



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 08:46 PM EST

PDB ID : 9DLL
BMRB ID : 31202
Title : NMR structures of small molecules bound to a model of an RNA CAG repeat expansion.
Authors : Chen, J.L.; Taghavi, A.; Disney, M.D.; Fountain, M.A.; Childs-Disney, J.L.
Deposited on : 2024-09-11

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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

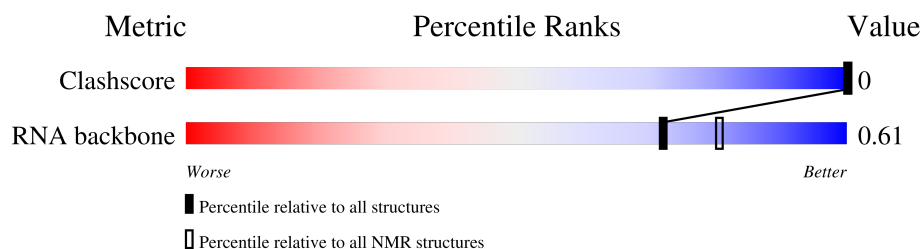
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

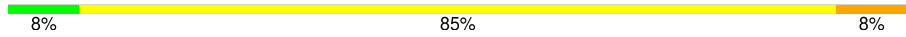
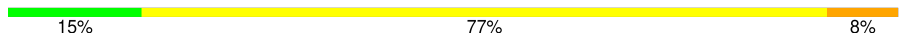
The overall completeness of chemical shifts assignment is 15%.

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	210492	14027
RNA backbone	6643	756

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

Mol	Chain	Length	Quality of chain
1	A	13	 8% 85% 8%
1	B	13	 15% 77% 8%

2 Ensemble composition and analysis ⓘ

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

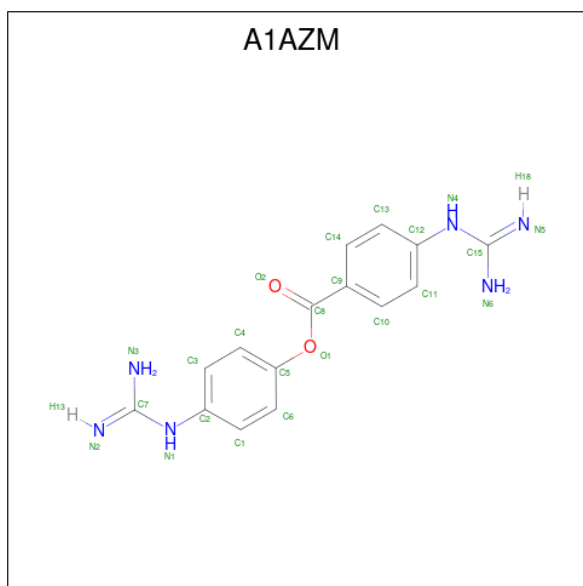
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 877 atoms, of which 304 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3').

Mol	Chain	Residues	Atoms						Trace
1	A	13	Total	C	H	N	O	P	0
			418	124	143	51	88	12	
1	B	13	Total	C	H	N	O	P	0
			418	124	143	51	88	12	

- Molecule 2 is 4-carbamimidamidophenyl 4-carbamimidamidobenzoate (three-letter code: A1AZM) (formula: C₁₅H₁₆N₆O₂) (labeled as "Ligand of Interest" by depositor).



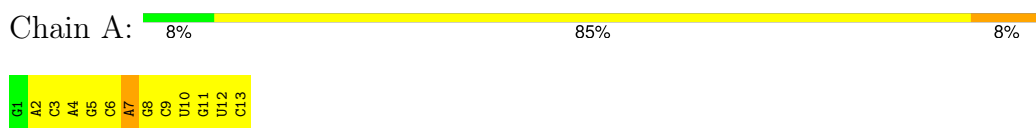
Mol	Chain	Residues	Atoms				
2	B	1	Total	C	H	N	O
			41	15	18	6	2

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: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



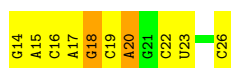


4.2.2 Score per residue for model 2

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

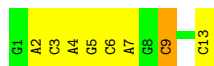


- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



4.2.3 Score per residue for model 3

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



4.2.4 Score per residue for model 4

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')





- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



4.2.5 Score per residue for model 5

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



4.2.6 Score per residue for model 6

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



4.2.7 Score per residue for model 7

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain A:  31% 62% 8%



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain B:  23% 69% 8%



4.2.8 Score per residue for model 8

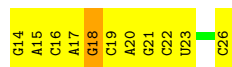
- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain A:  15% 77% 8%



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

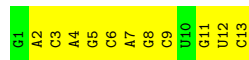
Chain B:  15% 77% 8%



4.2.9 Score per residue for model 9

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain A:  15% 85%



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

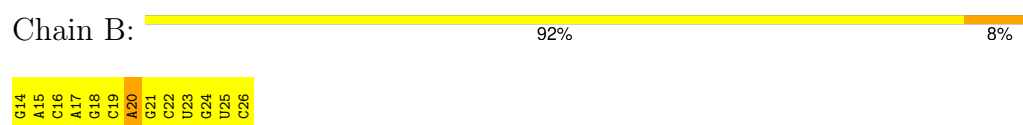


4.2.10 Score per residue for model 10

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



4.2.11 Score per residue for model 11

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



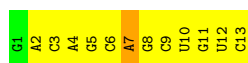
- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



4.2.12 Score per residue for model 12

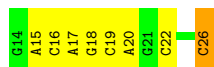
- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')





- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

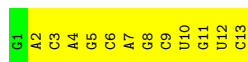
Chain B: 38% 54% 8%



4.2.13 Score per residue for model 13

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain A: 8% 92%



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

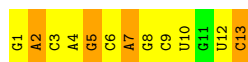
Chain B: 8% 92%



4.2.14 Score per residue for model 14

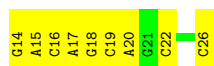
- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain A: 8% 62% 31%



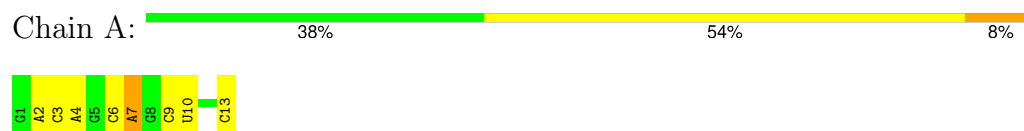
- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain B: 31% 69%



4.2.15 Score per residue for model 15

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

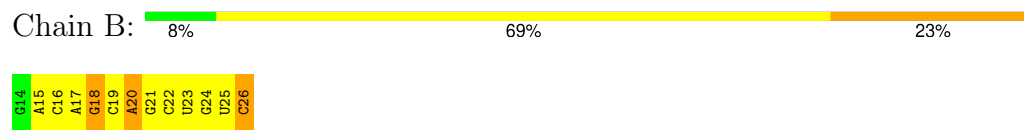


4.2.16 Score per residue for model 16

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

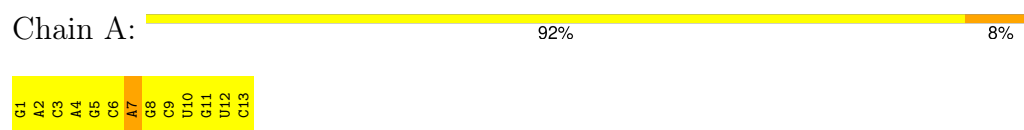


- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



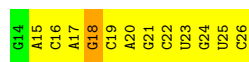
4.2.17 Score per residue for model 17

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain B:  8% 85% 8%




4.2.18 Score per residue for model 18

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain A:  15% 69% 15%



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain B:  8% 69% 23%



4.2.19 Score per residue for model 19

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain A:  8% 77% 15%



- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain B:  23% 69% 8%



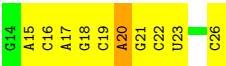
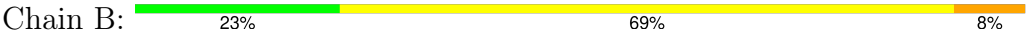
4.2.20 Score per residue for model 20

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain A:  15% 77% 8%



● Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
Amber	structure calculation	20

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	85
Number of shifts mapped to atoms	85
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	15%

