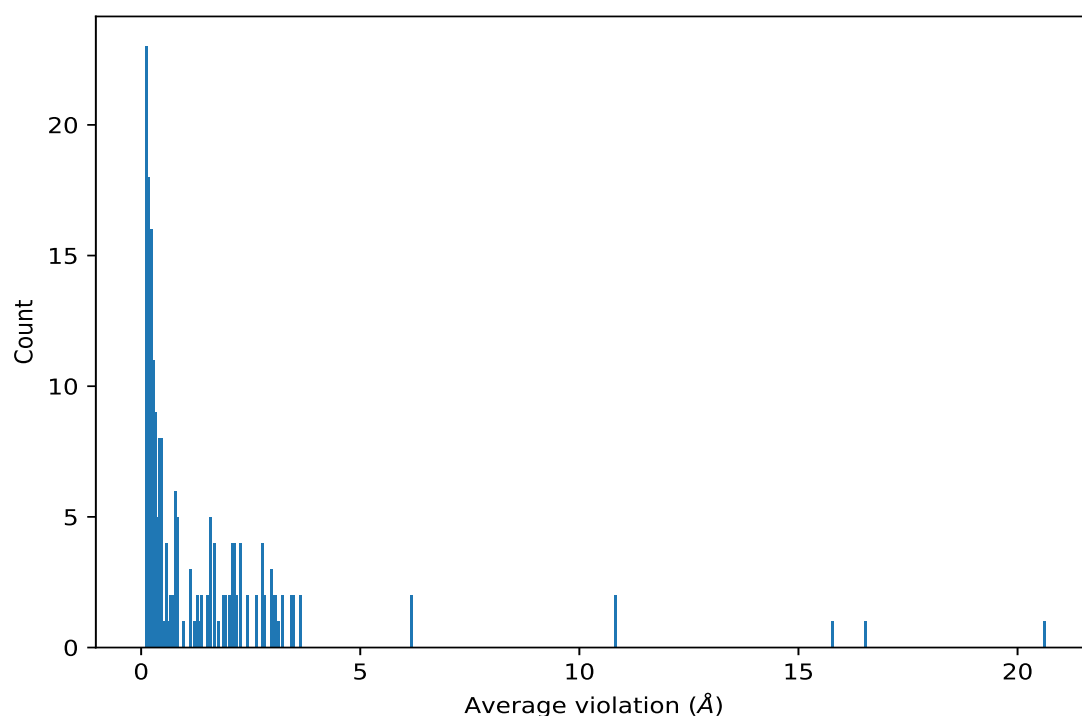
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	26	20.61	0.17	20.62
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	26	16.51	0.18	16.48
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	26	15.77	0.24	15.81
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	26	10.84	0.13	10.84
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	26	10.84	0.13	10.84
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	26	6.15	0.13	6.14
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	26	6.15	0.13	6.14
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	26	3.61	0.02	3.61
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	26	3.61	0.02	3.61
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	26	3.45	0.02	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	26	3.45	0.02	3.45
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	26	3.42	0.08	3.4
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	26	3.42	0.08	3.4
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	26	3.21	0.11	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	26	3.21	0.11	3.24
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	26	3.11	0.13	3.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	26	3.08	0.01	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	26	3.08	0.01	3.08
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	26	3.01	0.01	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	26	3.01	0.01	3.01
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	26	2.97	0.11	2.98
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	26	2.96	0.15	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	26	2.96	0.15	3.03
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	26	2.81	0.08	2.82
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	26	2.81	0.08	2.82
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	26	2.79	0.01	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	26	2.79	0.01	2.79
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	26	2.77	0.01	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	26	2.77	0.01	2.78
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	26	2.63	0.08	2.62
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	26	2.63	0.08	2.62
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	26	2.42	0.07	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	26	2.42	0.07	2.43
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	26	2.28	0.07	2.28
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	26	2.28	0.07	2.28
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	26	2.28	0.08	2.28
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	26	2.28	0.08	2.28
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	26	2.19	0.1	2.17
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	26	2.17	0.33	2.02
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	26	2.13	0.01	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	26	2.13	0.01	2.13
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	26	2.11	0.05	2.12
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	26	2.11	0.05	2.12
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	26	2.09	0.08	2.09
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	26	2.09	0.08	2.09
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	26	2.07	0.08	2.08
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	26	2.07	0.08	2.08
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	26	2.02	0.01	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	26	2.02	0.01	2.02
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	26	1.92	0.01	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	26	1.92	0.01	1.92
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	26	1.88	0.07	1.9
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	26	1.88	0.07	1.9
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	26	1.79	0.1	1.81
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	26	1.65	0.08	1.66
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	26	1.65	0.08	1.66
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	26	1.65	0.08	1.65
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	26	1.65	0.08	1.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	26	1.58	0.15	1.63
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	26	1.58	0.15	1.63
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	26	1.56	0.02	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	26	1.56	0.02	1.55
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	26	1.51	0.01	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	26	1.51	0.01	1.51
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	26	1.38	0.01	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	26	1.38	0.01	1.38
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	26	1.33	0.06	1.33
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	26	1.28	0.1	1.24
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	26	1.28	0.1	1.24
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	26	1.21	0.03	1.21
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	26	1.14	0.02	1.14
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	26	1.1	0.33	0.94
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	26	1.1	0.33	0.94
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	26	0.99	0.13	0.99
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	26	0.84	0.39	0.64
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	26	0.84	0.39	0.64
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	26	0.8	0.04	0.79
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	26	0.79	0.02	0.79
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	26	0.76	0.23	0.7
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	26	0.76	0.23	0.7
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	26	0.76	0.13	0.76
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	26	0.75	0.21	0.66
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	26	0.75	0.21	0.66
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	26	0.69	0.02	0.7
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	26	0.69	0.04	0.69
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	26	0.62	0.02	0.62
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	26	0.59	0.11	0.58
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	26	0.59	0.04	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	26	0.58	0.01	0.58
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	26	0.57	0.02	0.57
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	26	0.52	0.05	0.51
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	26	0.49	0.03	0.49
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	26	0.49	0.02	0.48
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	26	0.46	0.02	0.46
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	26	0.45	0.06	0.46
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	26	0.45	0.01	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	26	0.45	0.01	0.45
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	26	0.44	0.01	0.44
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	26	0.42	0.02	0.42
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	26	0.41	0.06	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	26	0.41	0.04	0.42
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	26	0.41	0.05	0.43
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	26	0.4	0.01	0.4
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	26	0.37	0.01	0.36
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	26	0.37	0.03	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	26	0.37	0.01	0.37
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	26	0.36	0.02	0.37
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	26	0.36	0.04	0.36
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	26	0.34	0.02	0.34
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	26	0.33	0.03	0.34
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	26	0.33	0.02	0.34
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	26	0.33	0.08	0.3
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	26	0.33	0.08	0.3
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	26	0.32	0.04	0.32
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	26	0.31	0.19	0.2
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	26	0.29	0.04	0.28
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	26	0.28	0.02	0.28
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	26	0.27	0.03	0.27
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	26	0.27	0.04	0.26
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	26	0.27	0.07	0.24
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	26	0.26	0.02	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	26	0.26	0.02	0.25
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	26	0.25	0.03	0.26
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	26	0.25	0.06	0.28
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	26	0.24	0.03	0.22
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	26	0.24	0.02	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	26	0.24	0.03	0.24
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	26	0.22	0.01	0.22
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	26	0.22	0.03	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	26	0.22	0.01	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	26	0.22	0.01	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	26	0.22	0.02	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	26	0.22	0.01	0.22
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	26	0.21	0.01	0.21
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	26	0.21	0.02	0.21
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	26	0.21	0.01	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	26	0.2	0.01	0.2
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	26	0.19	0.01	0.19
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	26	0.19	0.01	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	26	0.19	0.01	0.19
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	26	0.19	0.02	0.19
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	26	0.18	0.01	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	26	0.17	0.02	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	26	0.16	0.0	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	26	0.16	0.01	0.16
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	26	0.14	0.01	0.14
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	26	0.13	0.01	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	26	0.12	0.01	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	26	0.12	0.01	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	26	0.12	0.01	0.12
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	26	0.11	0.0	0.11
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	25	0.34	0.11	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	25	0.34	0.11	0.4
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	25	0.23	0.05	0.24
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	25	0.17	0.04	0.17
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	24	0.4	0.06	0.38
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	24	0.4	0.06	0.38
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	24	0.12	0.02	0.12
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	23	0.2	0.04	0.2
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	23	0.15	0.02	0.15
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	23	0.13	0.02	0.13
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	22	0.23	0.07	0.22
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	22	0.17	0.04	0.18
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	22	0.11	0.01	0.11
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	20	0.74	0.14	0.78
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	20	0.74	0.14	0.78
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	20	0.16	0.03	0.16
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	19	0.17	0.05	0.17
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	19	0.15	0.01	0.15
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	17	0.27	0.05	0.27
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	17	0.27	0.05	0.27
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	17	0.12	0.02	0.11
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	16	0.11	0.01	0.11
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	15	0.12	0.01	0.12
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	13	0.17	0.04	0.16
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	13	0.17	0.04	0.16
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	12	0.12	0.02	0.12
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	11	0.12	0.02	0.12
(1,68)	2:7:2:DG:H5''	2:6:2:DT:H1'	7	1.56	0.31	1.71
(1,212)	2:6:2:DT:H4'	2:7:2:DG:H8	7	0.15	0.02	0.14
(1,92)	2:9:2:DA:H3'	2:9:2:DA:H1'	7	0.1	0.0	0.1
(1,72)	2:8:2:DT:H2'	2:8:2:DT:H2''	6	0.1	0.0	0.1
(1,223)	2:7:2:DG:H2'	2:7:2:DG:H8	4	0.13	0.01	0.14
(1,209)	2:6:2:DT:H4'	2:6:2:DT:H1'	4	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

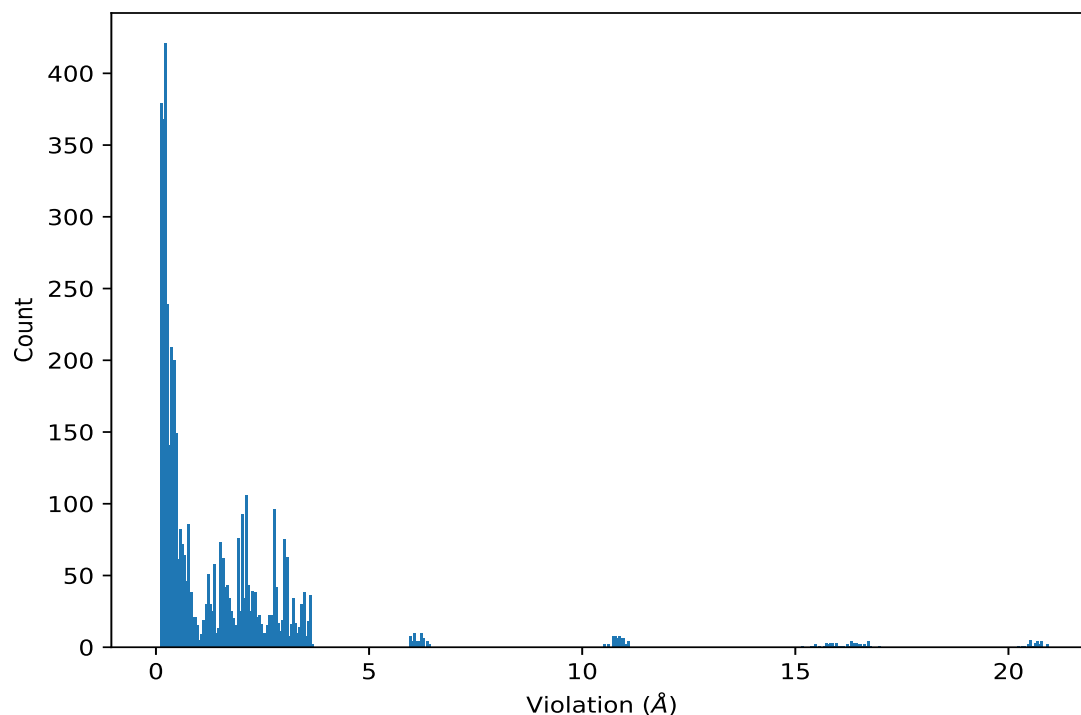
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,188)	2:5:2:DG:H3'	2:5:2:DG:H8	3	0.18	0.01	0.18
(1,303)	2:5:2:DG:H2'	2:5:2:DG:H5'	3	0.12	0.02	0.11
(1,303)	2:5:2:DG:H2'	2:5:2:DG:H5''	3	0.12	0.02	0.11
(1,390)	2:5:2:DG:H2'	2:5:2:DG:H3'	3	0.12	0.0	0.12
(1,99)	2:10:2:DC:H2''	2:11:2:DG:H5'	2	0.81	0.15	0.81
(1,99)	2:10:2:DC:H2''	2:11:2:DG:H5''	2	0.81	0.15	0.81
(1,107)	2:11:2:DG:H2''	2:11:2:DG:H5'	2	0.47	0.01	0.47
(1,107)	2:11:2:DG:H2''	2:11:2:DG:H5''	2	0.47	0.01	0.47
(1,366)	2:6:2:DT:H5'	2:6:2:DT:H3'	2	0.14	0.02	0.14
(1,135)	2:2:2:DC:H3'	2:2:2:DC:H1'	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	20	20.91
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	11	20.9
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	21	20.78
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	10	20.77
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	24	20.76
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	12	20.75
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	4	20.73
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	9	20.73
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	25	20.69
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	26	20.68
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	22	20.67
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	1	20.65
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	23	20.63
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	3	20.6
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	5	20.6
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	17	20.59
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	8	20.54
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	7	20.53
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	15	20.53
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	16	20.52
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	19	20.51
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	6	20.46
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	14	20.46
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	13	20.36
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	2	20.3
(1,94)	2:10:2:DC:H1'	2:3:2:DA:H2	18	20.2
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	11	16.97
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	5	16.78
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	22	16.72
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	23	16.72
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	12	16.71
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	20	16.71
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	26	16.66
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	4	16.62
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	16	16.6
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	24	16.59
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	1	16.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	25	16.51
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	10	16.48
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	21	16.48
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	9	16.44
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	14	16.42
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	6	16.41
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	8	16.38
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	19	16.38
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	3	16.35
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	7	16.33
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	13	16.32
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	15	16.32
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	2	16.3
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	18	16.27
(1,82)	2:9:2:DA:H1'	2:3:2:DA:H2	17	16.23
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	21	16.22
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	20	16.11
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	24	16.06
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	3	16.02
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	10	15.99
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	15	15.97
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	25	15.95
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	11	15.9
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	8	15.87
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	26	15.86
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	1	15.85
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	7	15.84
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	9	15.81
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	22	15.81
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	17	15.76
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	16	15.75
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	12	15.74
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	4	15.71
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	19	15.71
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	13	15.65
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	2	15.59
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	6	15.45
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	23	15.45
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	14	15.43
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	5	15.38
(1,22)	2:3:2:DA:H1'	2:9:2:DA:H2	18	15.19
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	5	11.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	5	11.08
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	11	11.08
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	11	11.08
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	23	11.03
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	23	11.03
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	16	10.97
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	16	10.97
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	22	10.97
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	22	10.97
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	26	10.96
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	26	10.96
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	12	10.93
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	12	10.93
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	14	10.92
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	14	10.92
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	20	10.91
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	20	10.91
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	6	10.89
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	6	10.89
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	1	10.87
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	1	10.87
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	4	10.87
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	4	10.87
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	24	10.85
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	24	10.85
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	21	10.82
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	21	10.82
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	2	10.81
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	2	10.81
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	18	10.81
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	18	10.81
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	25	10.77
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	25	10.77
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	13	10.76
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	13	10.76
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	19	10.76
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	19	10.76
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	9	10.75
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	9	10.75
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	10	10.73
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	10	10.73
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	7	10.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	7	10.72
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	8	10.72
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	8	10.72
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	3	10.7
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	3	10.7
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	15	10.63
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	15	10.63
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2'	17	10.52
(1,156)	2:4:2:DT:H1'	2:8:2:DT:H2''	17	10.52
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	21	6.43
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	21	6.43
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	15	6.38
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	15	6.38
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	25	6.35
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	25	6.35
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	8	6.26
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	8	6.26
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	24	6.26
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	24	6.26
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	20	6.25
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	20	6.25
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	2	6.23
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	2	6.23
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	18	6.22
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	18	6.22
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	17	6.21
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	17	6.21
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	16	6.2
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	16	6.2
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	26	6.2
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	26	6.2
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	9	6.19
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	9	6.19
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	1	6.15
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	1	6.15
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	3	6.12
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	3	6.12
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	11	6.11
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	11	6.11
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	5	6.09
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	5	6.09
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	13	6.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	13	6.08
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	19	6.08
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	19	6.08
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	4	6.06
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	4	6.06
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	7	6.05
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	7	6.05
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	14	6.02
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	14	6.02
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	10	6.0
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	10	6.0
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	6	5.98
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	6	5.98
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	23	5.98
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	23	5.98
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	12	5.97
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	12	5.97
(1,44)	2:5:2:DG:H5'	3:12:1:A4A:H9	22	5.96
(1,44)	2:5:2:DG:H5''	3:12:1:A4A:H9	22	5.96
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	25	3.67
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	25	3.67
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	3	3.64
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	3	3.64
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	8	3.64
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	8	3.64
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	4	3.63
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	4	3.63
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	5	3.63
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	5	3.63
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	7	3.63
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	7	3.63
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	2	3.62
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	2	3.62
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	10	3.62
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	10	3.62
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	23	3.62
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	23	3.62
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	15	3.61
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	15	3.61
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	20	3.61
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	20	3.61
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	21	3.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	21	3.61
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	24	3.61
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	24	3.61
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	26	3.61
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	26	3.61
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	16	3.61
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	16	3.61
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	1	3.6
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	1	3.6
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	6	3.6
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	6	3.6
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	18	3.6
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	18	3.6
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	19	3.6
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	19	3.6
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	11	3.59
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	11	3.59
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	12	3.59
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	12	3.59
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	16	3.59
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	16	3.59
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	17	3.59
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	17	3.59
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	9	3.58
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	9	3.58
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	13	3.58
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	13	3.58
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	14	3.58
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	14	3.58
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H61	22	3.58
(1,90)	2:9:2:DA:H2''	2:9:2:DA:H62	22	3.58
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	26	3.57
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	26	3.57
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	11	3.54
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	11	3.54
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	25	3.53
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	25	3.53
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	15	3.52
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	15	3.52
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	3	3.52
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	3	3.52
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	2	3.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	2	3.49
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	5	3.48
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	5	3.48
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	25	3.48
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	25	3.48
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	8	3.47
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	8	3.47
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	7	3.47
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	7	3.47
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	21	3.47
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	21	3.47
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	1	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	1	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	2	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	2	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	8	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	8	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	16	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	16	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	24	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	24	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	26	3.46
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	26	3.46
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	1	3.45
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	1	3.45
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	5	3.45
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	5	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	4	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	4	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	6	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	6	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	10	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	10	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	15	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	15	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	20	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	20	3.45
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	13	3.44
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	13	3.44
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	14	3.44
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	14	3.44
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	18	3.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	18	3.44
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	22	3.44
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	22	3.44
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	18	3.43
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	18	3.43
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	23	3.43
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	23	3.43
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	23	3.43
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	23	3.43
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	12	3.42
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	12	3.42
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	22	3.41
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	22	3.41
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	9	3.41
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	9	3.41
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	11	3.41
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	11	3.41
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	17	3.41
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	17	3.41
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H61	19	3.41
(1,27)	2:3:2:DA:H2''	2:3:2:DA:H62	19	3.41
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	12	3.4
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	12	3.4
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	14	3.4
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	14	3.4
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	3	3.38
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	3	3.38
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	4	3.38
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	4	3.38
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	20	3.38
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	20	3.38
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	7	3.37
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	7	3.37
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	10	3.36
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	10	3.36
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	13	3.36
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	13	3.36
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	19	3.35
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	19	3.35
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	6	3.34
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	6	3.34
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	17	3.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	17	3.34
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	24	3.33
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	24	3.33
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	9	3.32
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	9	3.32
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	21	3.31
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	21	3.31
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	10	3.28
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	10	3.28
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	16	3.28
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	16	3.28
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	23	3.28
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	23	3.28
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	9	3.28
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2'	9	3.28
(1,55)	2:7:2:DG:H1'	2:6:2:DT:H2''	9	3.28
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	1	3.27
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	1	3.27
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	2	3.27
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	2	3.27
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	5	3.27
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	5	3.27
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	6	3.25
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	6	3.25
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	12	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	12	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	18	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	18	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	19	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	19	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	22	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	22	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	26	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	26	3.24
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	3	3.24
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	7	3.23
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	7	3.23
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	8	3.23
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	8	3.23
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	24	3.23
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	24	3.23
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	7	3.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	17	3.23
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	25	3.22
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	25	3.22
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	10	3.22
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	4	3.21
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	4	3.21
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	21	3.21
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	21	3.21
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	3	3.2
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	3	3.2
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	11	3.2
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	11	3.2
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	17	3.2
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	17	3.2
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	20	3.2
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	20	3.2
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	4	3.19
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	25	3.19
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	15	3.18
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	15	3.18
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	14	3.18
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	22	3.18
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	12	3.16
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	18	3.16
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	19	3.16
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	24	3.16
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	1	3.15
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	1	3.15
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	13	3.15
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	20	3.15
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	21	3.15
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	23	3.15
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	6	3.14
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	5	3.13
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	1	3.11
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	10	3.1
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	10	3.1
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	18	3.1
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	18	3.1
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	20	3.1
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	4	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	4	3.09

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	6	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	6	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	8	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	8	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	9	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	9	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	11	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	11	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	21	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	21	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	23	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	23	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	26	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	26	3.09
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	2	3.09
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	12	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	12	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	14	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	14	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	17	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	17	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	19	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	19	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	20	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	20	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	24	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	24	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	25	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	25	3.08
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	2	3.07
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	2	3.07
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	13	3.07
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	13	3.07
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	15	3.07
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	15	3.07
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	18	3.07
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	26	3.07
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	5	3.06
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	5	3.06
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	13	3.06
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	13	3.06
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	19	3.06

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	19	3.06
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	1	3.06
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	1	3.06
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	5	3.06
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	5	3.06
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	7	3.06
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	7	3.06
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	16	3.06
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	16	3.06
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	22	3.06
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	22	3.06
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	21	3.06
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	6	3.05
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	6	3.05
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	20	3.05
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	20	3.05
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	21	3.05
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	21	3.05
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	11	3.05
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	12	3.04
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	12	3.04
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	18	3.04
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	18	3.04
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	24	3.04
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	24	3.04
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H61	3	3.04
(1,93)	2:9:2:DA:H3'	2:9:2:DA:H62	3	3.04
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	16	3.04
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	17	3.04
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	3	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	3	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	4	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	4	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	7	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	7	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	10	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	10	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	14	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	14	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	22	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	22	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	23	3.03

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	23	3.03
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	8	3.03
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	26	3.03
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	26	3.03
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	17	3.02
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	17	3.02
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	2	3.02
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	2	3.02
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	6	3.02
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	6	3.02
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	16	3.02
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	16	3.02
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	8	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	5	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	5	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	8	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	8	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	12	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	12	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	14	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	14	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	15	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	15	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	18	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	18	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	19	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	19	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	21	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	21	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	22	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	22	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	23	3.01
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	23	3.01
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	9	3.0
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	9	3.0
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	15	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	1	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	1	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	3	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	3	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	4	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	4	3.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	7	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	7	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	9	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	9	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	13	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	13	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	24	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	24	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	25	3.0
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	25	3.0
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	15	2.99
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	15	2.99
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	1	2.99
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	3	2.99
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	10	2.99
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	10	2.99
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	11	2.99
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	11	2.99
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	17	2.99
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	17	2.99
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H61	20	2.99
(1,30)	2:3:2:DA:H3'	2:3:2:DA:H62	20	2.99
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	19	2.97
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	16	2.96
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	16	2.96
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	5	2.96
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	16	2.95
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	4	2.95
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	22	2.95
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	12	2.94
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	24	2.94
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	2	2.93
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	10	2.93
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	13	2.92
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	13	2.92
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	22	2.91
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	22	2.91
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	15	2.91
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	23	2.91
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	7	2.9
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	9	2.89
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	9	2.89

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	11	2.89
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	11	2.89
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	17	2.89
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	17	2.89
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	11	2.89
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	9	2.89
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	14	2.88
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	14	2.88
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	13	2.87
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	13	2.87
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	23	2.87
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	23	2.87
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	25	2.87
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	6	2.85
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	6	2.85
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	12	2.83
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	12	2.83
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	19	2.83
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	19	2.83
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	8	2.83
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	26	2.83
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	25	2.82
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	25	2.82
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	24	2.82
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	24	2.82
(1,57)	2:7:2:DG:H2'	2:6:2:DT:H2''	26	2.82
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	4	2.81
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	4	2.81
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	8	2.81
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	8	2.81
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	11	2.81
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	11	2.81
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	23	2.81
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	23	2.81
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	5	2.81
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	5	2.81
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	13	2.81
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	25	2.8
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	25	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	6	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	6	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	9	2.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	9	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	10	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	10	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	15	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	15	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	20	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	20	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	21	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	21	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	26	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	26	2.8
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	18	2.8
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	18	2.8
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	3	2.8
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	3	2.8
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	5	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	5	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	7	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	7	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	12	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	12	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	13	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	13	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	17	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	17	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	18	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	18	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	19	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	19	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	24	2.79
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	24	2.79
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	26	2.79
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	26	2.79
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	11	2.79
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	14	2.79
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	2	2.79
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	2	2.79
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	5	2.79
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	5	2.79
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	16	2.79
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	16	2.79
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	26	2.79

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	26	2.79
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5'	14	2.78
(1,338)	2:11:2:DG:H3'	2:11:2:DG:H5''	14	2.78
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	8	2.78
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	8	2.78
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	1	2.78
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	1	2.78
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	2	2.78
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	2	2.78
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	14	2.78
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	14	2.78
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	16	2.78
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	16	2.78
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	20	2.78
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	20	2.78
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	21	2.78
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	21	2.78
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	15	2.78
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	15	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	6	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	6	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	7	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	7	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	8	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	8	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	15	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	15	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	18	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	18	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	21	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	21	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	22	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	22	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	25	2.78
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	25	2.78
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	3	2.77
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	3	2.77
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H61	22	2.77
(1,87)	2:9:2:DA:H2'	2:9:2:DA:H62	22	2.77
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	1	2.77
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	1	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	1	2.77