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: A1AZM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.55±0.04	0±1/307 (0.1± 0.2%)	2.35±0.05	23±3/477 (4.9± 0.6%)
1	B	1.54±0.04	0±0/307 (0.1± 0.1%)	2.34±0.06	24±3/477 (5.0± 0.6%)
All	All	1.54	10/12280 (0.1%)	2.35	943/19080 (4.9%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.9
1	B	0.0±0.0	1.1±0.9
All	All	0	40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	4	A	N3-C4	6.48	1.38	1.34	20	1
1	A	4	A	N7-C5	5.85	1.42	1.39	11	1
1	B	20	A	N7-C5	5.72	1.42	1.39	5	1
1	B	16	C	C4-N4	-5.45	1.29	1.33	12	2
1	A	7	A	N3-C4	5.30	1.38	1.34	4	2
1	A	13	C	N3-C4	-5.26	1.30	1.33	11	1
1	B	14	G	C2-N2	-5.19	1.29	1.34	11	1
1	A	6	C	C4-N4	-5.08	1.29	1.33	16	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
1	B	20	A	N1-C6-N6	-12.54	111.08	118.60	9	20
1	A	7	A	N1-C6-N6	-12.23	111.26	118.60	13	20
1	B	15	A	N1-C6-N6	-10.46	112.32	118.60	17	20
1	B	17	A	N1-C6-N6	-10.05	112.57	118.60	1	20
1	A	4	A	N1-C6-N6	-9.82	112.71	118.60	16	20
1	A	4	A	C5-C6-N1	9.62	122.51	117.70	10	18
1	A	7	A	C5-C6-N1	9.52	122.46	117.70	13	20
1	A	2	A	N1-C6-N6	-9.52	112.89	118.60	3	20
1	B	26	C	N3-C2-O2	-9.05	115.57	121.90	8	20
1	B	15	A	C4-C5-C6	-8.97	112.51	117.00	17	17
1	B	22	C	N3-C2-O2	-8.96	115.63	121.90	19	20
1	B	17	A	C5-C6-N1	8.95	122.17	117.70	10	18
1	A	9	C	N3-C2-O2	-8.94	115.64	121.90	11	19
1	B	16	C	N3-C2-O2	-8.91	115.66	121.90	12	19
1	B	20	A	C5-C6-N1	8.88	122.14	117.70	10	20
1	A	7	A	C4-C5-C6	-8.84	112.58	117.00	13	19
1	A	13	C	N3-C2-O2	-8.79	115.75	121.90	17	20
1	B	17	A	C4-C5-C6	-8.71	112.64	117.00	16	17
1	A	11	G	N1-C6-O6	-8.69	114.69	119.90	5	4
1	A	3	C	N3-C2-O2	-8.50	115.95	121.90	17	19
1	A	2	A	C5-C6-N1	8.32	121.86	117.70	20	19
1	B	15	A	C5-C6-N1	8.32	121.86	117.70	2	19
1	A	4	A	C4-C5-C6	-8.25	112.87	117.00	2	19
1	A	6	C	N3-C2-O2	-8.25	116.13	121.90	5	20
1	A	2	A	C4-C5-C6	-8.15	112.93	117.00	20	16
1	B	22	C	N1-C2-O2	8.05	123.73	118.90	19	13
1	B	20	A	C4-C5-C6	-8.00	113.00	117.00	12	18
1	B	19	C	N3-C2-O2	-7.96	116.33	121.90	2	20
1	A	9	C	N1-C2-O2	7.87	123.62	118.90	1	13
1	B	26	C	N1-C2-O2	7.84	123.60	118.90	6	16
1	B	23	U	O4'-C1'-N1	7.65	114.32	108.20	10	15
1	A	6	C	N1-C2-O2	7.62	123.47	118.90	5	14
1	B	19	C	N1-C2-O2	7.51	123.41	118.90	8	14
1	B	16	C	O4'-C1'-N1	7.50	114.20	108.20	19	14
1	B	18	G	N1-C6-O6	-7.28	115.53	119.90	1	10
1	B	16	C	N1-C2-O2	7.17	123.20	118.90	7	14
1	A	13	C	N1-C2-O2	7.13	123.18	118.90	1	14
1	A	12	U	O4'-C1'-N1	7.13	113.90	108.20	18	9
1	A	10	U	O4'-C1'-N1	7.08	113.86	108.20	17	15
1	A	10	U	N3-C2-O2	-7.07	117.25	122.20	5	9
1	B	22	C	N3-C4-C5	6.93	124.67	121.90	5	3
1	A	3	C	O4'-C1'-N1	6.92	113.73	108.20	11	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	C	O4'-C1'-N1	6.82	113.66	108.20	8	5
1	B	20	A	C6-C5-N7	6.79	137.05	132.30	13	6
1	A	13	C	N3-C4-C5	6.74	124.60	121.90	9	5
1	B	17	A	N1-C2-N3	-6.65	125.97	129.30	9	3
1	A	6	C	N3-C4-C5	6.64	124.56	121.90	10	3
1	A	7	A	C6-C5-N7	6.64	136.95	132.30	6	2
1	B	23	U	C5-C6-N1	-6.62	119.39	122.70	19	2
1	B	25	U	O4'-C1'-N1	6.54	113.43	108.20	4	9
1	B	22	C	O4'-C1'-N1	6.53	113.42	108.20	15	14
1	B	20	A	O4'-C1'-N9	6.52	113.42	108.20	14	2
1	A	3	C	N1-C2-O2	6.39	122.73	118.90	11	13
1	A	9	C	O4'-C1'-N1	6.37	113.30	108.20	4	9
1	B	14	G	C5-C6-N1	6.32	114.66	111.50	1	3
1	A	3	C	N3-C4-C5	6.32	124.43	121.90	2	6
1	B	26	C	O4'-C1'-N1	6.30	113.24	108.20	11	8
1	B	21	G	N3-C4-C5	-6.30	125.45	128.60	10	5
1	B	14	G	N1-C6-O6	-6.22	116.17	119.90	6	5
1	A	11	G	C5-C6-N1	6.22	114.61	111.50	5	3
1	A	8	G	N3-C4-C5	-6.17	125.51	128.60	14	8
1	B	25	U	C5-C6-N1	-6.12	119.64	122.70	16	3
1	B	18	G	C5-C6-N1	6.11	114.56	111.50	17	2
1	B	21	G	N1-C6-O6	-6.05	116.27	119.90	6	5
1	B	18	G	C8-N9-C4	-6.04	103.98	106.40	5	2
1	A	1	G	N1-C6-O6	-6.03	116.28	119.90	4	5
1	B	23	U	N3-C2-O2	-6.00	118.00	122.20	18	4
1	B	16	C	N3-C4-C5	5.95	124.28	121.90	14	2
1	A	5	G	N1-C6-O6	-5.95	116.33	119.90	9	9
1	B	18	G	N9-C4-C5	5.95	107.78	105.40	5	1
1	A	1	G	C5-C6-N1	5.94	114.47	111.50	17	2
1	B	20	A	C2-N3-C4	5.89	113.55	110.60	10	3
1	A	7	A	O4'-C1'-N9	5.89	112.91	108.20	13	2
1	A	12	U	N3-C2-O2	-5.88	118.08	122.20	17	3
1	A	4	A	C6-C5-N7	5.84	136.39	132.30	10	4
1	A	6	C	N3-C4-N4	-5.84	113.91	118.00	10	1
1	A	5	G	O4'-C1'-N9	5.83	112.86	108.20	11	2
1	A	10	U	C5-C6-N1	-5.82	119.79	122.70	20	1
1	A	8	G	N3-C2-N2	-5.80	115.84	119.90	20	3
1	B	25	U	N3-C2-O2	-5.79	118.15	122.20	1	4
1	B	14	G	N3-C4-C5	-5.79	125.70	128.60	8	2
1	B	24	G	N3-C4-C5	-5.76	125.72	128.60	10	1
1	B	24	G	N1-C6-O6	-5.76	116.45	119.90	16	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	5	G	C8-N9-C4	-5.74	104.10	106.40	1	1
1	A	9	C	N3-C4-C5	5.72	124.19	121.90	12	2
1	B	26	C	N3-C4-C5	5.72	124.19	121.90	3	5
1	A	3	C	N3-C4-N4	-5.63	114.06	118.00	2	1
1	A	11	G	O4'-C1'-N9	5.63	112.70	108.20	19	1
1	A	8	G	N1-C6-O6	-5.62	116.53	119.90	16	6
1	B	21	G	N3-C2-N2	-5.61	115.97	119.90	15	1
1	B	14	G	N3-C2-N2	-5.61	115.97	119.90	11	1
1	B	18	G	N3-C2-N2	-5.60	115.98	119.90	1	1
1	B	24	G	C4'-C3'-C2'	-5.58	97.02	102.60	11	1
1	A	12	U	C5-C6-N1	-5.55	119.92	122.70	20	2
1	A	3	C	C5'-C4'-O4'	5.50	115.70	109.10	15	1
1	B	22	C	C6-N1-C2	-5.50	118.10	120.30	6	1
1	A	4	A	N1-C2-N3	-5.48	126.56	129.30	2	1
1	B	17	A	C6-C5-N7	5.46	136.12	132.30	14	2
1	A	4	A	C2-N3-C4	5.44	113.32	110.60	2	1
1	A	1	G	N3-C4-C5	-5.44	125.88	128.60	4	1
1	B	19	C	C2-N3-C4	-5.44	117.18	119.90	18	1
1	B	21	G	N9-C4-C5	5.44	107.57	105.40	3	1
1	A	2	A	C6-C5-N7	5.40	136.08	132.30	3	6
1	B	26	C	N3-C4-N4	-5.39	114.22	118.00	17	1
1	B	19	C	N3-C4-C5	5.39	124.05	121.90	14	3
1	B	18	G	C5-C6-O6	5.38	131.82	128.60	1	1
1	A	12	U	N1-C2-N3	5.36	118.12	114.90	20	3
1	A	1	G	C8-N9-C4	-5.32	104.27	106.40	6	1
1	A	10	U	N1-C2-N3	5.30	118.08	114.90	1	1
1	B	25	U	N1-C2-N3	5.30	118.08	114.90	5	1
1	A	3	C	C4'-C3'-C2'	-5.29	97.31	102.60	16	1
1	B	24	G	C5-C6-N1	5.28	114.14	111.50	1	1
1	B	15	A	C6-C5-N7	5.28	136.00	132.30	2	2
1	B	24	G	N9-C4-C5	5.28	107.51	105.40	10	1
1	B	24	G	O4'-C1'-N9	5.27	112.42	108.20	19	1
1	B	26	C	C2-N3-C4	-5.24	117.28	119.90	10	1
1	B	16	C	C5'-C4'-O4'	5.24	115.38	109.10	4	1
1	A	11	G	N3-C4-C5	-5.22	125.99	128.60	9	1
1	B	19	C	N3-C4-N4	-5.22	114.35	118.00	2	2
1	B	24	G	N3-C2-N2	-5.22	116.25	119.90	19	1
1	A	8	G	C5-C6-N1	5.21	114.11	111.50	9	2
1	A	2	A	O4'-C1'-N9	5.21	112.36	108.20	1	1
1	A	4	A	O4'-C1'-N9	5.17	112.34	108.20	16	2
1	B	18	G	O4'-C1'-N9	5.17	112.33	108.20	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	23	U	C4-C5-C6	5.16	122.80	119.70	19	1
1	B	18	G	C6-C5-N7	5.15	133.49	130.40	15	1
1	A	8	G	C8-N9-C4	-5.15	104.34	106.40	1	2
1	A	11	G	C8-N9-C4	-5.14	104.34	106.40	9	2
1	A	8	G	N9-C4-C5	5.13	107.45	105.40	8	1
1	A	11	G	N9-C4-C5	5.11	107.44	105.40	4	1
1	B	17	A	C2-N3-C4	5.08	113.14	110.60	7	2
1	B	18	G	N7-C8-N9	5.05	115.62	113.10	9	1
1	B	25	U	C4-C5-C6	5.01	122.71	119.70	9	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	B	18	G	Sidechain	13
1	A	5	G	Sidechain	11
1	A	11	G	Sidechain	3
1	B	26	C	Sidechain	3
1	A	8	G	Sidechain	2
1	B	24	G	Sidechain	2
1	B	25	U	Sidechain	1
1	A	2	A	Sidechain	1
1	A	13	C	Sidechain	1
1	B	20	A	Sidechain	1
1	A	7	A	Sidechain	1
1	B	21	G	Sidechain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	11460	6080	5710	-

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 -.

There are no clashes.

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](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	12/13 (92%)	1±0 (5±4%)	0±0 (0±0%)	0.61±0.05
1	B	12/13 (92%)	1±1 (5±5%)	0±0 (0±2%)	0.60±0.03
All	All	480/520 (92%)	24 (5%)	1 (0%)	0.61

The overall RNA backbone suiteness is 0.61.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	20	A	11
1	A	7	A	10
1	A	9	C	1
1	B	21	G	1
1	B	22	C	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	21	G	1

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

There are no oligosaccharides in this entry.

6.6 Ligand geometry

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
2	A1AZM	B	101	-	24,24,24	1.25±0.09	2±1 (9±2%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	A1AZM	B	101	-	30,32,32	1.03±0.12	1±0 (4±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
2	A1AZM	B	101	-	-	0±0,16,16,16	0±0,2,2,2

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
2	B	101	A1AZM	C15-N4	3.54	1.33	1.38	19	20
2	B	101	A1AZM	C7-N1	3.52	1.33	1.38	8	19
2	B	101	A1AZM	C14-C9	2.21	1.42	1.39	7	1
2	B	101	A1AZM	C1-C2	2.21	1.43	1.39	16	1
2	B	101	A1AZM	C14-C13	2.14	1.42	1.38	4	2
2	B	101	A1AZM	O1-C5	2.04	1.36	1.41	15	1
2	B	101	A1AZM	C4-C3	2.01	1.42	1.38	17	1

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

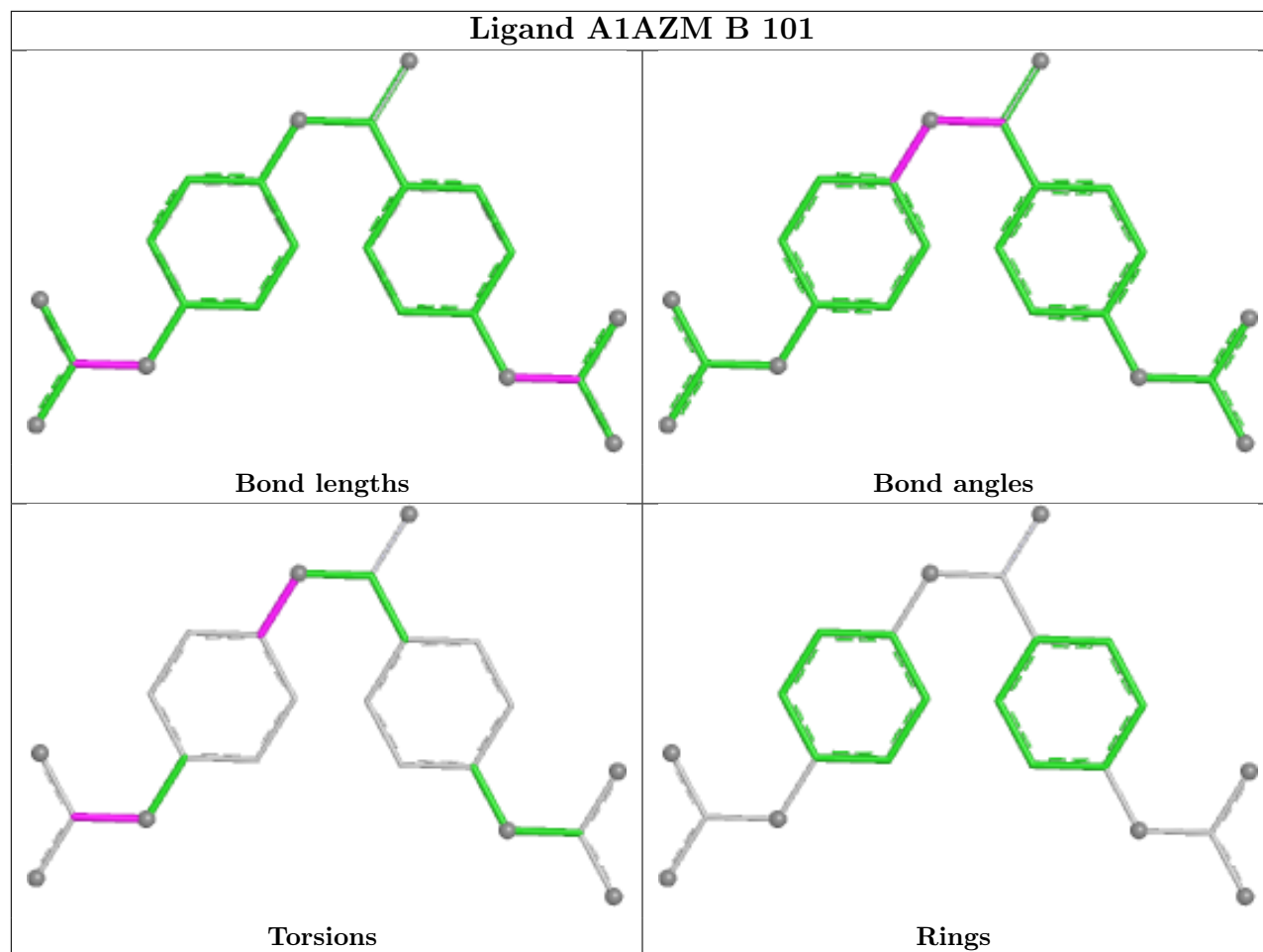
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	101	A1AZM	C5-O1-C8	5.02	131.66	118.39	7	20
2	B	101	A1AZM	O1-C5-C4	2.22	125.32	119.09	4	1
2	B	101	A1AZM	C12-N4-C15	2.19	132.96	127.84	13	3

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 15% for the well-defined parts and 15% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *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	85
Number of shifts mapped to atoms	85
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 15%, i.e. 75 atoms were assigned a chemical shift out of a possible 494. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	44/286 (15%)	44/156 (28%)	0/130 (0%)	0/0 (—%)
Base	31/208 (15%)	31/130 (24%)	0/44 (0%)	0/34 (0%)
Overall	75/494 (15%)	75/286 (26%)	0/174 (0%)	0/34 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 15%, i.e. 75 atoms were assigned a chemical shift out of a possible 494. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Sugar	44/286 (15%)	44/156 (28%)	0/130 (0%)	0/0 (—%)
Base	31/208 (15%)	31/130 (24%)	0/44 (0%)	0/34 (0%)
Overall	75/494 (15%)	75/286 (26%)	0/174 (0%)	0/34 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	224
Intra-residue ($ i-j =0$)	53
Sequential ($ i-j =1$)	35
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	5
Inter-chain	96
Hydrogen bond restraints	35
Disulfide bond restraints	0
Total dihedral-angle restraints	16
Number of unmapped restraints	0
Number of restraints per residue	8.9
Number of long range restraints per residue ¹	0.2

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)	None	None
0.2-0.5 (Medium)	None	None
>0.5 (Large)	99.0	37.06

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 ⓘ

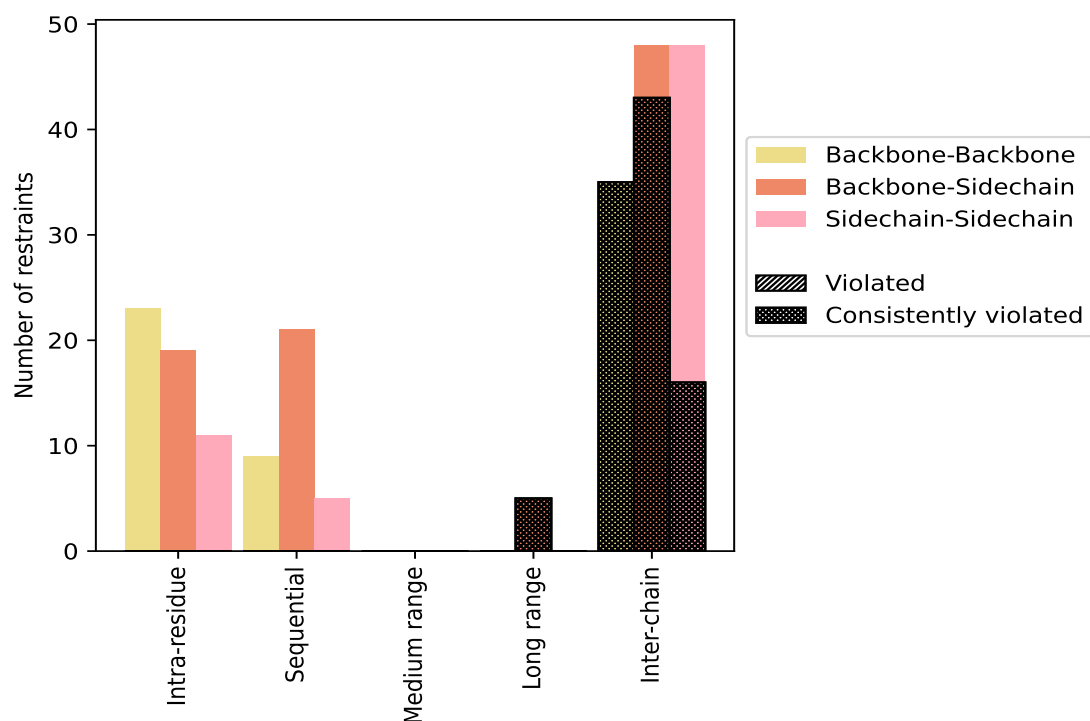
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	53	23.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	23	10.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	19	8.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	11	4.9	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	35	15.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	9	4.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	21	9.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	5	2.2	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	5	2.2	5	100.0	2.2	5	100.0	2.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	5	2.2	5	100.0	2.2	5	100.0	2.2
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	96	42.9	91	94.8	40.6	91	94.8	40.6
Backbone-Backbone	35	15.6	35	100.0	15.6	35	100.0	15.6
Backbone-Sidechain	48	21.4	43	89.6	19.2	43	89.6	19.2
Sidechain-Sidechain	13	5.8	13	100.0	5.8	13	100.0	5.8
Hydrogen bond	35	15.6	3	8.6	1.3	3	8.6	1.3
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	224	100.0	99	44.2	44.2	99	44.2	44.2
Backbone-Backbone	67	29.9	35	52.2	15.6	35	52.2	15.6
Backbone-Sidechain	93	41.5	48	51.6	21.4	48	51.6	21.4
Sidechain-Sidechain	64	28.6	16	25.0	7.1	16	25.0	7.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations [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	0	0	0	5	94	99	19.33	36.59	8.29	19.2
2	0	0	0	5	94	99	19.45	36.66	8.43	19.14
3	0	0	0	5	94	99	18.81	36.88	8.3	18.13
4	0	0	0	5	94	99	18.67	35.44	8.06	17.7
5	0	0	0	5	94	99	18.38	34.65	7.8	17.43
6	0	0	0	5	94	99	19.04	36.45	8.41	18.56
7	0	0	0	5	94	99	18.76	35.63	8.01	18.34
8	0	0	0	5	94	99	19.22	36.75	8.28	18.86
9	0	0	0	5	94	99	18.71	34.46	7.86	18.68
10	0	0	0	5	94	99	18.48	34.9	7.89	17.77

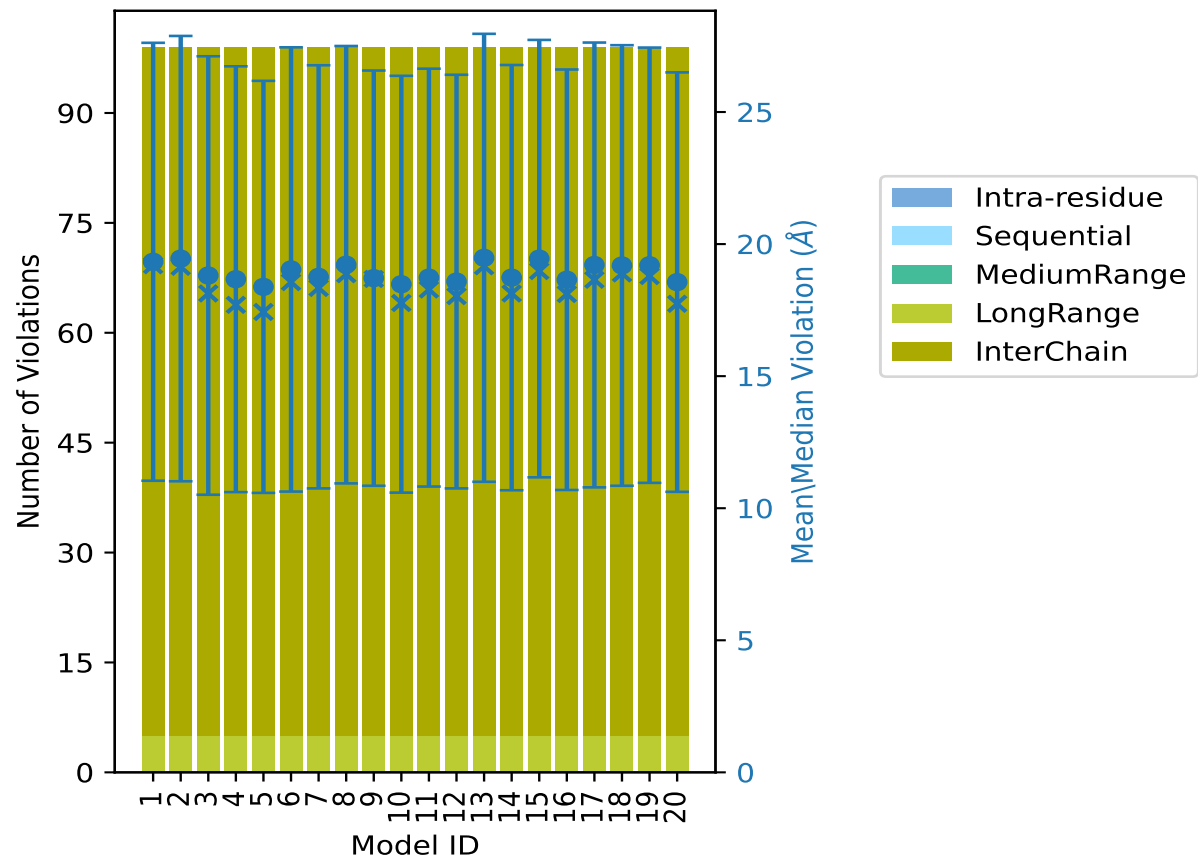
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	5	94	99	18.73	35.75	7.91	18.28
12	0	0	0	5	94	99	18.58	34.75	7.83	18.03
13	0	0	0	5	94	99	19.48	37.06	8.48	19.16
14	0	0	0	5	94	99	18.73	36.29	8.05	18.13
15	0	0	0	5	94	99	19.45	36.4	8.28	18.98
16	0	0	0	5	94	99	18.65	34.98	7.96	18.11
17	0	0	0	5	94	99	19.21	36.46	8.42	18.65
18	0	0	0	5	94	99	19.19	36.98	8.34	18.89
19	0	0	0	5	94	99	19.2	35.87	8.24	18.79
20	0	0	0	5	94	99	18.56	35.31	7.94	17.74