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	1	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	4	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	4	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	13	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	13	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	14	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	14	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	23	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	23	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	24	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	24	2.77
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	10	2.76
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	10	2.76
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	12	2.76
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	12	2.76
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	17	2.76
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	17	2.76
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	19	2.76
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	19	2.76
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	20	2.76
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	20	2.76
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	2	2.75
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	2	2.75
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	9	2.75
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	9	2.75
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H61	11	2.75
(1,25)	2:3:2:DA:H2'	2:3:2:DA:H62	11	2.75
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	2	2.74
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	2	2.74
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	25	2.74
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	25	2.74
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	16	2.74
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	16	2.74
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	4	2.73
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	4	2.73
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	15	2.73
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	11	2.72
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	11	2.72
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	7	2.71
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	7	2.71
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	2	2.71
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	8	2.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	8	2.7
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	9	2.7
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	9	2.7
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	22	2.7
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	22	2.7
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	23	2.7
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	23	2.7
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	11	2.69
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	11	2.69
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	14	2.69
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	14	2.69
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	17	2.69
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	17	2.69
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	15	2.68
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	15	2.68
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	26	2.68
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	26	2.68
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	10	2.68
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	10	2.68
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	6	2.68
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	6	2.68
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	12	2.66
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	12	2.66
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5'	16	2.65
(1,315)	2:7:2:DG:H3'	2:7:2:DG:H5''	16	2.65
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H61	3	2.65
(1,75)	2:8:2:DT:H2''	2:9:2:DA:H62	3	2.65
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	13	2.65
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	13	2.65
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	19	2.64
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	19	2.64
(1,36)	2:5:2:DG:H1'	3:12:1:A4A:H8	6	2.64
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	24	2.63
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	24	2.63
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	5	2.62
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	5	2.62
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	18	2.62
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	18	2.62
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	26	2.62
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	26	2.62
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	20	2.6
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	20	2.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	21	2.6
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	21	2.6
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	1	2.59
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	1	2.59
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	15	2.57
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	15	2.57
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	4	2.57
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	4	2.57
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	16	2.55
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	16	2.55
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	25	2.55
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	25	2.55
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	2	2.54
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	2	2.54
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	7	2.53
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	7	2.53
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	10	2.52
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	10	2.52
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	8	2.51
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	8	2.51
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	22	2.5
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	22	2.5
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	9	2.49
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	9	2.49
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	14	2.49
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	14	2.49
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	23	2.49
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	23	2.49
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	6	2.48
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	6	2.48
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	17	2.48
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	17	2.48
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	11	2.47
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	11	2.47
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	16	2.47
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H61	3	2.46
(1,73)	2:8:2:DT:H2'	2:9:2:DA:H62	3	2.46
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	16	2.46
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	12	2.44
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	12	2.44
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	5	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	5	2.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	13	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	13	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	18	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	18	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	19	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	19	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	24	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	24	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	26	2.43
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	26	2.43
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	18	2.42
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	18	2.42
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	17	2.41
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	17	2.41
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	21	2.4
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	21	2.4
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	15	2.4
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	15	2.4
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	1	2.39
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	1	2.39
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	9	2.39
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	9	2.39
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	20	2.38
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	20	2.38
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	18	2.38
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	18	2.38
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	4	2.37
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	4	2.37
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	2	2.37
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	2	2.37
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	16	2.37
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	16	2.37
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	19	2.37
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	19	2.37
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	2	2.36
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	2	2.36
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	11	2.36
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	6	2.36
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	6	2.36
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	7	2.34
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	7	2.34
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	25	2.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	25	2.34
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	2	2.34
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	11	2.34
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	11	2.34
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	14	2.34
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	14	2.34
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	10	2.33
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	10	2.33
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	21	2.33
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	21	2.33
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	16	2.33
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	16	2.33
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	22	2.33
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	22	2.33
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	8	2.32
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	8	2.32
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	10	2.32
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	10	2.32
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	25	2.32
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	8	2.32
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	8	2.32
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	20	2.32
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	20	2.32
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	9	2.32
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	9	2.32
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	23	2.32
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	23	2.32
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	1	2.31
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	5	2.31
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	5	2.31
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	26	2.3
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	12	2.3
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	12	2.3
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	2	2.3
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	2	2.3
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	8	2.29
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	3	2.29
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	3	2.29
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	4	2.29
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	4	2.29
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	5	2.29
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	5	2.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	11	2.29
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	11	2.29
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	1	2.28
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	1	2.28
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	19	2.28
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	19	2.28
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	22	2.28
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	22	2.28
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	23	2.28
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	23	2.28
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	26	2.28
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	26	2.28
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	8	2.28
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	8	2.28
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	13	2.28
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	13	2.28
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H61	3	2.27
(1,77)	2:8:2:DT:H3'	2:9:2:DA:H62	3	2.27
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	25	2.27
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	25	2.27
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	7	2.26
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	7	2.26
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	24	2.26
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	24	2.26
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	19	2.25
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	15	2.25
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	14	2.25
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	14	2.25
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	17	2.25
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	17	2.25
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	1	2.25
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	1	2.25
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	18	2.24
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	18	2.24
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	13	2.23
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	13	2.23
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	26	2.23
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	26	2.23
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	15	2.22
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	15	2.22
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	17	2.22
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	17	2.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	25	2.22
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	25	2.22
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	15	2.21
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	15	2.21
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	15	2.21
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	15	2.21
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	1	2.21
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	7	2.21
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	7	2.21
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	4	2.2
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	4	2.2
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	10	2.2
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	10	2.2
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	12	2.2
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	12	2.2
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	16	2.19
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	16	2.19
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	14	2.18
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	14	2.18
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	6	2.18
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	6	2.18
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	19	2.18
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	19	2.18
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	16	2.18
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	16	2.18
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	19	2.18
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	24	2.18
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	24	2.18
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	6	2.17
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	6	2.17
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	22	2.17
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	22	2.17
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	9	2.17
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	9	2.17
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	17	2.17
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	17	2.17
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	3	2.17
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	5	2.17
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	10	2.17
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	20	2.17
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	22	2.17
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	20	2.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	20	2.17
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	22	2.16
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	22	2.16
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	12	2.16
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	12	2.16
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	7	2.16
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	13	2.16
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	9	2.15
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	9	2.15
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	23	2.15
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	23	2.15
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	22	2.15
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	22	2.15
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	4	2.15
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	14	2.15
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	23	2.15
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	11	2.14
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	11	2.14
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	12	2.14
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	12	2.14
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	17	2.14
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	17	2.14
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	24	2.14
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	24	2.14
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	14	2.14
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	14	2.14
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	12	2.14
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	17	2.14
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	11	2.14
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	11	2.14
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	20	2.14
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	20	2.14
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	25	2.14
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	25	2.14
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	21	2.14
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	21	2.14
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	23	2.13
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	23	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	1	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	1	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	2	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	2	2.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	3	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	3	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	4	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	4	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	5	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	5	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	6	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	6	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	9	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	9	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	12	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	12	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	13	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	13	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	15	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	15	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	16	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	16	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	17	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	17	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	18	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	18	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	19	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	19	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	21	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	21	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	22	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	22	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	23	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	23	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	26	2.13
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	26	2.13
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	5	2.12
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	5	2.12
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	13	2.12
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	13	2.12
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	19	2.12
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	19	2.12
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	21	2.12
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	21	2.12
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	2	2.12
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	2	2.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	9	2.12
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	9	2.12
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	16	2.12
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	16	2.12
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	23	2.12
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	23	2.12
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	11	2.12
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	11	2.12
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	14	2.12
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	14	2.12
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	7	2.12
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	7	2.12
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	8	2.12
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	8	2.12
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	10	2.12
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	10	2.12
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	14	2.12
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	14	2.12
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2'	24	2.12
(1,46)	2:6:2:DT:H1'	2:6:2:DT:H2''	24	2.12
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	26	2.11
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	26	2.11
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	19	2.11
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	19	2.11
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	9	2.11
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	18	2.11
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	1	2.1
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	1	2.1
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	18	2.1
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	18	2.1
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	5	2.1
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	5	2.1
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	8	2.1
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	8	2.1
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	6	2.1
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	6	2.1
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	15	2.1
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	15	2.1
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	7	2.09
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	7	2.09
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	20	2.09
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	20	2.09

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	11	2.09
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	11	2.09
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	13	2.09
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	13	2.09
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	13	2.09
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	13	2.09
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	24	2.09
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	24	2.09
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H61	3	2.09
(1,15)	2:2:2:DC:H2'	2:3:2:DA:H62	3	2.09
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	20	2.08
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	4	2.07
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	4	2.07
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	24	2.07
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	24	2.07
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	21	2.07
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	21	2.07
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	21	2.07
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2'	6	2.07
(1,40)	2:5:2:DG:H2''	2:6:2:DT:H2''	6	2.07
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	20	2.06
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	20	2.06
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	26	2.06
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	26	2.06
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	1	2.05
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	1	2.05
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	26	2.05
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	26	2.05
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	6	2.05
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	21	2.05
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	8	2.04
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	8	2.04
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	25	2.04
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	25	2.04
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	1	2.04
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	1	2.04
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	8	2.04
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	8	2.04
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	3	2.04
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	13	2.04
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	2	2.03
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	2	2.03

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	10	2.03
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	10	2.03
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	18	2.03
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	18	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	2	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	2	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	5	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	5	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	7	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	7	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	15	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	15	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	18	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	18	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	25	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	25	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	26	2.03
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	26	2.03
(1,54)	2:7:2:DG:H1'	2:6:2:DT:H1'	24	2.03
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	4	2.02
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	4	2.02
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	7	2.02
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	7	2.02
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	25	2.02
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	25	2.02
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	15	2.02
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	15	2.02
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	4	2.02
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	4	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	1	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	1	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	3	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	3	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	4	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	4	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	10	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	10	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	11	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	11	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	12	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	12	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	14	2.02

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	14	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	16	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	16	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	19	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	19	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	20	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	20	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	21	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	21	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	22	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	22	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	23	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	23	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	24	2.02
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	24	2.02
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	7	2.02
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	9	2.02
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	17	2.02
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	24	2.02
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H61	3	2.01
(1,331)	2:9:2:DA:H5'	2:9:2:DA:H62	3	2.01
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	12	2.01
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	12	2.01
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	7	2.01
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	7	2.01
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	6	2.01
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	6	2.01
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	13	2.01
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	13	2.01
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	10	2.0
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	10	2.0
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	5	2.0
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	5	2.0
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	9	2.0
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	9	2.0
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2'	17	2.0
(1,69)	2:8:2:DT:H1'	2:8:2:DT:H2''	17	2.0
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	6	2.0
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	10	2.0
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	10	1.99
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	10	1.99
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	20	1.98

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	20	1.98
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	21	1.97
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	21	1.97
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	16	1.97
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	16	1.97
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	4	1.97
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	9	1.96
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	9	1.96
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	12	1.96
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	12	1.96
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	5	1.96
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	12	1.96
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	3	1.96
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	17	1.95
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	17	1.95
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	22	1.95
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	22	1.95
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	2	1.95
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	2	1.95
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	25	1.95
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	25	1.95
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	9	1.95
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	2	1.94
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	2	1.94
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	7	1.94
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	7	1.94
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	26	1.94
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	26	1.94
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	11	1.94
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	11	1.94
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	8	1.94
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	8	1.94
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	14	1.94
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	3	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	3	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	5	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	5	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	8	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	8	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	10	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	10	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	16	1.93

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	16	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	18	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	18	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	22	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	22	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	23	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	23	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	24	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	24	1.93
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	23	1.93
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	23	1.93
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	22	1.93
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	1	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	1	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	4	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	4	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	6	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	6	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	12	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	12	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	13	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	13	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	14	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	14	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	15	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	15	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	19	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	19	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	20	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	20	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	21	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	21	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	25	1.92
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	25	1.92
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	14	1.92
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	14	1.92
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H61	3	1.91
(1,288)	2:2:2:DC:H3'	2:3:2:DA:H62	3	1.91
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	11	1.91
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	11	1.91
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	17	1.91
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	17	1.91

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	6	1.91
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	6	1.91
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	19	1.91
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	19	1.91
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H61	3	1.91
(1,70)	2:8:2:DT:H1'	2:9:2:DA:H62	3	1.91
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	23	1.91
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	7	1.91
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2'	9	1.9
(1,282)	2:4:2:DT:H1'	2:4:2:DT:H2''	9	1.9
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	24	1.9
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	24	1.9
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	26	1.9
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	26	1.9
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	13	1.89
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	13	1.89
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	21	1.89
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	21	1.89
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	10	1.89
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	17	1.89
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	20	1.88
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	20	1.88
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	19	1.88
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	4	1.86
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	1	1.85
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	1	1.85
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	4	1.85
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	4	1.85
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	20	1.85
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	18	1.84
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	18	1.84
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	14	1.83
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	22	1.83
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	7	1.82
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	7	1.82
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	10	1.82
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	10	1.82
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	18	1.82
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	13	1.82
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	5	1.81
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	5	1.81
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	1	1.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	12	1.81
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	20	1.81
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	20	1.81
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	5	1.8
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	21	1.8
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	18	1.8
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	18	1.8
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	25	1.79
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	25	1.79
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	8	1.78
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	8	1.78
(1,68)	2:7:2:DG:H5''	2:6:2:DT:H1'	15	1.78
(1,67)	2:7:2:DG:H5'	2:6:2:DT:H1'	25	1.78
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	6	1.78
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	23	1.78
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	26	1.78
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	26	1.78
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	15	1.78
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	15	1.78
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	17	1.78
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	17	1.78
(1,68)	2:7:2:DG:H5''	2:6:2:DT:H1'	26	1.77
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	24	1.77
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	8	1.76
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	8	1.76
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	15	1.76
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	15	1.76
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	2	1.75
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	2	1.75
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	18	1.75
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	19	1.75
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	19	1.75
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	6	1.74
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	6	1.74
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	19	1.74
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	19	1.74
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	22	1.74
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	22	1.74
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	6	1.74
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	6	1.74
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	15	1.74
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	15	1.74