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 ⓘ



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

9.3 Distance violation statistics for the ensemble

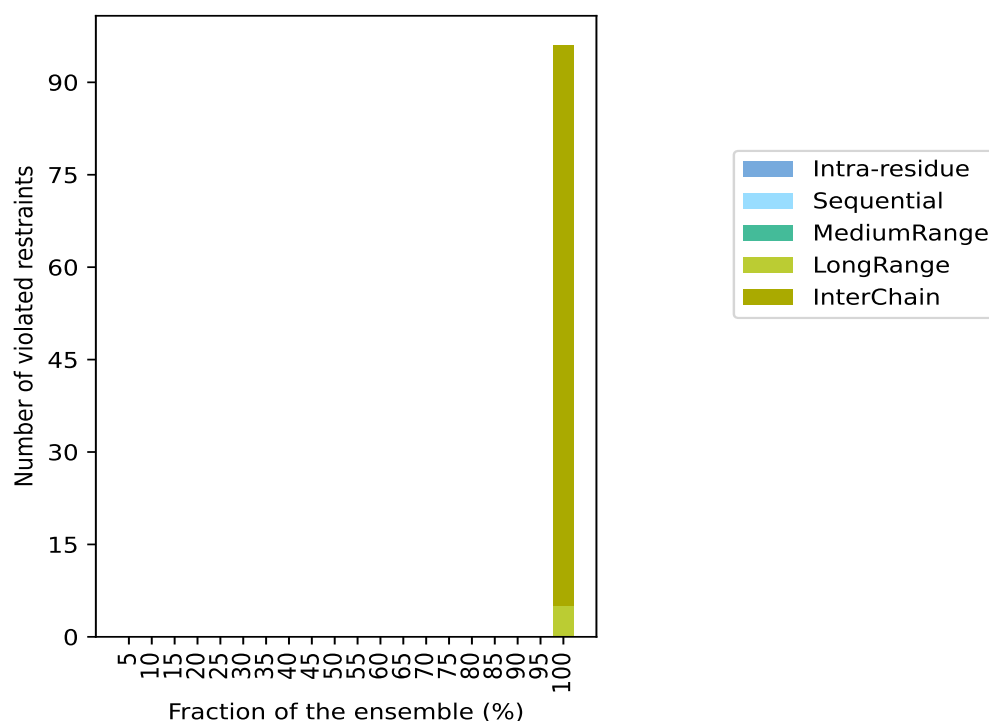
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 93(IR:53, SQ:35, MR:0, LR:0, IC:5) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	5	91	96	20	100.0

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

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

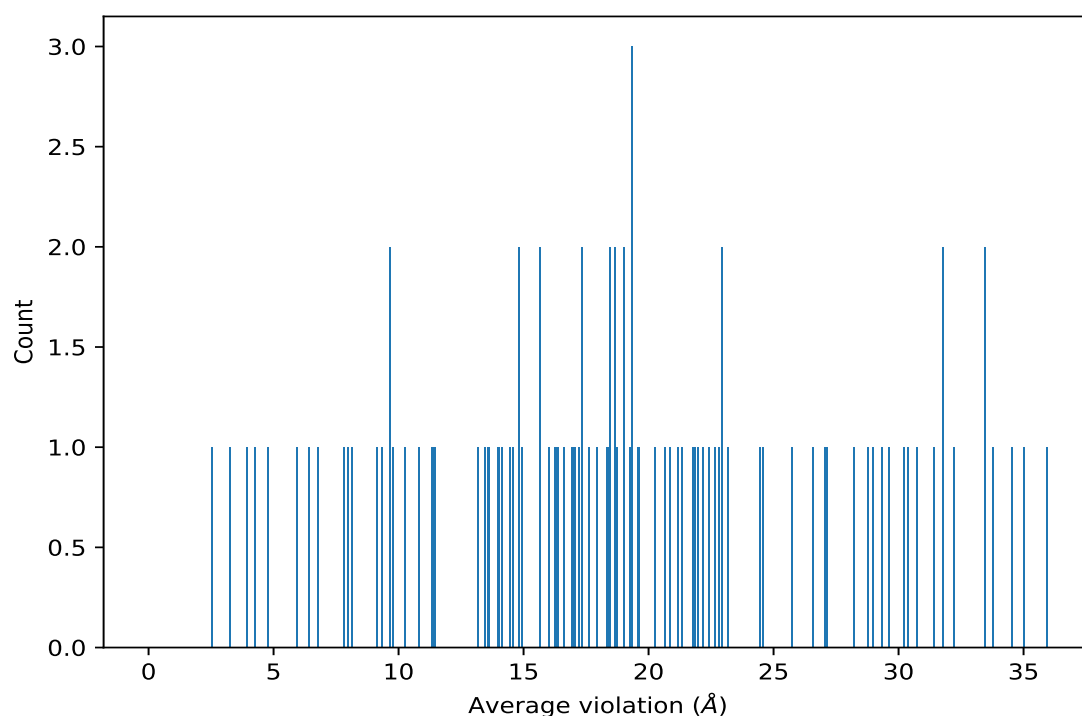
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	20	35.91	0.83	36.08
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	20	35.05	0.79	35.22
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	20	34.53	0.62	34.46
(1,186)	1:26:B:C:H5	1:13:A:C:H42	20	33.79	0.78	33.72
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	20	33.48	0.65	33.4
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	20	33.47	0.78	33.59
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	20	32.22	0.65	32.31
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	20	31.79	0.45	31.61
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	20	31.79	0.58	31.72
(1,153)	1:25:B:U:H6	1:13:A:C:H5	20	31.41	0.59	31.3
(1,175)	1:14:B:G:H1	1:1:A:G:H22	20	30.71	0.97	31.12
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	20	30.35	0.48	30.32
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	20	30.22	0.63	30.2
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	20	29.6	0.39	29.42
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	20	29.32	1.43	29.52
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	20	28.96	1.6	29.02

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	20	28.76	0.41	28.74
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	20	28.24	0.38	28.2
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	20	27.15	1.41	27.31
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	20	27.07	0.38	26.98
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	20	26.59	1.43	26.74
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	20	25.73	0.32	25.78
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	20	24.58	0.34	24.62
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	20	24.46	1.41	24.62
(1,190)	1:15:B:A:N7	1:2:A:A:H62	20	23.18	0.88	23.28
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	20	22.93	0.32	22.9
(1,178)	1:24:B:G:H1	1:11:A:G:H22	20	22.92	0.47	22.93
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	20	22.82	1.4	22.94
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	20	22.66	0.31	22.67
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	20	22.42	1.39	22.46
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	20	22.17	0.73	22.15
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	20	21.99	1.06	22.07
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	20	21.88	0.75	21.78
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	20	21.78	0.52	21.7
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	20	21.34	0.34	21.36
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	20	21.17	0.3	21.16
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	20	20.87	1.09	21.24
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	20	20.67	1.18	20.86
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	20	20.26	0.9	20.37
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	20	19.64	0.63	19.65
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	20	19.59	0.33	19.56
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	20	19.33	0.95	19.41
(1,164)	1:1:A:G:H1	1:8:A:G:H1'	20	19.33	0.95	19.41
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	20	19.32	0.72	19.24
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	20	19.26	0.48	19.28
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	20	19.01	0.55	18.81
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	20	19.01	0.62	18.98
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	20	18.7	0.94	18.63
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	20	18.69	1.08	18.9
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	20	18.66	0.58	18.72
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	20	18.48	0.63	18.38
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	20	18.45	0.52	18.44
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	20	18.41	1.05	18.34
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	20	18.32	0.59	18.14
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	20	17.94	1.05	18.03
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	20	17.6	0.82	17.53
(1,183)	1:16:B:C:H5	1:3:A:C:H42	20	17.34	0.83	17.38
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	20	17.32	0.65	17.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	20	17.2	0.89	17.29
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	20	17.07	1.05	17.27
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	20	17.01	0.73	17.08
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	20	16.94	0.66	16.82
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	20	16.61	0.61	16.56
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	20	16.39	0.56	16.3
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	20	16.34	0.31	16.24
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	20	16.25	0.67	16.19
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	20	16.0	0.59	16.04
(1,166)	1:1:A:G:H5'	1:20:B:A:H8	20	15.68	1.08	15.53
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	20	15.68	1.08	15.53
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	20	14.9	0.27	14.9
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	20	14.82	0.9	14.84
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	20	14.82	0.9	14.84
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	20	14.56	0.44	14.75
(1,176)	1:18:B:G:H1	1:5:A:G:H22	20	14.46	0.42	14.39
(1,191)	1:17:B:A:N7	1:4:A:A:H62	20	14.13	0.47	14.04
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	20	14.04	0.34	14.1
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	20	13.98	0.28	14.0
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	20	13.62	0.45	13.72
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	20	13.59	0.25	13.58
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	20	13.46	0.43	13.52
(1,136)	1:22:B:C:H6	1:10:A:U:H5	20	13.19	0.26	13.18
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	20	11.49	0.19	11.5
(1,185)	1:22:B:C:H5	1:9:A:C:H42	20	11.4	0.35	11.39
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	20	11.34	0.22	11.3
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	20	10.84	0.41	10.86
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	20	10.25	0.23	10.23
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	20	9.78	0.11	9.77
(1,126)	1:20:B:A:H8	1:6:A:C:H6	20	9.69	0.33	9.73
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	20	9.65	0.32	9.74
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	20	9.33	0.3	9.3
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	20	9.12	0.11	9.14
(1,177)	1:21:B:G:H1	1:8:A:G:H22	20	8.14	0.19	8.16
(1,184)	1:19:B:C:H5	1:6:A:C:H42	20	7.95	0.37	7.95
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	20	7.82	0.36	7.76
(1,131)	1:21:B:G:H8	1:9:A:C:H5	20	6.79	0.48	6.71
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	20	6.44	0.37	6.37
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	20	5.9	0.39	5.93
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	20	4.78	0.45	4.74
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	20	4.25	0.15	4.25
(1,127)	1:20:B:A:H8	1:8:A:G:H8	20	3.93	0.28	3.92

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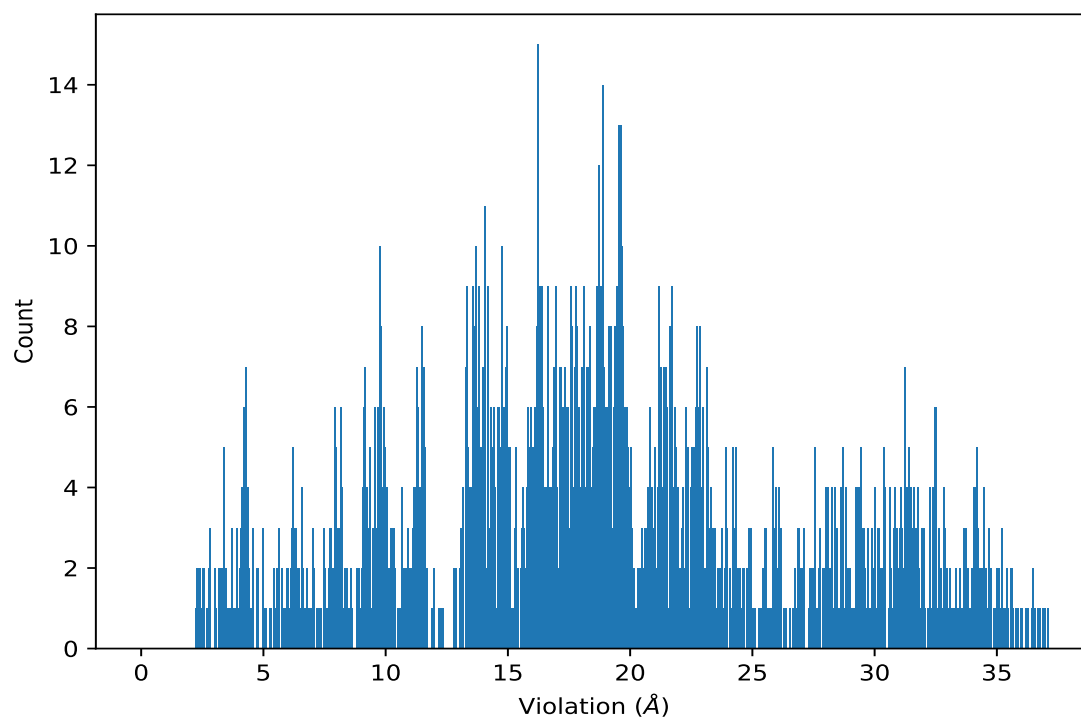
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,192)	1:20:B:A:N7	1:7:A:A:H62	20	3.28	0.17	3.32
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	20	2.51	0.19	2.5