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	18	1.74
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	18	1.74
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H61	3	1.73
(1,79)	2:8:2:DT:H4'	2:9:2:DA:H62	3	1.73
(1,68)	2:7:2:DG:H5''	2:6:2:DT:H1'	11	1.73
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	8	1.73
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	17	1.73
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	17	1.73
(1,68)	2:7:2:DG:H5''	2:6:2:DT:H1'	8	1.71
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	11	1.71
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	11	1.71
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	25	1.71
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	25	1.71
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	14	1.71
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	14	1.71
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	23	1.71
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	23	1.71
(1,68)	2:7:2:DG:H5''	2:6:2:DT:H1'	2	1.7
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	22	1.7
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	22	1.7
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	2	1.7
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	2	1.7
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	9	1.7
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	9	1.7
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	2	1.69
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	2	1.69
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	2	1.69
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	3	1.69
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	3	1.69
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	9	1.69
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	9	1.69
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	13	1.69
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	13	1.69
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	23	1.69
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	23	1.69
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	16	1.69
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	16	1.69
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	22	1.69
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	22	1.69
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	16	1.68
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	10	1.68
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	10	1.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	14	1.68
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	14	1.68
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	16	1.68
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	16	1.68
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	2	1.68
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	2	1.68
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	8	1.68
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	8	1.68
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	8	1.67
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	8	1.67
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	2	1.66
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	2	1.66
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	4	1.66
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	4	1.66
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	8	1.66
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	8	1.66
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	13	1.66
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	13	1.66
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	19	1.66
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	19	1.66
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	26	1.66
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	26	1.66
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	25	1.65
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	11	1.65
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	11	1.65
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	11	1.64
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	1	1.64
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	1	1.64
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	11	1.64
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	11	1.64
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	12	1.64
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	12	1.64
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	11	1.64
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	11	1.64
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	12	1.64
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	12	1.64
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	5	1.63
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	5	1.63
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	26	1.63
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	26	1.63
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	13	1.62
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	13	1.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	7	1.62
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	7	1.62
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	1	1.62
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	1	1.62
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	1	1.62
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	1	1.62
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	13	1.62
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	13	1.62
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	14	1.61
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	14	1.61
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	5	1.61
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	5	1.61
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	23	1.61
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	23	1.61
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	26	1.61
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	26	1.61
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	24	1.61
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	24	1.61
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	5	1.61
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	5	1.61
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	24	1.61
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	24	1.61
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	15	1.6
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	12	1.6
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	12	1.6
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	18	1.59
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	18	1.59
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	16	1.59
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	16	1.59
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	4	1.59
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	4	1.59
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	25	1.59
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	25	1.59
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	7	1.59
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	7	1.59
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	6	1.58
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	6	1.58
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	8	1.58
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	8	1.58
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	15	1.58
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	15	1.58
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	21	1.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	21	1.58
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	26	1.58
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	26	1.58
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	4	1.58
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	4	1.58
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	10	1.58
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	10	1.58
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	2	1.57
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	2	1.57
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	4	1.57
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	4	1.57
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	7	1.57
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	7	1.57
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	21	1.57
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	21	1.57
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	10	1.56
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	10	1.56
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	13	1.56
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	13	1.56
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	22	1.56
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	22	1.56
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	25	1.56
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	25	1.56
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	20	1.56
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	20	1.56
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	25	1.56
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	25	1.56
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	5	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	5	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	7	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	7	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	14	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	14	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	20	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	20	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	23	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	23	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	24	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	24	1.55
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	13	1.55
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	13	1.55
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	10	1.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	10	1.55
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	21	1.55
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	21	1.55
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	1	1.54
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	1	1.54
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	3	1.54
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	3	1.54
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	12	1.54
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	12	1.54
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	16	1.54
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	16	1.54
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	19	1.54
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	19	1.54
(1,56)	2:7:2:DG:H2'	2:6:2:DT:H1'	26	1.54
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	21	1.54
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	21	1.54
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	9	1.53
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	9	1.53
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	11	1.53
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	11	1.53
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H61	17	1.53
(1,330)	2:9:2:DA:H4'	2:9:2:DA:H62	17	1.53
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	24	1.52
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	24	1.52
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	6	1.52
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	6	1.52
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	21	1.52
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	21	1.52
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	26	1.52
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	26	1.52
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	20	1.52
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	20	1.52
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	2	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	2	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	3	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	3	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	5	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	5	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	7	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	7	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	8	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	8	1.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	12	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	12	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	14	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	14	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	15	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	15	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	16	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	16	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	18	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	18	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	22	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	22	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	24	1.51
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	24	1.51
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	6	1.5
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	6	1.5
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	14	1.5
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	14	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	1	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	1	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	4	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	4	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	10	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	10	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	13	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	13	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	19	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	19	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	20	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	20	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	23	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	23	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	25	1.5
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	25	1.5
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	14	1.49
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	14	1.49
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	3	1.49
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	9	1.49
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	9	1.49
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	11	1.49
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	11	1.49
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H61	17	1.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	2:3:2:DA:H1'	2:3:2:DA:H62	17	1.49
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H61	3	1.48
(1,17)	2:2:2:DC:H2''	2:3:2:DA:H62	3	1.48
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	9	1.47
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	9	1.47
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	2	1.43
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	13	1.43
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	16	1.43
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	16	1.43
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H61	3	1.43
(1,11)	2:2:2:DC:H1'	2:3:2:DA:H62	3	1.43
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	18	1.4
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	18	1.4
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	22	1.4
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	22	1.4
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	8	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	2	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	2	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	4	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	4	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	8	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	8	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	21	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	21	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	23	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	23	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	24	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	24	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	25	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	25	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	26	1.39
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	26	1.39
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	7	1.38
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	22	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	3	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	3	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	5	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	5	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	6	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	6	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	7	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	7	1.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	10	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	10	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	12	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	12	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	13	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	13	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	15	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	15	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	20	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	20	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	22	1.38
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	22	1.38
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	21	1.38
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	21	1.38
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	5	1.37
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	1	1.37
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	1	1.37
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	11	1.37
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	11	1.37
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	14	1.37
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	14	1.37
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	17	1.37
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	17	1.37
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	19	1.37
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	19	1.37
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	25	1.36
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	9	1.36
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	9	1.36
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H61	16	1.36
(1,81)	2:9:2:DA:H1'	2:9:2:DA:H62	16	1.36
(1,68)	2:7:2:DG:H5''	2:6:2:DT:H1'	16	1.36
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	16	1.34
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	18	1.34
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	8	1.34
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	8	1.34
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	1	1.33
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	10	1.33
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	19	1.33
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	21	1.33
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	3	1.33
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	3	1.33
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	4	1.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	5	1.32
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	5	1.32
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	9	1.32
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	9	1.32
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	20	1.31
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	24	1.31
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	16	1.31
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	16	1.31
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	20	1.31
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	20	1.31
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	15	1.3
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	26	1.3
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	2	1.3
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	2	1.3
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	12	1.29
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	17	1.29
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	22	1.29
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	22	1.29
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	11	1.28
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	8	1.28
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	8	1.28
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	10	1.28
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	10	1.28
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	25	1.28
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	25	1.28
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	3	1.27
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	23	1.27
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	3	1.27
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	3	1.27
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	1	1.26
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	14	1.26
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	7	1.26
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	7	1.26
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	21	1.26
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	21	1.26
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	14	1.26
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	14	1.26
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	18	1.26
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	18	1.26
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	5	1.25
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	25	1.25
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	9	1.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	17	1.25
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	17	1.25
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	2	1.24
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	10	1.24
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	1	1.24
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	1	1.24
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	9	1.24
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	9	1.24
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	18	1.24
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	18	1.24
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	23	1.24
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	23	1.24
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	4	1.23
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	16	1.23
(1,102)	2:10:2:DC:H4'	2:9:2:DA:H1'	6	1.23
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	15	1.23
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	15	1.23
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	19	1.23
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	19	1.23
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	15	1.23
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	15	1.23
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	13	1.22
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	17	1.22
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	19	1.22
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	20	1.22
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	4	1.22
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	4	1.22
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	6	1.22
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	6	1.22
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	24	1.22
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	24	1.22
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	9	1.21
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	11	1.21
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	18	1.21
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	11	1.21
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	11	1.21
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	12	1.21
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	12	1.21
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	20	1.21
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	20	1.21
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	26	1.21
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	26	1.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	7	1.2
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	8	1.2
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	14	1.2
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	24	1.2
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	26	1.2
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	8	1.2
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	8	1.2
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	26	1.2
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	26	1.2
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	23	1.2
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	23	1.2
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	21	1.19
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	22	1.19
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	23	1.19
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5'	17	1.19
(1,101)	2:10:2:DC:H3'	2:11:2:DG:H5''	17	1.19
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	3	1.19
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	6	1.19
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	6	1.19
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	6	1.17
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	19	1.17
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	6	1.16
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	7	1.16
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	12	1.16
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	21	1.16
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	26	1.16
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	12	1.16
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	2	1.15
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	3	1.15
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	5	1.15
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	8	1.15
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	13	1.15
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	22	1.15
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	23	1.15
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	25	1.15
(1,127)	2:2:2:DC:H2'	2:1:2:DG:H2''	15	1.15
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	9	1.15
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	11	1.15
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	11	1.15
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	19	1.15
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	19	1.15
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	1	1.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	4	1.14
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	10	1.14
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	14	1.14
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	18	1.14
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	20	1.14
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	17	1.14
(1,45)	2:5:2:DG:H5'	2:4:2:DT:H1'	18	1.14
(1,45)	2:5:2:DG:H5''	2:4:2:DT:H1'	18	1.14
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	16	1.13
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	24	1.13
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	20	1.13
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	15	1.12
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	19	1.12
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	9	1.11
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	11	1.11
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	7	1.11
(1,134)	2:2:2:DC:H2''	2:3:2:DA:H8	17	1.1
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	10	1.1
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	1	1.09
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	1	1.09
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	15	1.08
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	15	1.08
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	4	1.07
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	21	1.06
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	1	1.05
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	2	1.05
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	2	1.05
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	13	1.04
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	19	1.02
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	19	1.02
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	24	1.01
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	14	1.0
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	12	0.98
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	22	0.98
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	9	0.98
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	9	0.98
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	17	0.98
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	17	0.98
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	6	0.97
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	23	0.97
(1,99)	2:10:2:DC:H2''	2:11:2:DG:H5'	13	0.96
(1,99)	2:10:2:DC:H2''	2:11:2:DG:H5''	13	0.96