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 [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	13	37.06
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	18	36.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	3	36.88
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	8	36.75
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	2	36.66
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	1	36.59
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	17	36.46
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	6	36.45
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	15	36.4
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	14	36.29
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	18	36.2
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	2	36.15
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	3	36.02
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	13	35.97
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	19	35.87
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	11	35.75
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	1	35.68
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	7	35.63
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	8	35.61
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	17	35.56
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	19	35.56
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	17	35.49
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	4	35.44
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	13	35.44
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	11	35.39
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	20	35.31
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	15	35.26
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	2	35.24
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	6	35.24
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	15	35.2
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	6	35.17
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	8	35.09
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	1	35.07
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	14	35.05
(1,186)	1:26:B:C:H5	1:13:A:C:H42	2	35.02
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	16	34.98
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	10	34.9
(1,186)	1:26:B:C:H5	1:13:A:C:H42	13	34.89
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	3	34.79
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	12	34.75
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	13	34.7
(1,186)	1:26:B:C:H5	1:13:A:C:H42	8	34.67
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	18	34.67
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	5	34.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	19	34.64
(1,186)	1:26:B:C:H5	1:13:A:C:H42	17	34.59
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	13	34.57
(1,186)	1:26:B:C:H5	1:13:A:C:H42	6	34.55
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	12	34.5
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	4	34.49
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	17	34.47
(1,160)	1:26:B:C:H6	1:13:A:C:H2'	9	34.46
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	7	34.46
(1,186)	1:26:B:C:H5	1:13:A:C:H42	1	34.39
(1,186)	1:26:B:C:H5	1:13:A:C:H42	3	34.39
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	8	34.34
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	18	34.34
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	7	34.28
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	15	34.27
(1,186)	1:26:B:C:H5	1:13:A:C:H42	15	34.24
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	17	34.22
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	14	34.21
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	1	34.19
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	8	34.19
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	6	34.18
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	9	34.17
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	20	34.16
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	2	34.11
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	15	34.11
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	1	34.11
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	10	34.1
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	4	34.09
(1,186)	1:26:B:C:H5	1:13:A:C:H42	19	34.07
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	6	34.07
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	16	34.07
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	10	34.01
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	3	33.99
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	16	33.99
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	2	33.93
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	5	33.89
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	9	33.81
(1,155)	1:26:B:C:H1'	1:13:A:C:H2'	20	33.81
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	11	33.8
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	3	33.8
(1,186)	1:26:B:C:H5	1:13:A:C:H42	18	33.73
(1,186)	1:26:B:C:H5	1:13:A:C:H42	4	33.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:26:B:C:H5	1:13:A:C:H42	14	33.71
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	14	33.69
(1,186)	1:26:B:C:H5	1:13:A:C:H42	7	33.65
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	12	33.65
(1,157)	1:26:B:C:H5	1:12:A:U:H3'	5	33.6
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	19	33.52
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	19	33.49
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	18	33.49
(1,186)	1:26:B:C:H5	1:13:A:C:H42	20	33.44
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	2	33.36
(1,186)	1:26:B:C:H5	1:13:A:C:H42	16	33.34
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	7	33.31
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	7	33.26
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	20	33.22
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	17	33.1
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	14	33.09
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	13	33.06
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	20	33.03
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	4	32.97
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	16	32.96
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	19	32.94
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	10	32.93
(1,186)	1:26:B:C:H5	1:13:A:C:H42	11	32.87
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	4	32.87
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	1	32.85
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	11	32.84
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	11	32.83
(1,186)	1:26:B:C:H5	1:13:A:C:H42	10	32.81
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	8	32.81
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	8	32.78
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	2	32.72
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	13	32.7
(1,186)	1:26:B:C:H5	1:13:A:C:H42	5	32.69
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	10	32.63
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	9	32.62
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	12	32.6
(1,186)	1:26:B:C:H5	1:13:A:C:H42	9	32.59
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	16	32.55
(1,156)	1:26:B:C:H5	1:12:A:U:H2'	5	32.55
(1,153)	1:25:B:U:H6	1:13:A:C:H5	8	32.55
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	12	32.54
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	8	32.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	2	32.5
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	3	32.48
(1,186)	1:26:B:C:H5	1:13:A:C:H42	12	32.47
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	13	32.47
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	1	32.46
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	6	32.45
(1,153)	1:25:B:U:H6	1:13:A:C:H5	2	32.45
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	15	32.42
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	18	32.37
(1,175)	1:14:B:G:H1	1:1:A:G:H22	2	32.36
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	5	32.35
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	15	32.35
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	17	32.33
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	17	32.28
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	1	32.26
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	12	32.25
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	7	32.25
(1,153)	1:25:B:U:H6	1:13:A:C:H5	13	32.2
(1,159)	1:26:B:C:H6	1:13:A:C:H1'	9	32.15
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	11	32.09
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	6	32.05
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	6	32.03
(1,153)	1:25:B:U:H6	1:13:A:C:H5	1	32.0
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	3	31.94
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	9	31.93
(1,153)	1:25:B:U:H6	1:13:A:C:H5	17	31.92
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	3	31.88
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	7	31.83
(1,153)	1:25:B:U:H6	1:13:A:C:H5	3	31.82
(1,175)	1:14:B:G:H1	1:1:A:G:H22	19	31.79
(1,175)	1:14:B:G:H1	1:1:A:G:H22	13	31.77
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	18	31.77
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	19	31.76
(1,153)	1:25:B:U:H6	1:13:A:C:H5	6	31.69
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	5	31.68
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	15	31.66
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	5	31.63
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	19	31.62
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	5	31.61
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	7	31.6
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	18	31.58
(1,175)	1:14:B:G:H1	1:1:A:G:H22	15	31.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:14:B:G:H1	1:1:A:G:H22	18	31.56
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	16	31.54
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	11	31.51
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	12	31.5
(1,153)	1:25:B:U:H6	1:13:A:C:H5	15	31.49
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	14	31.47
(1,153)	1:25:B:U:H6	1:13:A:C:H5	7	31.46
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	20	31.46
(1,175)	1:14:B:G:H1	1:1:A:G:H22	17	31.43
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	14	31.43
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	10	31.42
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	20	31.42
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	4	31.41
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	16	31.4
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	12	31.36
(1,153)	1:25:B:U:H6	1:13:A:C:H5	5	31.35
(1,175)	1:14:B:G:H1	1:1:A:G:H22	3	31.34
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	10	31.32
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	11	31.32
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	9	31.3
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	16	31.27
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	14	31.26
(1,175)	1:14:B:G:H1	1:1:A:G:H22	1	31.25
(1,153)	1:25:B:U:H6	1:13:A:C:H5	14	31.24
(1,175)	1:14:B:G:H1	1:1:A:G:H22	6	31.22
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	17	31.22
(1,153)	1:25:B:U:H6	1:13:A:C:H5	20	31.22
(1,154)	1:26:B:C:H1'	1:12:A:U:H2'	20	31.21
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	8	31.21
(1,150)	1:25:B:U:H5	1:12:A:U:H3'	4	31.21
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	2	31.2
(1,153)	1:25:B:U:H6	1:13:A:C:H5	19	31.17
(1,175)	1:14:B:G:H1	1:1:A:G:H22	4	31.14
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	13	31.13
(1,175)	1:14:B:G:H1	1:1:A:G:H22	8	31.11
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	13	31.08
(1,153)	1:25:B:U:H6	1:13:A:C:H5	18	31.07
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	9	31.07
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	2	31.06
(1,153)	1:25:B:U:H6	1:13:A:C:H5	16	31.02
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	6	31.01
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	2	31.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	13	30.99
(1,153)	1:25:B:U:H6	1:13:A:C:H5	11	30.98
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	8	30.95
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	17	30.94
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	1	30.92
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	10	30.89
(1,153)	1:25:B:U:H6	1:13:A:C:H5	4	30.87
(1,148)	1:25:B:U:H1'	1:12:A:U:H2'	4	30.85
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	1	30.8
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	6	30.8
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	15	30.8
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	6	30.8
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	18	30.78
(1,153)	1:25:B:U:H6	1:13:A:C:H5	12	30.77
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	13	30.75
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	15	30.72
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	6	30.68
(1,153)	1:25:B:U:H6	1:13:A:C:H5	10	30.67
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	17	30.65
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	17	30.62
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	18	30.62
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	19	30.6
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	15	30.59
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	18	30.45
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	15	30.45
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	3	30.44
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	7	30.44
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	5	30.38
(1,175)	1:14:B:G:H1	1:1:A:G:H22	14	30.37
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	19	30.37
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	4	30.37
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	3	30.36
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	2	30.34
(1,153)	1:25:B:U:H6	1:13:A:C:H5	9	30.3
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	20	30.29
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	2	30.25
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	19	30.22
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	4	30.21
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	8	30.2
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	18	30.19
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	15	30.18
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	12	30.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:14:B:G:H1	1:1:A:G:H22	11	30.11
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	17	30.11
(1,175)	1:14:B:G:H1	1:1:A:G:H22	16	30.05
(1,175)	1:14:B:G:H1	1:1:A:G:H22	7	30.04
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	7	30.04
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	13	30.03
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	11	30.01
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	1	29.99
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	14	29.97
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	19	29.93
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	16	29.91
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	6	29.89
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	20	29.86
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	1	29.85
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	9	29.83
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	10	29.78
(1,175)	1:14:B:G:H1	1:1:A:G:H22	10	29.73
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	12	29.73
(1,175)	1:14:B:G:H1	1:1:A:G:H22	9	29.71
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	16	29.66
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	14	29.62
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	3	29.61
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	9	29.58
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	3	29.58
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	11	29.55
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	3	29.54
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	5	29.53
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	8	29.51
(1,175)	1:14:B:G:H1	1:1:A:G:H22	20	29.49
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	9	29.46
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	14	29.45
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	5	29.44
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	4	29.43
(1,158)	1:26:B:C:H6	1:12:A:U:H1'	10	29.43
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	16	29.43
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	16	29.39
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	19	29.38
(1,152)	1:25:B:U:H6	1:12:A:U:H1'	4	29.37
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	12	29.35
(1,175)	1:14:B:G:H1	1:1:A:G:H22	12	29.34
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	18	29.34
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	5	29.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	7	29.32
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	20	29.29
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	14	29.26
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	1	29.23
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	10	29.22
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	11	29.21
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	7	29.21
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	2	29.17
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	1	29.1
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	12	29.05
(1,149)	1:25:B:U:H5	1:11:A:G:H2'	4	28.99
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	13	28.97
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	8	28.93
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	2	28.93
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	2	28.88
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	8	28.85
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	9	28.84
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	5	28.81
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	11	28.81
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	14	28.8
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	17	28.75
(1,175)	1:14:B:G:H1	1:1:A:G:H22	5	28.74
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	14	28.74
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	6	28.74
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	16	28.71
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	18	28.71
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	1	28.66
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	6	28.63
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	20	28.63
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	17	28.63
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	7	28.61
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	13	28.59
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	13	28.53
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	15	28.47
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	13	28.47
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	10	28.46
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	16	28.45
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	18	28.41
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	20	28.41
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	12	28.4
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	3	28.4
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	9	28.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	19	28.38
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	15	28.3
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	6	28.29
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	18	28.29
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	11	28.26
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	14	28.26
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	19	28.24
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	4	28.22
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	10	28.18
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	7	28.17
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	17	28.15
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	9	28.1
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	8	28.09
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	19	28.06
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	15	28.06
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	16	28.05
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	20	28.04
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	10	28.03
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	17	28.03
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	6	28.01
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	15	27.98
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	10	27.95
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	20	27.94
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	11	27.9
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	18	27.85
(1,144)	1:24:B:G:H1'	1:11:A:G:H2'	4	27.78
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	2	27.76
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	3	27.75
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	3	27.73
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	2	27.72
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	4	27.63
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	19	27.59
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	1	27.58
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	17	27.57
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	9	27.56
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	11	27.56
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	8	27.49
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	1	27.48
(1,145)	1:24:B:G:H1'	1:11:A:G:H3'	4	27.43
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	6	27.41
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	13	27.4
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	7	27.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	15	27.32
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	3	27.12
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	9	27.11
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	14	27.11
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	14	27.04
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	18	27.0
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	12	26.97
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	16	26.96
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	8	26.95
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	1	26.93
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	3	26.91
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	5	26.89
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	7	26.86
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	16	26.86
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	19	26.81
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	20	26.79
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	12	26.74
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	10	26.72
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	11	26.68
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	14	26.54
(1,84)	1:14:B:G:H8	1:1:A:G:H1'	5	26.39
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	16	26.34
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	5	26.29
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	7	26.19
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	2	26.18
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	20	26.17
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	18	26.09
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	12	26.09
(1,151)	1:25:B:U:H6	1:11:A:G:H1'	4	26.08
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	8	26.06
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	10	26.04
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	13	26.02
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	12	25.99
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	20	25.99
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	6	25.97
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	9	25.96
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	1	25.95
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	17	25.92
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	15	25.87
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	15	25.85
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	13	25.85
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	6	25.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	17	25.83
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	11	25.83
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	14	25.82
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	8	25.81
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	11	25.75
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	2	25.72
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	7	25.66
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	10	25.62
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	18	25.59
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	19	25.58
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	9	25.58
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	16	25.53
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	19	25.51
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	20	25.5
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	3	25.48
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	10	25.47
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	4	25.44
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	9	25.44
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	11	25.35
(1,83)	1:14:B:G:H1'	1:1:A:G:H4'	5	25.3
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	7	25.29
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	1	25.15
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	1	25.0
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	11	24.94
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	5	24.93
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	2	24.92
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	3	24.89
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	8	24.87
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	9	24.86
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	7	24.8
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	12	24.79
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	13	24.77
(1,147)	1:24:B:G:H8	1:11:A:G:H1'	4	24.69
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	18	24.68
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	2	24.63
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	12	24.6
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	14	24.57
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	16	24.47
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	17	24.47
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	15	24.42
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	18	24.42
(1,190)	1:15:B:A:N7	1:2:A:A:H62	15	24.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	16	24.34
(1,190)	1:15:B:A:N7	1:2:A:A:H62	2	24.33
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	6	24.33
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	6	24.32
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	19	24.31
(1,190)	1:15:B:A:N7	1:2:A:A:H62	13	24.29
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	14	24.28
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	17	24.25
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	20	24.24
(1,190)	1:15:B:A:N7	1:2:A:A:H62	18	24.23
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	10	24.23
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	15	24.22
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	13	24.21
(1,81)	1:14:B:G:H1'	1:1:A:G:H2'	5	24.1
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	18	24.08
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	8	24.06
(1,190)	1:15:B:A:N7	1:2:A:A:H62	6	23.99
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	2	23.99
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	17	23.96