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	16	0.95
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	18	0.95
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	5	0.95
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	3	0.95
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	3	0.95
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	2	0.94
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	8	0.94
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	10	0.94
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	10	0.94
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	13	0.94
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	13	0.94
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	21	0.94
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	21	0.94
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	7	0.93
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	7	0.93
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	20	0.93
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	20	0.93
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	24	0.93
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	24	0.93
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	4	0.92
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	4	0.92
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	2	0.91
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	13	0.91
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	25	0.91
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	25	0.91
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	2	0.9
(1,68)	2:7:2:DG:H5''	2:6:2:DT:H1'	25	0.89
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	12	0.89
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	12	0.89
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	14	0.89
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	14	0.89
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	22	0.89
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	22	0.89
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	6	0.88
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	6	0.88
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	23	0.88
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	23	0.88
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	18	0.87
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	21	0.86
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	18	0.86
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	5	0.86
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	5	0.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5'	18	0.86
(1,51)	2:6:2:DT:H2''	2:7:2:DG:H5''	18	0.86
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	1	0.86
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	1	0.86
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	8	0.85
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	16	0.84
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	22	0.84
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	11	0.84
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	25	0.84
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	13	0.84
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	13	0.84
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	8	0.83
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	15	0.83
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	1	0.83
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	1	0.83
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	6	0.82
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	1	0.82
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	11	0.82
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	5	0.81
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	10	0.81
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	12	0.81
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	13	0.81
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	17	0.81
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	20	0.81
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	5	0.81
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	9	0.81
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	14	0.81
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	17	0.81
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	20	0.81
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	20	0.81
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	1	0.8
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	15	0.8
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	3	0.8
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	4	0.8
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	11	0.8
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	23	0.8
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	5	0.8
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	5	0.8
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	9	0.8
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	9	0.8
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	25	0.8
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	13	0.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	13	0.8
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	10	0.79
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	19	0.79
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	5	0.79
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	7	0.79
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	9	0.79
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	14	0.79
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	19	0.79
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	22	0.79
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	25	0.79
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	15	0.79
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	16	0.79
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	16	0.79
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	1	0.79
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	16	0.79
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	19	0.79
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	23	0.79
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	26	0.79
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	3	0.79
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	3	0.79
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	17	0.79
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	17	0.79
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	19	0.79
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	19	0.79
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	26	0.78
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	6	0.78
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	8	0.78
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	16	0.78
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	18	0.78
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	21	0.78
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	24	0.78
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	26	0.78
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	18	0.78
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	18	0.78
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	6	0.78
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	10	0.78
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	15	0.78
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	20	0.78
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	4	0.78
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	4	0.78
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	10	0.78
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	10	0.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	21	0.78
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	21	0.78
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	23	0.78
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	23	0.78
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	23	0.77
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	23	0.77
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	3	0.77
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	4	0.77
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	24	0.77
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	26	0.77
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	5	0.77
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	5	0.77
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	7	0.77
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	7	0.77
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	24	0.77
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	24	0.77
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	4	0.76
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	11	0.76
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	20	0.76
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	2	0.76
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	8	0.76
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	2	0.76
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	2	0.76
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	10	0.76
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	10	0.76
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	12	0.76
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	12	0.76
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	21	0.76
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	12	0.76
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	12	0.76
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	14	0.76
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	14	0.76
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	18	0.76
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	18	0.76
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	22	0.76
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	22	0.76
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	19	0.76
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	19	0.76
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	23	0.75
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	24	0.75
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	2	0.75
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	22	0.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	22	0.75
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	6	0.75
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	6	0.75
(1,198)	2:6:2:DT:H2'	2:6:2:DT:H6	15	0.74
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	21	0.74
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	9	0.74
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	17	0.74
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	7	0.74
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	16	0.74
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	16	0.74
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	12	0.73
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	15	0.73
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	17	0.73
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	2	0.73
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	9	0.73
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	9	0.73
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	3	0.72
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	9	0.72
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	13	0.72
(1,84)	2:9:2:DA:H2'	2:8:2:DT:H2''	12	0.72
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	22	0.71
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	3	0.71
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	13	0.71
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	17	0.71
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	18	0.71
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	24	0.71
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	6	0.71
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	10	0.71
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	11	0.71
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	15	0.71
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	23	0.71
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	24	0.71
(1,63)	2:7:2:DG:H3'	2:6:2:DT:H1'	16	0.71
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	9	0.7
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	14	0.7
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	6	0.7
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	26	0.7
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	14	0.7
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	18	0.7
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	20	0.7
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	25	0.7
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	6	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	6	0.7
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	25	0.7
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	25	0.7
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	9	0.7
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	9	0.7
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	5	0.7
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	5	0.7
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	5	0.69
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	10	0.69
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	11	0.69
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	14	0.69
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	19	0.69
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	22	0.69
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	3	0.69
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	3	0.69
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	17	0.69
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	17	0.69
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	7	0.68
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	13	0.68
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	22	0.68
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	16	0.68
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	2	0.68
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	7	0.68
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	8	0.68
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	12	0.68
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	1	0.68
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	1	0.68
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	3	0.68
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	3	0.68
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	20	0.68
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	20	0.68
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	25	0.67
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	5	0.67
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	1	0.67
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	20	0.67
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	6	0.67
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	1	0.67
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	4	0.67
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	26	0.67
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	15	0.67
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	15	0.67
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	6	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	4	0.66
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	7	0.66
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	19	0.66
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	16	0.66
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	3	0.66
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	16	0.66
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	5	0.66
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	19	0.66
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	19	0.66
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	26	0.66
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	26	0.66
(1,99)	2:10:2:DC:H2''	2:11:2:DG:H5'	14	0.66
(1,99)	2:10:2:DC:H2''	2:11:2:DG:H5''	14	0.66
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	13	0.66
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	13	0.66
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	21	0.66
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	21	0.66
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	12	0.65
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	21	0.65
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	7	0.65
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	7	0.65
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	8	0.65
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	8	0.65
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	21	0.65
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	21	0.65
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	4	0.65
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	4	0.65
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	10	0.65
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	10	0.65
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	26	0.64
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	9	0.64
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	17	0.64
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	25	0.64
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	6	0.64
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	14	0.64
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	15	0.64
(1,117)	2:1:2:DG:H2''	2:1:2:DG:H8	5	0.64
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	21	0.64
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	7	0.64
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	7	0.64
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	24	0.64
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	24	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	11	0.63
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	15	0.63
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	1	0.63
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	2	0.63
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	17	0.63
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	18	0.63
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	19	0.63
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	24	0.63
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	1	0.63
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	19	0.63
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	22	0.63
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	22	0.63
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	22	0.63
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	16	0.62
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	25	0.62
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	18	0.62
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	15	0.62
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	24	0.62
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	5	0.62
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	7	0.62
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	8	0.62
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	23	0.62
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	25	0.62
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	16	0.62
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	24	0.62
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	24	0.62
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	5	0.62
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	5	0.62
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	12	0.62
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	12	0.62
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	14	0.62
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	14	0.62
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	23	0.62
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	23	0.62
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	2	0.61
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	23	0.61
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	9	0.61
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	10	0.61
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	11	0.61
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	12	0.61
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	13	0.61
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	21	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	22	0.61
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	26	0.61
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	20	0.61
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	3	0.61
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	4	0.61
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	4	0.61
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	4	0.61
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	11	0.6
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	3	0.6
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	4	0.6
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	3	0.6
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	2	0.6
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	9	0.6
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	6	0.6
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	6	0.6
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	18	0.6
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	18	0.6
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	8	0.59
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	23	0.59
(1,148)	2:3:2:DA:H2''	2:3:2:DA:H8	20	0.59
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	4	0.59
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	7	0.59
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	8	0.59
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	14	0.59
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	26	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	3	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	4	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	7	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	12	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	18	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	19	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	20	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	21	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	22	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	23	0.59
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	24	0.59
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	19	0.58
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	24	0.58
(1,194)	2:6:2:DT:H2'	3:12:1:A4A:H4	22	0.58
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	10	0.58
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	11	0.58
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	21	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	22	0.58
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	10	0.58
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	11	0.58
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	12	0.58
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	20	0.58
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	11	0.58
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	11	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	1	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	2	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	5	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	6	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	8	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	9	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	10	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	13	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	14	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	15	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	17	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	25	0.58
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	26	0.58
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	4	0.58
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	4	0.58
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	1	0.57
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	17	0.57
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	5	0.57
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	7	0.57
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	9	0.57
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	12	0.57
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	13	0.57
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	24	0.57
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	25	0.57
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	26	0.57
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	23	0.57
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	11	0.57
(1,61)	2:7:2:DG:H2''	2:7:2:DG:H1'	16	0.57
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	18	0.56
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	18	0.56
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	13	0.56
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	1	0.56
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	8	0.56
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	23	0.56
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	25	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	20	0.56
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	20	0.56
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	12	0.56
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	11	0.56
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	11	0.56
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	16	0.55
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	2	0.55
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	6	0.55
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	14	0.55
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	17	0.55
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	18	0.55
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	18	0.55
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	24	0.55
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5'	17	0.55
(1,105)	2:11:2:DG:H2'	2:11:2:DG:H5''	17	0.55
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	14	0.54
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	3	0.54
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	2	0.54
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	14	0.54
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	21	0.54
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	15	0.54
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	19	0.54
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	6	0.54
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	15	0.54
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	10	0.54
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	10	0.54
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	8	0.53
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	25	0.53
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	4	0.53
(1,145)	2:3:2:DA:H2'	2:3:2:DA:H8	16	0.53
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	13	0.53
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	15	0.53
(1,114)	2:1:2:DG:H2'	2:1:2:DG:H8	17	0.53
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	2	0.53
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	2	0.53
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	2	0.53
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	8	0.53
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	11	0.53
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	26	0.53
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	7	0.53
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	7	0.53
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	7	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	12	0.52
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	23	0.52
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	21	0.52
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	26	0.52
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	23	0.52
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	18	0.52
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	18	0.52
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	4	0.52
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	26	0.52
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	26	0.52
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	1	0.51
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	10	0.51
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	25	0.51
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	1	0.51
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	8	0.51
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	12	0.51
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	16	0.51
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	18	0.51
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	9	0.51
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	10	0.51
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	17	0.51
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	9	0.5
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	14	0.5
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	18	0.5
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	19	0.5
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	16	0.5
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	3	0.5
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	5	0.5
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	10	0.5
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	20	0.5
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	26	0.5
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	19	0.5
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	1	0.5
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	16	0.5
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	2	0.49
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	4	0.49
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	5	0.49
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	15	0.49
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	22	0.49
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	18	0.49
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	20	0.49
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	7	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	22	0.49
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	25	0.49
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	3	0.49
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	15	0.49
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	7	0.49
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	21	0.49
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	6	0.49
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	21	0.49
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	2	0.49
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	2	0.49
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	26	0.48
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	15	0.48
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	19	0.48
(1,107)	2:11:2:DG:H2''	2:11:2:DG:H5'	13	0.48
(1,107)	2:11:2:DG:H2''	2:11:2:DG:H5''	13	0.48
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	20	0.48
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	24	0.48
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	5	0.48
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	7	0.48
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	13	0.48
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	18	0.48
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	19	0.48
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	20	0.48
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	22	0.48
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	23	0.48
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	24	0.48
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	24	0.48
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	24	0.48
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	6	0.47
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	8	0.47
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	13	0.47
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	3	0.47
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	3	0.47
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	2	0.47
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	9	0.47
(1,177)	2:5:2:DG:H2'	3:12:1:A4A:H4	11	0.47
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	16	0.47
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	7	0.47
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	7	0.47
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	16	0.47
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	25	0.47
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	26	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	16	0.47
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	16	0.47
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	3	0.47
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	26	0.47
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	3	0.47
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	4	0.47
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	10	0.47
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	12	0.47
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	14	0.47
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	25	0.47
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	17	0.46
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	20	0.46
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	24	0.46
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	8	0.46
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	22	0.46
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	7	0.46
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	12	0.46
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	15	0.46
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	2	0.46
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	11	0.46
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	15	0.46
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	26	0.46
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	2	0.46
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	3	0.46
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	8	0.46
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	16	0.46
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	22	0.46
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	23	0.46
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	26	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	1	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	2	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	4	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	6	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	8	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	12	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	13	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	17	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	18	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	21	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	23	0.46
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	24	0.46
(1,107)	2:11:2:DG:H2''	2:11:2:DG:H5'	14	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	2:11:2:DG:H2''	2:11:2:DG:H5''	14	0.46
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	10	0.46
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	10	0.46
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	2	0.46
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	16	0.46
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	1	0.46
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	23	0.46
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	9	0.46
(1,64)	2:7:2:DG:H3'	2:7:2:DG:H1'	17	0.46
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	16	0.46
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	16	0.46
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	15	0.45
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	15	0.45
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	4	0.45
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	10	0.45
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	6	0.45
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	5	0.45
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	9	0.45
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	6	0.45
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	18	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	1	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	7	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	8	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	10	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	12	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	13	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	17	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	21	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	22	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	23	0.45
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	24	0.45
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	1	0.45
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	5	0.45
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	6	0.45
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	10	0.45
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	15	0.45
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	18	0.45
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	24	0.45
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	25	0.45
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	5	0.45
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	11	0.45
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	14	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	5	0.45
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	5	0.45
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	3	0.45
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	5	0.45
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	7	0.45
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	8	0.45
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	14	0.45
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	15	0.45
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	18	0.45
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	22	0.45
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	26	0.45
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	11	0.45
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	22	0.45
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	1	0.45
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	1	0.45
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	9	0.44
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	9	0.44
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	24	0.44
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	24	0.44
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	3	0.44
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	8	0.44
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	25	0.44
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	21	0.44
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	26	0.44
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	4	0.44
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	4	0.44
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	7	0.44
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	14	0.44
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	17	0.44
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	18	0.44
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	20	0.44
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	6	0.44
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	21	0.44
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	4	0.44
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	6	0.44
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	9	0.44
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	18	0.44
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	19	0.44
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	20	0.44
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	25	0.44
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	4	0.44
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	12	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	13	0.44
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	14	0.44
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	19	0.44
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	20	0.44
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	21	0.44
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	10	0.44
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	20	0.44
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	22	0.44
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	6	0.44
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	6	0.44
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	21	0.44
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	21	0.44
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	1	0.44
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	6	0.44
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	10	0.44
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	19	0.44
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	21	0.44
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	23	0.44
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	24	0.44
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	25	0.44
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	6	0.44
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	15	0.44
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	12	0.44
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	12	0.44
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	17	0.43
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	17	0.43
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	2	0.43
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	7	0.43
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	9	0.43
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	11	0.43
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	13	0.43
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	17	0.43
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	19	0.43
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	20	0.43
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	11	0.43
(1,273)	2:11:2:DG:H2'	2:11:2:DG:H8	21	0.43
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	5	0.43
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	10	0.43
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	10	0.43
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	21	0.43
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	22	0.43
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	23	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	24	0.43
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	9	0.43
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	13	0.43
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	17	0.43
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	24	0.43
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	3	0.43
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	14	0.43
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	11	0.43
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	17	0.43
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	19	0.43
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	4	0.43
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	12	0.43
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	16	0.43
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	1	0.43
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	1	0.43
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	18	0.43
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	11	0.42
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	1	0.42
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	6	0.42
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	12	0.42
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	13	0.42
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	19	0.42
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	2	0.42
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	11	0.42
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	14	0.42
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	16	0.42
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	20	0.42
(1,166)	2:4:2:DT:H2''	2:4:2:DT:H6	5	0.42
(1,165)	2:4:2:DT:H2''	2:4:2:DT:H1'	9	0.42
(1,120)	2:1:2:DG:H3'	2:1:2:DG:H1'	9	0.42
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	8	0.42
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	8	0.42
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	9	0.42
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	13	0.42
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	17	0.42
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	20	0.42
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	5	0.42
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	25	0.42
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	15	0.42
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	21	0.41
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	21	0.41
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	1	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	18	0.41
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	1	0.41
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	9	0.41
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	19	0.41
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	24	0.41
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	7	0.41
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	26	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	1	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	2	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	6	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	7	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	8	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	10	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	12	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	13	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	14	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	16	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	21	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	24	0.41
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	26	0.41
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	1	0.41
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	1	0.41
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	19	0.41
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	19	0.41
(1,89)	2:9:2:DA:H2''	2:9:2:DA:H1'	11	0.41
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	8	0.41
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	14	0.41
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	22	0.41
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	3	0.41
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	3	0.41
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	5	0.41
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	5	0.41
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	13	0.41
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	15	0.41
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	15	0.41
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	17	0.41
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	17	0.41
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5'	25	0.41
(1,8)	2:1:2:DG:H2'	2:1:2:DG:H5''	25	0.41
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	15	0.4
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	5	0.4
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	12	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	22	0.4
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	14	0.4
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	1	0.4
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	3	0.4
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	4	0.4
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	8	0.4
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	12	0.4
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	25	0.4
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	4	0.4
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	5	0.4
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	11	0.4
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	19	0.4
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	22	0.4
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	23	0.4
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	25	0.4
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	23	0.4
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	23	0.4
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	18	0.4
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	18	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	4	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	4	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	7	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	7	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	10	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	10	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	12	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	12	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	13	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	13	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	14	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	14	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	17	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	17	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	18	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	18	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	19	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	19	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	20	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	20	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	22	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	22	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	23	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	23	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	24	0.4
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	24	0.4
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	13	0.4
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	17	0.4
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	9	0.39
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	18	0.39
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	21	0.39
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	21	0.39
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	23	0.39
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	24	0.39
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	26	0.39
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	4	0.39
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	15	0.39
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	17	0.39
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	24	0.39
(1,242)	2:8:2:DT:H6	2:9:2:DA:H8	10	0.39
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	5	0.39
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	10	0.39
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	19	0.39
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	22	0.39
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	16	0.39
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	3	0.39
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	9	0.39
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	15	0.39
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	20	0.39
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	9	0.39
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	23	0.39
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	14	0.39
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	17	0.39
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	20	0.39
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	24	0.39
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	26	0.39
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	26	0.39
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	6	0.39
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	6	0.39
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	21	0.39
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	21	0.39
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5'	25	0.39
(1,49)	2:6:2:DT:H2'	2:7:2:DG:H5''	25	0.39
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	2	0.39
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	6	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	8	0.39
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	14	0.39
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	6	0.39
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	9	0.38
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	18	0.38
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	6	0.38
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	6	0.38
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	3	0.38
(1,213)	2:6:2:DT:H5'	3:12:1:A4A:H4	23	0.38
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	1	0.38
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	2	0.38
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	9	0.38
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	11	0.38
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	13	0.38
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	17	0.38
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	4	0.38
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	23	0.38
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	18	0.38
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	22	0.38
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	7	0.38
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	11	0.38
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	21	0.38
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	26	0.38
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	4	0.38
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	4	0.38
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	22	0.38
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	22	0.38
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	9	0.38
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	9	0.38
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	4	0.38
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	16	0.38
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	20	0.38
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	25	0.38
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	17	0.38
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	17	0.37
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	6	0.37
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	24	0.37
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	14	0.37
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	23	0.37
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	3	0.37
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	4	0.37
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	8	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	10	0.37
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	18	0.37
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	25	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	1	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	6	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	7	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	9	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	11	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	12	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	13	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	14	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	15	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	18	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	20	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	21	0.37
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	22	0.37
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	7	0.37
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	19	0.37
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	9	0.37
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	13	0.37
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	18	0.37
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	22	0.37
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	3	0.37
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	4	0.37
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	6	0.37
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	7	0.37
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	8	0.37
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	13	0.37
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	15	0.37
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	19	0.37
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	9	0.37
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	9	0.37
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	11	0.37
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	11	0.37
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	12	0.37
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	12	0.37
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	17	0.37
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	17	0.37
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	1	0.37
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	23	0.37
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	26	0.37
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	2	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	5	0.37
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	8	0.37
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	15	0.37
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	23	0.37
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	13	0.36
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	15	0.36
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	14	0.36
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	14	0.36
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	7	0.36
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	25	0.36
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	8	0.36
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	21	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	5	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	6	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	7	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	12	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	15	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	19	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	20	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	21	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	22	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	23	0.36
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	26	0.36
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	6	0.36
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	2	0.36
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	5	0.36
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	8	0.36
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	10	0.36
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	16	0.36
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	19	0.36
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	24	0.36
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	25	0.36
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	26	0.36
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	1	0.36
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	13	0.36
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	21	0.36
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	1	0.36
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	2	0.36
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	18	0.36
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	18	0.36
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	3	0.36
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	5	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	7	0.36
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	10	0.36
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	11	0.36
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	12	0.36
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	19	0.36
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	20	0.36
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	25	0.36
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	26	0.36
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	14	0.35
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	20	0.35
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	22	0.35
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	23	0.35
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	6	0.35
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	12	0.35
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	20	0.35
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	25	0.35
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	14	0.35
(1,201)	2:6:2:DT:H2''	2:6:2:DT:H3'	24	0.35
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	6	0.35
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	7	0.35
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	21	0.35
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	23	0.35
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	25	0.35
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	13	0.35
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	3	0.35
(1,169)	2:4:2:DT:H3'	2:4:2:DT:H1'	17	0.35
(1,149)	2:3:2:DA:H2''	2:4:2:DT:H6	17	0.35
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	5	0.35
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	10	0.35
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	11	0.35
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	14	0.35
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	23	0.35
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	5	0.35
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	12	0.35
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	16	0.35
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	22	0.35
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	25	0.35
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	20	0.35
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	20	0.35
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	24	0.35
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	24	0.35
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	22	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	9	0.35
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	12	0.35
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	14	0.35
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	19	0.35
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	6	0.34
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	7	0.34
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	10	0.34
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	11	0.34
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	25	0.34
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	6	0.34
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	2	0.34
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	4	0.34
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	5	0.34
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	12	0.34
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	13	0.34
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	14	0.34
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	18	0.34
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	20	0.34
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	22	0.34
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	26	0.34
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	2	0.34
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	4	0.34
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	16	0.34
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	20	0.34
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	10	0.34
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	14	0.34
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	15	0.34
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	20	0.34
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	23	0.34
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	15	0.34
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	15	0.34
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	13	0.34
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	24	0.34
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	4	0.34
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	7	0.34
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	2	0.33
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	8	0.33
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	12	0.33
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	19	0.33
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	24	0.33
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	11	0.33
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	1	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	3	0.33
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	8	0.33
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	15	0.33
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	19	0.33
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	24	0.33
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	15	0.33
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	18	0.33
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	25	0.33
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	6	0.33
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	24	0.33
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	9	0.33
(1,106)	2:11:2:DG:H2''	2:11:2:DG:H1'	10	0.33
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	11	0.33
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	21	0.33
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	4	0.32
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	26	0.32
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	16	0.32
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	16	0.32
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	16	0.32
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	15	0.32
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	15	0.32
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	15	0.32
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	25	0.32
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	26	0.32
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	10	0.32
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	11	0.32
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	2	0.32
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	17	0.32
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	18	0.32
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	24	0.32
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	3	0.32
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	8	0.32
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	15	0.32
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	24	0.32
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	18	0.32
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	2	0.32
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	11	0.32
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	3	0.32
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	3	0.32
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	23	0.32
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	23	0.32
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	21	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	1	0.32
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	3	0.32
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	10	0.32
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	26	0.31
(1,339)	2:11:2:DG:H4'	2:10:2:DC:H1'	13	0.31
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	12	0.31
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	12	0.31
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	23	0.31
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	23	0.31
(1,283)	2:9:2:DA:H2'	2:9:2:DA:H8	16	0.31
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	15	0.31
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	17	0.31
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	1	0.31
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	9	0.31
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	6	0.31
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	12	0.31
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	17	0.31
(1,121)	2:1:2:DG:H3'	2:1:2:DG:H8	26	0.31
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	16	0.31
(1,88)	2:9:2:DA:H2''	2:8:2:DT:H1'	2	0.31
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	14	0.31
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	14	0.31
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	22	0.31
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	22	0.31
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	24	0.31
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	1	0.3
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	5	0.3
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	16	0.3
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	21	0.3
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	2	0.3
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	1	0.3
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	1	0.3
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	4	0.3
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	4	0.3
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	7	0.3
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	7	0.3
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	11	0.3
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	11	0.3
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	13	0.3
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	2	0.3
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	8	0.3
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	11	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	26	0.3
(1,225)	2:7:2:DG:H2''	2:7:2:DG:H8	16	0.3
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	18	0.3
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	3	0.3
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	19	0.3
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	9	0.3
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	7	0.3
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	10	0.3
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	13	0.3
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	17	0.3
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	23	0.3
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	25	0.3
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	23	0.3
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	25	0.3
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	25	0.3
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	6	0.3
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	6	0.3
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	9	0.3
(1,41)	2:5:2:DG:H3'	2:5:2:DG:H1'	18	0.3
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	4	0.29
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	12	0.29
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	23	0.29
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	5	0.29
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	23	0.29
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	26	0.29
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	5	0.29
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	5	0.29
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	19	0.29
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	19	0.29
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	26	0.29
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	26	0.29
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	11	0.29
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	16	0.29
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	9	0.29
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	11	0.29
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	20	0.29
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	2	0.29
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	16	0.29
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	21	0.29
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	2	0.29
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	5	0.29
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	14	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	20	0.29
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	22	0.29
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	17	0.29
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	19	0.29
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5'	7	0.29
(1,97)	2:10:2:DC:H2'	2:11:2:DG:H5''	7	0.29
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	5	0.29
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	5	0.29
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	12	0.29
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	12	0.29
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	24	0.29
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	24	0.29
(1,23)	2:3:2:DA:H2'	2:2:2:DC:H2''	16	0.29
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	3	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	5	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	7	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	9	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	10	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	14	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	17	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	18	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	20	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	21	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	22	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	24	0.28
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	2	0.28
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	3	0.28
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	7	0.28
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	11	0.28
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	12	0.28
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	16	0.28
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	19	0.28
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	20	0.28
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	22	0.28
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	25	0.28
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	15	0.28
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	16	0.28
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	13	0.28
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	13	0.28
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	2	0.28
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	21	0.28
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	24	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	18	0.28
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	26	0.28
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	5	0.28
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	6	0.28
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	17	0.28
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	4	0.28
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	8	0.28
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	11	0.28
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	14	0.28
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	6	0.28
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	9	0.28
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	22	0.28
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	6	0.28
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	9	0.28
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	11	0.28
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	19	0.28
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	24	0.28
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	3	0.28
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	4	0.28
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	25	0.28
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	5	0.28
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	9	0.28