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	12	23.95
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	3	23.94
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	19	23.93
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	13	23.91
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	15	23.91
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	6	23.87
(1,143)	1:24:B:G:H1'	1:10:A:U:H2'	4	23.85
(1,178)	1:24:B:G:H1	1:11:A:G:H22	13	23.83
(1,190)	1:15:B:A:N7	1:2:A:A:H62	19	23.78
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	4	23.78
(1,190)	1:15:B:A:N7	1:2:A:A:H62	17	23.76
(1,178)	1:24:B:G:H1	1:11:A:G:H22	8	23.74
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	19	23.73
(1,178)	1:24:B:G:H1	1:11:A:G:H22	2	23.68
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	2	23.66
(1,190)	1:15:B:A:N7	1:2:A:A:H62	4	23.58
(1,190)	1:15:B:A:N7	1:2:A:A:H62	1	23.55
(1,178)	1:24:B:G:H1	1:11:A:G:H22	1	23.53
(1,82)	1:14:B:G:H1'	1:1:A:G:H3'	5	23.49
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	20	23.48
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	15	23.47
(1,190)	1:15:B:A:N7	1:2:A:A:H62	3	23.41
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	10	23.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	13	23.4
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	2	23.4
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	5	23.34
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	1	23.34
(1,178)	1:24:B:G:H1	1:11:A:G:H22	15	23.33
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	7	23.3
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	11	23.29
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	15	23.27
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	2	23.25
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	8	23.24
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	19	23.21
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	13	23.21
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	7	23.19
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	1	23.19
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	3	23.19
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	12	23.18
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	13	23.17
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	7	23.15
(1,190)	1:15:B:A:N7	1:2:A:A:H62	14	23.14
(1,190)	1:15:B:A:N7	1:2:A:A:H62	8	23.12
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	9	23.12
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	11	23.12
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	15	23.11
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	1	23.11
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	13	23.09
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	15	23.06
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	12	23.04
(1,178)	1:24:B:G:H1	1:11:A:G:H22	18	22.99
(1,178)	1:24:B:G:H1	1:11:A:G:H22	19	22.99
(1,178)	1:24:B:G:H1	1:11:A:G:H22	3	22.97
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	20	22.97
(1,178)	1:24:B:G:H1	1:11:A:G:H22	6	22.96
(1,178)	1:24:B:G:H1	1:11:A:G:H22	17	22.96
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	9	22.93
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	8	22.93
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	4	22.93
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	11	22.92
(1,178)	1:24:B:G:H1	1:11:A:G:H22	7	22.9
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	18	22.9
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	1	22.89
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	8	22.88
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	3	22.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	10	22.87
(1,190)	1:15:B:A:N7	1:2:A:A:H62	16	22.86
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	8	22.86
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	5	22.84
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	17	22.84
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	17	22.84
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	15	22.84
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	17	22.81
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	19	22.79
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	2	22.79
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	1	22.78
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	1	22.77
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	14	22.77
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	19	22.76
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	18	22.74
(1,178)	1:24:B:G:H1	1:11:A:G:H22	9	22.73
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	9	22.73
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	2	22.73
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	19	22.72
(1,178)	1:24:B:G:H1	1:11:A:G:H22	11	22.71
(1,178)	1:24:B:G:H1	1:11:A:G:H22	14	22.71
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	14	22.71
(1,190)	1:15:B:A:N7	1:2:A:A:H62	7	22.7
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	16	22.68
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	3	22.68
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	10	22.67
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	17	22.67
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	6	22.66
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	14	22.65
(1,178)	1:24:B:G:H1	1:11:A:G:H22	12	22.63
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	18	22.63
(1,190)	1:15:B:A:N7	1:2:A:A:H62	11	22.61
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	20	22.6
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	2	22.59
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	19	22.55
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	1	22.55
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	13	22.53
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	8	22.52
(1,190)	1:15:B:A:N7	1:2:A:A:H62	20	22.51
(1,178)	1:24:B:G:H1	1:11:A:G:H22	5	22.5
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	19	22.5
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	3	22.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	6	22.47
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	8	22.47
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	16	22.46
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	3	22.43
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	6	22.4
(1,178)	1:24:B:G:H1	1:11:A:G:H22	20	22.39
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	16	22.36
(1,178)	1:24:B:G:H1	1:11:A:G:H22	16	22.35
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	13	22.35
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	15	22.32
(1,178)	1:24:B:G:H1	1:11:A:G:H22	10	22.27
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	18	22.27
(1,138)	1:23:B:U:H1'	1:10:A:U:H2'	4	22.27
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	2	22.26
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	16	22.26
(1,178)	1:24:B:G:H1	1:11:A:G:H22	4	22.25
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	8	22.24
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	6	22.23
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	17	22.2
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	2	22.19
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	3	22.19
(1,140)	1:23:B:U:H1'	1:10:A:U:H4'	4	22.18
(1,190)	1:15:B:A:N7	1:2:A:A:H62	10	22.14
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	18	22.13
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	3	22.13
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	14	22.09
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	17	22.06
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	12	22.01
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	4	22.01
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	13	21.99
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	18	21.98
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	18	21.97
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	1	21.96
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	6	21.94
(1,190)	1:15:B:A:N7	1:2:A:A:H62	9	21.92
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	1	21.91
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	14	21.9
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	19	21.87
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	17	21.87
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	13	21.86
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	11	21.85
(1,190)	1:15:B:A:N7	1:2:A:A:H62	12	21.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	15	21.84
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	16	21.83
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	7	21.83
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	9	21.82
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	20	21.82
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	12	21.78
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	9	21.77
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	15	21.76
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	11	21.76
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	9	21.74
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	15	21.74
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	10	21.74
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	4	21.74
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	7	21.73
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	14	21.73
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	18	21.72
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	17	21.71
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	6	21.71
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	11	21.69
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	6	21.69
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	8	21.68
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	15	21.66
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	19	21.66
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	4	21.65
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	4	21.64
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	7	21.64
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	7	21.63
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	14	21.63
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	4	21.62
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	12	21.61
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	6	21.6
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	13	21.58
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	5	21.54
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	8	21.54
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	18	21.53
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	10	21.52
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	10	21.51
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	11	21.5
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	5	21.49
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	3	21.48
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	9	21.48
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	18	21.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	7	21.47
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	19	21.47
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	14	21.46
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	11	21.45
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	9	21.45
(1,190)	1:15:B:A:N7	1:2:A:A:H62	5	21.43
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	20	21.42
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	15	21.41
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	11	21.41
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	8	21.4
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	20	21.36
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	1	21.35
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	12	21.35
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	16	21.35
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	1	21.35
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	3	21.35
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	15	21.33
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	7	21.33
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	9	21.32
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	9	21.31
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	17	21.29
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	4	21.29
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	16	21.28
(1,90)	1:15:B:A:H8	1:1:A:G:H1'	5	21.28
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	3	21.27
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	7	21.27
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	13	21.25
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	12	21.24
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	10	21.22
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	16	21.22
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	10	21.2
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	8	21.2
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	20	21.2
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	3	21.19
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	12	21.19
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	11	21.19
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	19	21.18
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	2	21.17
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	20	21.16
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	6	21.13
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	13	21.11
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	7	21.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	11	21.1
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	18	21.08
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	2	21.05
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	17	21.04
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	10	21.02
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	14	21.01
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	14	21.01
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	16	21.01
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	1	20.99
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	10	20.98
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	8	20.97
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	19	20.94
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	9	20.91
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	16	20.87
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	15	20.87
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	19	20.86
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	20	20.85
(1,162)	1:1:A:G:H1	1:7:A:A:H2'	5	20.84
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	19	20.84
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	20	20.84
(1,9)	1:2:A:A:H2	1:16:B:C:H1'	5	20.83
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	20	20.82
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	5	20.81
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	16	20.79
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	9	20.76
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	17	20.74
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	8	20.74
(1,88)	1:15:B:A:H2	1:3:A:C:H1'	10	20.74
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	14	20.73
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	4	20.7
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	14	20.69
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	4	20.68
(1,146)	1:24:B:G:H8	1:10:A:U:H1'	3	20.65
(1,139)	1:23:B:U:H1'	1:10:A:U:H3'	6	20.63
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	15	20.62
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	1	20.59
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	12	20.57
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	6	20.52
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	2	20.49
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	16	20.48
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	1	20.46
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	10	20.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	12	20.42
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	15	20.37
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	16	20.37
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	2	20.32
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	7	20.32
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	18	20.27
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	13	20.21
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	1	20.18
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	2	20.16
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	20	20.11
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	12	20.1
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	5	20.09
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	8	20.09
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	12	20.05
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	1	20.04
(1,164)	1:1:A:G:H1	1:8:A:G:H1'	13	20.03
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	16	20.03
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	5	20.02
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	7	20.0
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	13	19.98
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	18	19.97
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	1	19.97
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	17	19.96
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	19	19.94
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	13	19.94
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	5	19.93
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	9	19.93
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	11	19.91
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	18	19.89
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	2	19.89
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	9	19.87
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	12	19.87
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	11	19.86
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	1	19.85
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	11	19.84
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	9	19.84
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	12	19.8
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	9	19.78
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	8	19.77
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	8	19.77
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	11	19.77
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	20	19.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	13	19.75
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	5	19.74
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	10	19.73
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	13	19.73
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	11	19.73
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	15	19.73
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	18	19.73
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	12	19.72
(1,92)	1:15:B:A:H8	1:1:A:G:H2'	5	19.71
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	1	19.7
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	12	19.7
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	4	19.69
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	12	19.69
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	20	19.69
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	6	19.67
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	14	19.67
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	13	19.67
(1,87)	1:15:B:A:H2	1:2:A:A:H1'	5	19.67
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	18	19.66
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	15	19.65
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	8	19.65
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	8	19.65
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	15	19.64
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	6	19.63
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	15	19.63
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	2	19.62
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	12	19.62
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	17	19.62
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	19	19.61
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	1	19.61
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	19	19.61
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	8	19.6
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	10	19.58
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	16	19.57
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	10	19.57
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	11	19.56
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	17	19.55
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	5	19.55
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	19	19.55
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	7	19.54
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	8	19.54
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	6	19.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	20	19.54
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	13	19.53
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	7	19.52
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	13	19.52
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	3	19.51
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	7	19.51
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	17	19.5
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	20	19.5
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	1	19.5
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	18	19.5
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	11	19.49
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	19	19.49
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	2	19.49
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	17	19.49
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	11	19.49
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	9	19.48
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	9	19.47
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	7	19.46
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	2	19.46
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	7	19.45
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	11	19.45
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	8	19.43
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	7	19.41
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	2	19.4
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	8	19.39
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	9	19.38
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	1	19.38
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	1	19.37
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	15	19.36
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	9	19.35
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	2	19.35
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	3	19.34
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	7	19.34
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	19	19.33
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	2	19.33
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	12	19.33
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	10	19.32
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	20	19.28
(1,85)	1:15:B:A:H1'	1:1:A:G:H2'	5	19.26
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	3	19.25
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	5	19.24
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	10	19.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	15	19.23
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	6	19.22
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	8	19.22
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	14	19.21
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	6	19.21
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	20	19.21
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	13	19.2
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	16	19.2
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	1	19.2
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	18	19.17
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	13	19.16
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	2	19.15
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	19	19.15
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	2	19.14
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	6	19.13
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	16	19.13
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	1	19.12
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	17	19.11
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	18	19.1
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	7	19.08
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	13	19.07
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	16	19.06
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	14	19.06
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	2	19.06
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	4	19.05
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	4	19.04
(1,142)	1:23:B:U:H6	1:10:A:U:H1'	4	19.04
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	10	19.03
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	2	19.03
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	9	19.0
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	13	19.0
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	15	18.98
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	20	18.97
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	17	18.96
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	3	18.94
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	3	18.92
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	9	18.92
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	19	18.92
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	13	18.92
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	13	18.91
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	18	18.91
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	18	18.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	18	18.89
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	4	18.88
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	20	18.88
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	11	18.88
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	12	18.88
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	1	18.87
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	11	18.86
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	12	18.86
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	14	18.86
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	8	18.86
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	3	18.85
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	14	18.85
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	3	18.85
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	5	18.83
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	11	18.83
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	2	18.82
(1,183)	1:16:B:C:H5	1:3:A:C:H42	15	18.81
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	14	18.81
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	15	18.81
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	9	18.8
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	9	18.8
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	17	18.8
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	18	18.79
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	19	18.79
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	15	18.79
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	4	18.77
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	17	18.76
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	5	18.76
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	3	18.76
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	10	18.74
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	2	18.74
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	13	18.74