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	10	0.28
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	12	0.28
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	6	0.27
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	13	0.27
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	19	0.27
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	17	0.27
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	1	0.27
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	8	0.27
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	10	0.27
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	15	0.27
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	23	0.27
(1,340)	2:11:2:DG:H5'	2:10:2:DC:H1'	13	0.27
(1,340)	2:11:2:DG:H5''	2:10:2:DC:H1'	13	0.27
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	8	0.27
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	8	0.27
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	17	0.27
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	6	0.27
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	11	0.27
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	21	0.27
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	22	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	26	0.27
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	2	0.27
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	1	0.27
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	16	0.27
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	1	0.27
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	4	0.27
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	7	0.27
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	10	0.27
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	12	0.27
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	13	0.27
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	22	0.27
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	26	0.27
(1,197)	2:6:2:DT:H2'	2:6:2:DT:H3'	16	0.27
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	20	0.27
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	15	0.27
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	1	0.27
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	3	0.27
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	15	0.27
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	1	0.27
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	8	0.27
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	19	0.27
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	4	0.27
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	4	0.27
(1,398)	2:2:2:DC:H2''	2:2:2:DC:H6	3	0.26
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	1	0.26
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	14	0.26
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	6	0.26
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	13	0.26
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	4	0.26
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	6	0.26
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	14	0.26
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	7	0.26
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	18	0.26
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	26	0.26
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	2	0.26
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	2	0.26
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	10	0.26
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	10	0.26
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	8	0.26
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	24	0.26
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	9	0.26
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	12	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	18	0.26
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	20	0.26
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	23	0.26
(1,261)	2:10:2:DC:H2'	2:11:2:DG:H8	13	0.26
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	26	0.26
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	6	0.26
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	21	0.26
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	11	0.26
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	12	0.26
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	13	0.26
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	17	0.26
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	8	0.26
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	14	0.26
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	15	0.26
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	23	0.26
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	3	0.26
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	10	0.26
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	22	0.26
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	23	0.26
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	5	0.26
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	4	0.26
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	8	0.26
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	16	0.26
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	12	0.26
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	21	0.26
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	26	0.26
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	2	0.26
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	6	0.26
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	16	0.26
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	18	0.26
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	25	0.26
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	2	0.25
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	4	0.25
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	11	0.25
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	15	0.25
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	16	0.25
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	20	0.25
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	25	0.25
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	2	0.25
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	3	0.25
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	13	0.25
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	22	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	22	0.25
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	2	0.25
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	16	0.25
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	13	0.25
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	20	0.25
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	1	0.25
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	3	0.25
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	7	0.25
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	17	0.25
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	5	0.25
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	7	0.25
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	13	0.25
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	18	0.25
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	19	0.25
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	20	0.25
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	22	0.25
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	23	0.25
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	24	0.25
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	2	0.25
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	9	0.25
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	20	0.25
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	18	0.25
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	21	0.25
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	24	0.25
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	5	0.25
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	7	0.25
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	12	0.25
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	19	0.25
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	24	0.25
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	25	0.25
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	26	0.25
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	8	0.25
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	23	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	1	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	3	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	4	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	7	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	11	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	13	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	15	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	20	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	21	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	22	0.25
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	24	0.25
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	10	0.25
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	10	0.25
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	3	0.25
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	15	0.25
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	25	0.24
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	8	0.24
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	23	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	1	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	3	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	5	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	7	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	8	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	10	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	12	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	14	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	19	0.24
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	22	0.24
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	17	0.24
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	20	0.24
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	24	0.24
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	1	0.24
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	1	0.24
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	25	0.24
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	25	0.24
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	6	0.24
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	4	0.24
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	14	0.24
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	8	0.24
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	3	0.24
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	4	0.24
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	10	0.24
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	12	0.24
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	14	0.24
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	25	0.24
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	3	0.24
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	8	0.24
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	14	0.24
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	23	0.24
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	25	0.24
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	2	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	1	0.24
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	3	0.24
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	14	0.24
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	18	0.24
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	3	0.24
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	10	0.24
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	11	0.24
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	24	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	4	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	5	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	6	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	10	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	11	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	14	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	16	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	18	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	20	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	21	0.24
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	24	0.24
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	26	0.24
(1,115)	2:1:2:DG:H2'	2:2:2:DC:H5	5	0.24
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	8	0.24
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	14	0.24
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	17	0.24
(1,108)	2:11:2:DG:H3'	2:11:2:DG:H1'	26	0.24
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	7	0.24
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	7	0.24
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	21	0.24
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	21	0.24
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	21	0.24
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	14	0.23
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	7	0.23
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	23	0.23
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	26	0.23
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	4	0.23
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	14	0.23
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	3	0.23
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	3	0.23
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	25	0.23
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	25	0.23
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	12	0.23
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	12	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	8	0.23
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	18	0.23
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	2	0.23
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	4	0.23
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	26	0.23
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	19	0.23
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	3	0.23
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	14	0.23
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	8	0.23
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	9	0.23
(1,226)	2:7:2:DG:H3'	2:7:2:DG:H1'	17	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	3	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	4	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	7	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	12	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	18	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	19	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	20	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	21	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	22	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	23	0.23
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	24	0.23
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	10	0.23
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	5	0.23
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	11	0.23
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	12	0.23
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	22	0.23
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	23	0.23
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	17	0.23
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	4	0.23
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	9	0.23
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	16	0.23
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	20	0.23
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	1	0.23
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	2	0.23
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	3	0.23
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	12	0.23
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	15	0.23
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	21	0.23
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	18	0.23
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	23	0.23
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	9	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	9	0.23
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	13	0.23
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	13	0.23
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	15	0.23
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	9	0.23
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	11	0.23
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	14	0.23
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	17	0.23
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	18	0.23
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	19	0.23
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	22	0.23
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	23	0.23
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	7	0.23
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	16	0.23
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	25	0.23
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	26	0.23
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	10	0.22
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	17	0.22
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	19	0.22
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	12	0.22
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	24	0.22
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	13	0.22
(1,358)	2:5:2:DG:H2'	2:5:2:DG:H3'	17	0.22
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	1	0.22
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	25	0.22
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	3	0.22
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	15	0.22
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	3	0.22
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	15	0.22
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	19	0.22
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	22	0.22
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	7	0.22
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	8	0.22
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	1	0.22
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	6	0.22
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	7	0.22
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	2	0.22
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	5	0.22
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	7	0.22
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	15	0.22
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	18	0.22
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	25	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	26	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	1	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	2	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	5	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	6	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	8	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	9	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	10	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	13	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	14	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	15	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	17	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	25	0.22
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	26	0.22
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	1	0.22
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	4	0.22
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	5	0.22
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	7	0.22
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	19	0.22
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	3	0.22
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	7	0.22
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	10	0.22
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	13	0.22
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	16	0.22
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	17	0.22
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	19	0.22
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	25	0.22
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	26	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	1	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	4	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	6	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	7	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	8	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	9	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	13	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	19	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	20	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	24	0.22
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	25	0.22
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	1	0.22
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	5	0.22
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	7	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	25	0.22
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	26	0.22
(1,119)	2:1:2:DG:H2''	2:2:2:DC:H6	12	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	1	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	2	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	4	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	5	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	6	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	7	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	8	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	11	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	13	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	15	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	20	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	21	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	22	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	24	0.22
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	26	0.22
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	17	0.22
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	17	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	1	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	2	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	4	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	6	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	8	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	12	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	13	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	15	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	16	0.22
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	26	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	1	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	2	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	4	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	6	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	8	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	12	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	13	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	17	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	18	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	21	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	23	0.22
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	24	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	1	0.21
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	5	0.21
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	9	0.21
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	11	0.21
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	12	0.21
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	13	0.21
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	22	0.21
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	25	0.21
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	17	0.21
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	20	0.21
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	25	0.21
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	3	0.21
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	12	0.21
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	7	0.21
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	21	0.21
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	24	0.21
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	23	0.21
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	1	0.21
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	9	0.21
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	14	0.21
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	5	0.21
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	8	0.21
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	15	0.21
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	18	0.21
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	24	0.21
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	26	0.21
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	2	0.21
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	25	0.21
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	25	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	3	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	4	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	10	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	11	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	12	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	14	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	16	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	19	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	20	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	21	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	22	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	23	0.21
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	24	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	11	0.21
(1,224)	2:7:2:DG:H2''	2:7:2:DG:H1'	16	0.21
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	22	0.21
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	2	0.21
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	4	0.21
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	20	0.21
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	2	0.21
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	10	0.21
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	15	0.21
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	22	0.21
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	23	0.21
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	13	0.21
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	14	0.21
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	17	0.21
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	19	0.21
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	25	0.21
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	7	0.21
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	17	0.21
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	15	0.21
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	16	0.21
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	2	0.21
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	3	0.21
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	9	0.21
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	10	0.21
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	12	0.21
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	14	0.21
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	16	0.21
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	17	0.21
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	19	0.21
(1,98)	2:10:2:DC:H2''	2:10:2:DC:H1'	25	0.21
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	2	0.21
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	9	0.21
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	5	0.21
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	7	0.21
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	10	0.21
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	20	0.21
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	21	0.21
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	24	0.21
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	25	0.21
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	5	0.21
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	11	0.21
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	14	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	2	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	3	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	4	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	6	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	7	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	8	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	15	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	18	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	20	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	21	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	23	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	24	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	26	0.2
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	3	0.2
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	4	0.2
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	9	0.2
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	11	0.2
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	12	0.2
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	24	0.2
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	26	0.2
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	5	0.2
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	11	0.2
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	24	0.2
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	8	0.2
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	3	0.2
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	5	0.2
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	6	0.2
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	10	0.2
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	14	0.2
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	18	0.2
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	22	0.2
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	23	0.2
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5'	20	0.2
(1,301)	2:4:2:DT:H2'	2:5:2:DG:H5''	20	0.2
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	17	0.2
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	17	0.2
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	18	0.2
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	10	0.2
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	25	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	1	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	2	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	3	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	6	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	12	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	14	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	19	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	21	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	22	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	23	0.2
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	25	0.2
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	5	0.2
(1,263)	2:10:2:DC:H2''	2:10:2:DC:H6	10	0.2
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	15	0.2
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	16	0.2
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	22	0.2
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	1	0.2
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	6	0.2
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	13	0.2
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	22	0.2
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	4	0.2
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	19	0.2
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	20	0.2
(1,202)	2:6:2:DT:H2''	2:6:2:DT:H6	16	0.2
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	21	0.2
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	8	0.2
(1,179)	2:5:2:DG:H2'	2:5:2:DG:H8	14	0.2
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	11	0.2
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	12	0.2
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	16	0.2
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	21	0.2
(1,163)	2:4:2:DT:H2'	2:4:2:DT:H6	26	0.2
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	15	0.2
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	21	0.2
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	23	0.2
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	13	0.2
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	7	0.2
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	12	0.2
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	23	0.2
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	24	0.2
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	25	0.2
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	16	0.2
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	12	0.2
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	3	0.2
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	3	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	3	0.2
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	4	0.2
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	23	0.2
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	26	0.2
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	10	0.2
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	20	0.2
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	22	0.2
(1,383)	2:10:2:DC:H2'	2:10:2:DC:H4'	16	0.19
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	1	0.19
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	7	0.19
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	8	0.19
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	15	0.19
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	19	0.19
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	21	0.19
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	23	0.19
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	1	0.19
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	5	0.19
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	10	0.19
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	11	0.19
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	4	0.19
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	12	0.19
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	13	0.19
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	19	0.19
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	20	0.19
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	8	0.19
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	13	0.19
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	22	0.19
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	10	0.19
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	26	0.19
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	5	0.19
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	9	0.19
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	10	0.19
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	12	0.19
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	5	0.19
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	7	0.19
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	18	0.19
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	4	0.19
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	9	0.19
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	10	0.19
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	13	0.19
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	16	0.19
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	5	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	13	0.19
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	21	0.19
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	24	0.19
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	9	0.19
(1,235)	2:8:2:DT:H2''	2:8:2:DT:H1'	17	0.19
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	11	0.19
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	23	0.19
(1,212)	2:6:2:DT:H4'	2:7:2:DG:H8	16	0.19
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	9	0.19
(1,188)	2:5:2:DG:H3'	2:5:2:DG:H8	9	0.19
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	9	0.19
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	20	0.19
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	8	0.19
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	12	0.19
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	26	0.19
(1,124)	2:1:2:DG:H4'	2:1:2:DG:H8	19	0.19
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	1	0.19
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	2	0.19
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	3	0.19
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	13	0.19
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	16	0.19
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	17	0.19
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	18	0.19
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	20	0.19
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	26	0.19
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	10	0.19
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	13	0.19
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	22	0.19
(1,66)	2:7:2:DG:H5'	2:6:2:DT:H1'	20	0.19
(1,66)	2:7:2:DG:H5''	2:6:2:DT:H1'	20	0.19
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	8	0.19
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	14	0.19
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	16	0.19
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	26	0.19
(1,29)	2:3:2:DA:H3'	2:3:2:DA:H1'	3	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	1	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	2	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	3	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	5	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	6	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	7	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	8	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	10	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	14	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	15	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	16	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	18	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	20	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	21	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	22	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	24	0.19
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	26	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	1	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	2	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	5	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	6	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	7	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	8	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	9	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	10	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	11	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	12	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	14	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	16	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	17	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	18	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	19	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	20	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	21	0.19
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	25	0.19
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	19	0.19
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	6	0.18
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	10	0.18
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	16	0.18
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	18	0.18
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	21	0.18
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	1	0.18
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	9	0.18
(1,317)	2:7:2:DG:H5'	2:7:2:DG:H1'	17	0.18
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	15	0.18
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	15	0.18
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	16	0.18
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	16	0.18
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	1	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	5	0.18
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	26	0.18
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	7	0.18
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	25	0.18
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	19	0.18
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	3	0.18
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	12	0.18
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	16	0.18
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	11	0.18
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	17	0.18
(1,272)	2:11:2:DG:H1'	2:11:2:DG:H8	20	0.18
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	10	0.18
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	23	0.18
(1,188)	2:5:2:DG:H3'	2:5:2:DG:H8	21	0.18
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	17	0.18
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	2	0.18
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	6	0.18
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	13	0.18
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	4	0.18
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	6	0.18
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	8	0.18
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	10	0.18
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	19	0.18
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	21	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	1	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	5	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	8	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	9	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	11	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	12	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	15	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	18	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	19	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	21	0.18
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	23	0.18
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	24	0.18
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	25	0.18
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	11	0.18
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	4	0.18
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	9	0.18
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	11	0.18
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	12	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	13	0.18
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	19	0.18
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	23	0.18
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	25	0.18
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	13	0.18
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	15	0.18
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	22	0.18
(1,19)	2:2:2:DC:H3'	2:2:2:DC:H1'	24	0.18
(1,10)	2:1:2:DG:H3'	2:1:2:DG:H1'	9	0.18
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	13	0.17
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	4	0.17
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	19	0.17
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	20	0.17
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	22	0.17
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	25	0.17
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	21	0.17
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	6	0.17
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	14	0.17
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	1	0.17
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	5	0.17
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	6	0.17
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	21	0.17
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	2	0.17
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	6	0.17
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	16	0.17
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	18	0.17
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	25	0.17
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	4	0.17
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	5	0.17
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	6	0.17
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	18	0.17
(1,217)	2:6:2:DT:H5''	3:12:1:A4A:H4	16	0.17
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	7	0.17
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	10	0.17
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	13	0.17
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	25	0.17
(1,212)	2:6:2:DT:H4'	2:7:2:DG:H8	2	0.17
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	2	0.17
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	16	0.17
(1,188)	2:5:2:DG:H3'	2:5:2:DG:H8	18	0.17
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	11	0.17
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	18	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	22	0.17
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	18	0.17
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	5	0.17
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	9	0.17
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	11	0.17
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	14	0.17
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	3	0.17
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	4	0.17
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	6	0.17
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	7	0.17
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	14	0.17
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	17	0.17
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	20	0.17
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	25	0.17
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	26	0.17
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	12	0.17
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	24	0.17
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	1	0.17
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	18	0.17
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	19	0.17
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	20	0.17
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	2	0.17
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	3	0.17
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	4	0.17
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	18	0.17
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	20	0.17
(1,26)	2:3:2:DA:H2''	2:3:2:DA:H1'	17	0.17
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	1	0.16
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	5	0.16
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	14	0.16
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	16	0.16
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	18	0.16
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	22	0.16
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	1	0.16
(1,359)	2:5:2:DG:H2'	2:5:2:DG:H4'	9	0.16
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	2	0.16
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	2	0.16
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	24	0.16
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	24	0.16
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	7	0.16
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	21	0.16
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	24	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	1	0.16
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	3	0.16
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	4	0.16
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	7	0.16
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	11	0.16
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	13	0.16
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	15	0.16
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	20	0.16
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	21	0.16
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	22	0.16
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	24	0.16
(1,276)	2:11:2:DG:H2''	2:11:2:DG:H8	23	0.16
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	20	0.16
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	21	0.16
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	23	0.16
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	1	0.16
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	5	0.16
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	12	0.16
(1,212)	2:6:2:DT:H4'	2:7:2:DG:H8	25	0.16
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	15	0.16
(1,189)	2:5:2:DG:H3'	2:6:2:DT:H6	18	0.16
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	12	0.16
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	15	0.16
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	23	0.16
(1,110)	2:1:2:DG:H1'	2:1:2:DG:H8	22	0.16
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	15	0.16
(1,100)	2:10:2:DC:H3'	2:10:2:DC:H1'	24	0.16
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	8	0.16
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	8	0.16
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	11	0.16
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	11	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	1	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	2	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	3	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	4	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	5	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	6	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	7	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	8	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	9	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	10	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	11	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	13	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	14	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	15	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	16	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	17	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	18	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	19	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	20	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	21	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	22	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	23	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	25	0.16
(1,59)	2:7:2:DG:H2'	2:7:2:DG:H2''	26	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	1	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	5	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	7	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	8	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	9	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	12	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	13	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	16	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	21	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	23	0.16
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	26	0.16
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	22	0.16
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	2	0.15
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	3	0.15
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	9	0.15
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	10	0.15
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	19	0.15
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	23	0.15
(1,382)	2:10:2:DC:H2'	2:10:2:DC:H3'	2	0.15
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	11	0.15
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	10	0.15
(1,366)	2:6:2:DT:H5'	2:6:2:DT:H3'	16	0.15
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	22	0.15
(1,303)	2:5:2:DG:H2'	2:5:2:DG:H5'	6	0.15
(1,303)	2:5:2:DG:H2'	2:5:2:DG:H5''	6	0.15
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	26	0.15
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	26	0.15
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	25	0.15
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	4	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	8	0.15
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	14	0.15
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	17	0.15
(1,277)	2:11:2:DG:H3'	2:11:2:DG:H1'	26	0.15
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	2	0.15
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	20	0.15
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	1	0.15
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	4	0.15
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	7	0.15
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	12	0.15
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	14	0.15
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	22	0.15
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	24	0.15
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	3	0.15
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	14	0.15
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	17	0.15
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	12	0.15
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	25	0.15
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	6	0.15
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	10	0.15
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	25	0.15
(1,131)	2:2:2:DC:H2'	2:3:2:DA:H8	22	0.15
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	3	0.15
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	11	0.15
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	12	0.15
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	17	0.15
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	2	0.15
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	16	0.15
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	5	0.15
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	23	0.15
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	6	0.15
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	10	0.15
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	14	0.15
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	15	0.15
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	19	0.15
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	22	0.15
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	24	0.15
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	25	0.15
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	7	0.15
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	4	0.14
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	6	0.14
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	7	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	8	0.14
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	16	0.14
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	20	0.14
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	24	0.14
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	26	0.14
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	2	0.14
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	11	0.14
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	2	0.14
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	13	0.14
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	15	0.14
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	16	0.14
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	19	0.14
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	26	0.14
(1,367)	2:6:2:DT:H5''	2:5:2:DG:H1'	13	0.14
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	5	0.14
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	5	0.14
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	16	0.14
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	19	0.14
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	10	0.14
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	13	0.14
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	19	0.14
(1,223)	2:7:2:DG:H2'	2:7:2:DG:H8	16	0.14
(1,223)	2:7:2:DG:H2'	2:7:2:DG:H8	26	0.14
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	8	0.14
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	26	0.14
(1,212)	2:6:2:DT:H4'	2:7:2:DG:H8	11	0.14
(1,212)	2:6:2:DT:H4'	2:7:2:DG:H8	15	0.14
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	8	0.14
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	9	0.14
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	18	0.14
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	8	0.14
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	4	0.14
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	7	0.14
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	14	0.14
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	19	0.14
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	24	0.14
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	9	0.14
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	19	0.14
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	22	0.14
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	24	0.14
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	2	0.14
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	2	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	26	0.14
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	26	0.14
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	15	0.14
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	3	0.14
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	7	0.14
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	17	0.14
(1,42)	2:5:2:DG:H4'	2:4:2:DT:H1'	18	0.14
(1,39)	2:5:2:DG:H2''	2:5:2:DG:H1'	17	0.14
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	5	0.13
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	11	0.13
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	14	0.13
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	15	0.13
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	18	0.13
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	21	0.13
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	25	0.13
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	8	0.13
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	15	0.13
(1,370)	2:7:2:DG:H2'	2:7:2:DG:H4'	26	0.13
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	6	0.13
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	8	0.13
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	20	0.13
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	21	0.13
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	24	0.13
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	25	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	1	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	3	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	5	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	6	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	8	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	13	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	15	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	17	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	18	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	20	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	21	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	22	0.13
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	24	0.13
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	4	0.13
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	4	0.13
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	10	0.13
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	10	0.13
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5'	11	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	2:1:2:DG:H2''	2:1:2:DG:H5''	11	0.13
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	10	0.13
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	14	0.13
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	24	0.13
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	10	0.13
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	13	0.13
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	22	0.13
(1,247)	2:9:2:DA:H2'	2:10:2:DC:H5	12	0.13
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	3	0.13
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	17	0.13
(1,223)	2:7:2:DG:H2'	2:7:2:DG:H8	15	0.13
(1,212)	2:6:2:DT:H4'	2:7:2:DG:H8	8	0.13
(1,209)	2:6:2:DT:H4'	2:6:2:DT:H1'	6	0.13
(1,209)	2:6:2:DT:H4'	2:6:2:DT:H1'	24	0.13
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	21	0.13
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	24	0.13
(1,171)	2:4:2:DT:H3'	2:5:2:DG:H8	15	0.13
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	4	0.13
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	5	0.13
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	21	0.13
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	2	0.13
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	8	0.13
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	26	0.13
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	2	0.13
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	7	0.13
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	21	0.13
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	23	0.13
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	7	0.13
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	15	0.13
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	15	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	1	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	2	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	4	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	9	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	10	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	11	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	13	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	16	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	17	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	20	0.13
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	25	0.13
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	4	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	11	0.13
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	13	0.13
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	9	0.13
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	19	0.13
(1,390)	2:5:2:DG:H2'	2:5:2:DG:H3'	9	0.12
(1,390)	2:5:2:DG:H2'	2:5:2:DG:H3'	18	0.12
(1,390)	2:5:2:DG:H2'	2:5:2:DG:H3'	21	0.12
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	12	0.12
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	13	0.12
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	17	0.12
(1,386)	2:11:2:DG:H2'	2:11:2:DG:H3'	22	0.12
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	4	0.12
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	10	0.12
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	12	0.12
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	14	0.12
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	22	0.12
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	23	0.12
(1,366)	2:6:2:DT:H5'	2:6:2:DT:H3'	2	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	2	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	4	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	7	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	9	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	10	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	11	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	12	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	14	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	16	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	19	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	23	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	25	0.12
(1,298)	2:3:2:DA:H2'	2:3:2:DA:H3'	26	0.12
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	19	0.12
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	20	0.12
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	23	0.12
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	20	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	1	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	5	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	8	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	9	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	11	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	12	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	15	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	18	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	19	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	21	0.12
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	23	0.12
(1,212)	2:6:2:DT:H4'	2:7:2:DG:H8	26	0.12
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	1	0.12
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	6	0.12
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	11	0.12
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	13	0.12
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	17	0.12
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	26	0.12
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	3	0.12
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	6	0.12
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	7	0.12
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	8	0.12
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	14	0.12
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	21	0.12
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	23	0.12
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	24	0.12
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	26	0.12
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	2	0.12
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	6	0.12
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	9	0.12
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	16	0.12
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	22	0.12
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	26	0.12
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	1	0.12
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	3	0.12
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	19	0.12
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	26	0.12
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	21	0.12
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	7	0.12
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	15	0.12
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	18	0.12
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	22	0.12
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	23	0.12
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	1	0.12
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	4	0.12
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	5	0.12
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	10	0.12
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	20	0.12
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	4	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	9	0.12
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	15	0.12
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	17	0.12
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	19	0.12
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	21	0.12
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	24	0.12
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5'	16	0.12
(1,62)	2:7:2:DG:H2''	2:7:2:DG:H5''	16	0.12
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5'	25	0.12
(1,60)	2:7:2:DG:H2'	2:7:2:DG:H5''	25	0.12
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	8	0.12
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	9	0.12
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	18	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	3	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	5	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	6	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	7	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	8	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	12	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	15	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	18	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	19	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	21	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	22	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	23	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	24	0.12
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	26	0.12
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	22	0.12
(1,35)	2:5:2:DG:H1'	2:4:2:DT:H2'	15	0.12
(1,35)	2:5:2:DG:H1'	2:4:2:DT:H2''	15	0.12
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	2	0.12
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	14	0.12
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	15	0.12
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	23	0.12
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	3	0.11
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	5	0.11
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	7	0.11
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	17	0.11
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	18	0.11
(1,368)	2:6:2:DT:H5''	2:6:2:DT:H3'	15	0.11
(1,303)	2:5:2:DG:H2'	2:5:2:DG:H5'	17	0.11
(1,303)	2:5:2:DG:H2'	2:5:2:DG:H5''	17	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	2:9:2:DA:H3'	2:10:2:DC:H6	12	0.11
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	13	0.11
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	22	0.11
(1,284)	2:8:2:DT:H2''	2:9:2:DA:H8	23	0.11
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	3	0.11
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	4	0.11
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	6	0.11
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	7	0.11
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	14	0.11
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	17	0.11
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	20	0.11
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	25	0.11
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	26	0.11
(1,228)	2:7:2:DG:H3'	2:8:2:DT:H6	9	0.11
(1,223)	2:7:2:DG:H2'	2:7:2:DG:H8	11	0.11
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	9	0.11
(1,209)	2:6:2:DT:H4'	2:6:2:DT:H1'	15	0.11
(1,209)	2:6:2:DT:H4'	2:6:2:DT:H1'	21	0.11
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	3	0.11
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	4	0.11
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	5	0.11
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	7	0.11
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	10	0.11
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	14	0.11
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	19	0.11
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	22	0.11
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	23	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	1	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	2	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	4	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	5	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	10	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	11	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	12	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	15	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	16	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	18	0.11
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	20	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	1	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	3	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	4	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	5	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	7	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	8	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	10	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	11	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	12	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	13	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	14	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	15	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	17	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	18	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	19	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	20	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	21	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	23	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	24	0.11
(1,144)	2:3:2:DA:H2'	2:3:2:DA:H2''	25	0.11
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	2	0.11
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	10	0.11
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	16	0.11
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	17	0.11
(1,137)	2:2:2:DC:H5	2:1:2:DG:H8	18	0.11
(1,133)	2:2:2:DC:H2''	2:2:2:DC:H5	1	0.11
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	6	0.11
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	8	0.11
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	12	0.11
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	14	0.11
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	20	0.11
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	21	0.11
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	24	0.11
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	26	0.11
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	6	0.11
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	26	0.11
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	20	0.11
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	21	0.11
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	24	0.11
(1,48)	2:6:2:DT:H2'	2:6:2:DT:H2''	14	0.11
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	10	0.11
(1,43)	2:5:2:DG:H4'	2:5:2:DG:H1'	12	0.11
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	5	0.11
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	10	0.11
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	13	0.11
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	16	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	18	0.11
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	21	0.11
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	24	0.11
(1,369)	2:7:2:DG:H2'	2:7:2:DG:H3'	9	0.1
(1,350)	2:2:2:DC:H5	2:1:2:DG:H1'	9	0.1
(1,303)	2:5:2:DG:H2'	2:5:2:DG:H5'	13	0.1
(1,303)	2:5:2:DG:H2'	2:5:2:DG:H5''	13	0.1
(1,264)	2:10:2:DC:H3'	2:10:2:DC:H1'	24	0.1
(1,216)	2:6:2:DT:H5'	2:6:2:DT:H6	16	0.1
(1,205)	2:6:2:DT:H3'	2:6:2:DT:H1'	12	0.1
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	13	0.1
(1,154)	2:3:2:DA:H4'	2:3:2:DA:H8	19	0.1
(1,135)	2:2:2:DC:H3'	2:2:2:DC:H1'	3	0.1
(1,135)	2:2:2:DC:H3'	2:2:2:DC:H1'	4	0.1
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	4	0.1
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	10	0.1
(1,132)	2:2:2:DC:H2''	2:2:2:DC:H1'	19	0.1
(1,130)	2:2:2:DC:H2'	2:2:2:DC:H5	16	0.1
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	8	0.1
(1,103)	2:10:2:DC:H4'	2:10:2:DC:H1'	25	0.1
(1,92)	2:9:2:DA:H3'	2:9:2:DA:H1'	9	0.1
(1,92)	2:9:2:DA:H3'	2:9:2:DA:H1'	11	0.1
(1,92)	2:9:2:DA:H3'	2:9:2:DA:H1'	12	0.1
(1,92)	2:9:2:DA:H3'	2:9:2:DA:H1'	13	0.1
(1,92)	2:9:2:DA:H3'	2:9:2:DA:H1'	14	0.1
(1,92)	2:9:2:DA:H3'	2:9:2:DA:H1'	22	0.1
(1,92)	2:9:2:DA:H3'	2:9:2:DA:H1'	23	0.1
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	3	0.1
(1,83)	2:9:2:DA:H2'	2:8:2:DT:H1'	16	0.1
(1,72)	2:8:2:DT:H2'	2:8:2:DT:H2''	2	0.1
(1,72)	2:8:2:DT:H2'	2:8:2:DT:H2''	6	0.1
(1,72)	2:8:2:DT:H2'	2:8:2:DT:H2''	14	0.1
(1,72)	2:8:2:DT:H2'	2:8:2:DT:H2''	17	0.1
(1,72)	2:8:2:DT:H2'	2:8:2:DT:H2''	24	0.1
(1,72)	2:8:2:DT:H2'	2:8:2:DT:H2''	26	0.1
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	1	0.1
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	17	0.1
(1,52)	2:6:2:DT:H3'	2:6:2:DT:H1'	26	0.1
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	1	0.1
(1,9)	2:1:2:DG:H2''	2:1:2:DG:H1'	3	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found