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	6	18.73
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	19	18.71
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	6	18.71
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	11	18.71
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	19	18.71
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	18	18.7
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	3	18.7
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	12	18.7
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	20	18.7
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	7	18.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	9	18.68
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	16	18.68
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	17	18.67
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	17	18.65
(1,86)	1:15:B:A:H1'	1:2:A:A:H2'	5	18.65
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	6	18.64
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	18	18.64
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	6	18.62
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	8	18.62
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	8	18.61
(1,165)	1:1:A:G:H3'	1:7:A:A:H2	5	18.6
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	10	18.6
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	16	18.59
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	7	18.57
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	15	18.57
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	14	18.57
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	6	18.56
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	14	18.55
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	15	18.54
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	8	18.54
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	10	18.5
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	3	18.5
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	10	18.5
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	8	18.5
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	9	18.48
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	17	18.48
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	19	18.47
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	1	18.46
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	2	18.45
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	1	18.44
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	4	18.43
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	7	18.41
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	4	18.41
(1,183)	1:16:B:C:H5	1:3:A:C:H42	13	18.4
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	17	18.4
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	14	18.4
(1,183)	1:16:B:C:H5	1:3:A:C:H42	2	18.39
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	8	18.36
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	1	18.35
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	6	18.35
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	12	18.35
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	10	18.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	7	18.34
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	9	18.33
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	13	18.32
(1,104)	1:17:B:A:H2	1:5:A:G:H1'	4	18.31
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	19	18.31
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	9	18.3
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	16	18.28
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	16	18.28
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	13	18.28
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	11	18.28
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	18	18.24
(1,91)	1:15:B:A:H8	1:2:A:A:H1'	5	18.24
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	2	18.23
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	6	18.23
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	14	18.22
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	10	18.21
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	13	18.21
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	19	18.18
(1,183)	1:16:B:C:H5	1:3:A:C:H42	18	18.16
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	1	18.16
(1,102)	1:17:B:A:H1'	1:4:A:A:H4'	4	18.16
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	15	18.15
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	3	18.14
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	16	18.14
(1,110)	1:18:B:G:H1'	1:5:A:G:H2'	3	18.13
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	14	18.13
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	14	18.13
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	12	18.12
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	17	18.12
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	16	18.11
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	2	18.08
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	14	18.07
(1,183)	1:16:B:C:H5	1:3:A:C:H42	6	18.05
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	5	18.05
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	15	18.04
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	12	18.03
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	20	18.03
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	18	18.02
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	20	18.01
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	6	18.01
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	17	18.0
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	1	17.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	1:16:B:C:H5	1:3:A:C:H42	19	17.95
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	16	17.95
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	7	17.95
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	20	17.94
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	19	17.94
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	11	17.93
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	9	17.92
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	13	17.91
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	3	17.91
(1,183)	1:16:B:C:H5	1:3:A:C:H42	1	17.9
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	2	17.9
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	17	17.9
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	18	17.89
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	16	17.87
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	8	17.86
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	19	17.84
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	6	17.84
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	12	17.83
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	16	17.82
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	18	17.81
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	8	17.8
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	9	17.8
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	7	17.8
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	15	17.78
(1,183)	1:16:B:C:H5	1:3:A:C:H42	17	17.77
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	10	17.77
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	11	17.77
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	17	17.77
(1,161)	1:1:A:G:H1	1:7:A:A:H1'	3	17.75
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	6	17.75
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	8	17.75
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	4	17.75
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	20	17.74
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	12	17.74
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	15	17.72
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	10	17.71
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	14	17.7
(1,100)	1:17:B:A:H1'	1:4:A:A:H2'	4	17.7
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	1	17.7
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	16	17.68
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	17	17.68
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	4	17.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	12	17.66
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	9	17.63
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	1	17.63
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	20	17.63
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	7	17.61
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	4	17.61
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	20	17.61
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	1	17.6
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	6	17.6
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	5	17.59
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	15	17.58
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	3	17.58
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	20	17.58
(1,183)	1:16:B:C:H5	1:3:A:C:H42	4	17.57
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	6	17.57
(1,103)	1:17:B:A:H2	1:4:A:A:H1'	4	17.57
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	12	17.57
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	10	17.57
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	4	17.53
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	13	17.53
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	10	17.5
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	10	17.48
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	11	17.47
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	9	17.46
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	10	17.45
(1,109)	1:18:B:G:H1'	1:4:A:A:H2'	4	17.45
(1,94)	1:16:B:C:H1'	1:3:A:C:H2'	16	17.45
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	15	17.44
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	18	17.44
(1,164)	1:1:A:G:H3'	1:8:A:G:H1'	5	17.43
(1,163)	1:1:A:G:H1	1:7:A:A:H3'	5	17.43
(1,183)	1:16:B:C:H5	1:3:A:C:H42	3	17.42
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	17	17.42
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	19	17.4
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	19	17.38
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	20	17.37
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	9	17.37
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	3	17.37
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	3	17.35
(1,183)	1:16:B:C:H5	1:3:A:C:H42	14	17.34
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	11	17.34
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	1	17.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	2	17.33
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	13	17.33
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	14	17.33
(1,183)	1:16:B:C:H5	1:3:A:C:H42	8	17.3
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	7	17.28
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	13	17.28
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	1	17.26
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	14	17.25
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	12	17.25
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	19	17.25
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	12	17.24
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	7	17.24
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	3	17.23
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	6	17.23
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	12	17.23
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	8	17.2
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	5	17.19
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	5	17.19
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	9	17.18
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	2	17.18
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	11	17.16
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	8	17.16
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	7	17.16
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	1	17.15
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	12	17.15
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	5	17.15
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	18	17.14
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	8	17.13
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	7	17.13
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	8	17.1
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	4	17.08
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	11	17.07
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	8	17.03
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	11	17.03
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	12	17.01
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	14	17.01
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	7	16.99
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	12	16.99
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	17	16.99
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	20	16.98
(1,183)	1:16:B:C:H5	1:3:A:C:H42	11	16.96
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	15	16.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	11	16.95
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	1	16.95
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	15	16.95
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	8	16.94
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	15	16.93
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	4	16.93
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	18	16.9
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	6	16.88
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	14	16.88
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	2	16.87
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	14	16.87
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	11	16.86
(1,183)	1:16:B:C:H5	1:3:A:C:H42	16	16.85
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	5	16.84
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	7	16.83
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	13	16.82
(1,183)	1:16:B:C:H5	1:3:A:C:H42	7	16.8
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	9	16.8
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	14	16.79
(1,170)	1:1:A:G:H4'	1:20:B:A:H1'	3	16.77
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	7	16.77
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	7	16.75
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	13	16.74
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	7	16.72
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	3	16.71
(1,93)	1:16:B:C:H1'	1:2:A:A:H2'	5	16.71
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	13	16.67
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	4	16.66
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	18	16.66
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	11	16.65
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	15	16.65
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	16	16.64
(1,183)	1:16:B:C:H5	1:3:A:C:H42	20	16.63
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	12	16.63
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	5	16.62
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	19	16.61
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	19	16.61
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	16	16.6
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	20	16.58
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	10	16.57
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	9	16.57
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	11	16.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	3	16.53
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	2	16.52
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	5	16.5
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	14	16.48
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	20	16.47
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	14	16.47
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	10	16.46
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	9	16.44
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	18	16.44
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	17	16.44
(1,166)	1:1:A:G:H5'	1:20:B:A:H8	17	16.42
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	15	16.42
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	16	16.41
(1,183)	1:16:B:C:H5	1:3:A:C:H42	10	16.39
(1,166)	1:1:A:G:H5'	1:20:B:A:H8	6	16.38
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	5	16.38
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	12	16.38
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	8	16.37
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	6	16.37
(1,95)	1:16:B:C:H1'	1:3:A:C:H4'	20	16.37
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	2	16.35
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	20	16.35
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	14	16.34
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	20	16.34
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	12	16.34
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	9	16.34
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	17	16.34
(1,99)	1:17:B:A:H1'	1:3:A:C:H2'	4	16.33
(1,183)	1:16:B:C:H5	1:3:A:C:H42	9	16.32
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	9	16.32
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	10	16.3
(1,166)	1:1:A:G:H5'	1:20:B:A:H8	16	16.29
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	9	16.28
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	3	16.27
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	19	16.27
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	11	16.26
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	7	16.25
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	1	16.24
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	17	16.24
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	17	16.24
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	15	16.24
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	3	16.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	11	16.23
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	18	16.23
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	18	16.23
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	13	16.23
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	9	16.22
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	9	16.22
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	18	16.22
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	10	16.21
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	16	16.21
(1,97)	1:16:B:C:H6	1:2:A:A:H1'	5	16.21
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	2	16.19
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	2	16.19
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	16	16.19
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	14	16.18
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	7	16.18
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	5	16.17
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	19	16.17
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	18	16.16
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	11	16.15
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	11	16.14
(1,183)	1:16:B:C:H5	1:3:A:C:H42	12	16.13
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	3	16.13
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	12	16.13
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	9	16.11
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	4	16.09
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	6	16.09
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	17	16.08
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	7	16.05
(1,168)	1:1:A:G:H4'	1:20:B:A:H8	5	16.04
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	19	16.04
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	19	16.04
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	20	16.02
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	20	16.0
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	6	15.98
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	15	15.97
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	15	15.97
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	16	15.95
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	16	15.95
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	18	15.94
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	10	15.94
(1,166)	1:1:A:G:H5'	1:20:B:A:H8	10	15.93
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	18	15.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	3	15.89
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	14	15.89
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	19	15.88
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	3	15.88
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	3	15.87
(1,137)	1:23:B:U:H1'	1:9:A:C:H2'	6	15.85
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	5	15.85
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	10	15.85
(1,98)	1:16:B:C:H6	1:3:A:C:H1'	10	15.83
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	6	15.81
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	20	15.81
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	12	15.78
(1,169)	1:1:A:G:H4'	1:21:B:G:H1'	14	15.76
(1,166)	1:1:A:G:H5'	1:20:B:A:H8	1	15.76
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	19	15.75
(1,183)	1:16:B:C:H5	1:3:A:C:H42	5	15.74
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	10	15.73
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	17	15.7
(1,101)	1:17:B:A:H1'	1:4:A:A:H3'	4	15.7
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	14	15.65
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	20	15.64
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	12	15.62
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	12	15.62
(1,111)	1:18:B:G:H8	1:4:A:A:H1'	4	15.62
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	16	15.59
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	6	15.57
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	4	15.56
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	13	15.52
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	13	15.52
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	5	15.42
(1,176)	1:18:B:G:H1	1:5:A:G:H22	5	15.41
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	10	15.37
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	16	15.37
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	12	15.35
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	10	15.33
(1,112)	1:18:B:G:H8	1:5:A:G:H1'	4	15.32
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	5	15.32
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	2	15.3
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	15	15.29
(1,166)	1:1:A:G:H5'	1:20:B:A:H8	20	15.27
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	4	15.25
(1,107)	1:17:B:A:H8	1:3:A:C:H1'	20	15.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	20	15.17
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	10	15.08
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	5	15.08
(1,176)	1:18:B:G:H1	1:5:A:G:H22	12	15.07
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	16	15.07
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	16	15.07
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	8	15.03
(1,191)	1:17:B:A:N7	1:4:A:A:H62	13	15.02
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	17	15.02
(1,191)	1:17:B:A:N7	1:4:A:A:H62	15	15.01
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	12	15.01
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	17	14.99
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	17	14.99
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	1	14.97
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	11	14.97
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	1	14.97
(1,176)	1:18:B:G:H1	1:5:A:G:H22	11	14.96
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	6	14.96
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	6	14.96
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	12	14.94
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	16	14.94
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	7	14.92
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	7	14.92
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	19	14.91
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	4	14.9
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	14	14.9
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	11	14.87
(1,191)	1:17:B:A:N7	1:4:A:A:H62	1	14.85
(1,108)	1:17:B:A:H8	1:4:A:A:H1'	4	14.85
(1,176)	1:18:B:G:H1	1:5:A:G:H22	15	14.84
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	20	14.84
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	7	14.8
(1,96)	1:16:B:C:H5	1:2:A:A:H2'	5	14.8
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	18	14.79
(1,176)	1:18:B:G:H1	1:5:A:G:H22	1	14.78
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	10	14.78
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	7	14.77
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	10	14.76
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	10	14.76
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	19	14.76
(1,176)	1:18:B:G:H1	1:5:A:G:H22	8	14.75
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	4	14.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	17	14.75
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	18	14.73
(1,191)	1:17:B:A:N7	1:4:A:A:H62	8	14.71
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	9	14.71
(1,166)	1:1:A:G:H5'	1:20:B:A:H8	8	14.7
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	8	14.7
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	1	14.69
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	1	14.69
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	9	14.68
(1,176)	1:18:B:G:H1	1:5:A:G:H22	13	14.64
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	7	14.63
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	2	14.63
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	20	14.61
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	20	14.61
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	16	14.61
(1,176)	1:18:B:G:H1	1:5:A:G:H22	20	14.59
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	5	14.59
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	5	14.59
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	11	14.59
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	3	14.56
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	5	14.56
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	13	14.53
(1,132)	1:22:B:C:H1'	1:9:A:C:H2'	6	14.49
(1,166)	1:1:A:G:H5'	1:20:B:A:H8	14	14.47
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	14	14.47
(1,191)	1:17:B:A:N7	1:4:A:A:H62	2	14.46
(1,176)	1:18:B:G:H1	1:5:A:G:H22	14	14.45
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	5	14.45
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	12	14.44
(1,191)	1:17:B:A:N7	1:4:A:A:H62	3	14.43
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	2	14.42
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	7	14.41
(1,176)	1:18:B:G:H1	1:5:A:G:H22	17	14.39
(1,176)	1:18:B:G:H1	1:5:A:G:H22	7	14.38
(1,176)	1:18:B:G:H1	1:5:A:G:H22	9	14.37
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	5	14.36
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	5	14.36
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	8	14.34
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	16	14.34
(1,176)	1:18:B:G:H1	1:5:A:G:H22	18	14.32
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	11	14.32
(1,176)	1:18:B:G:H1	1:5:A:G:H22	10	14.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	1	14.31
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	1	14.29
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	11	14.29
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	13	14.26
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	2	14.24
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	12	14.24
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	15	14.21
(1,176)	1:18:B:G:H1	1:5:A:G:H22	19	14.2
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	9	14.19
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	15	14.19
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	8	14.19
(1,191)	1:17:B:A:N7	1:4:A:A:H62	18	14.18
(1,176)	1:18:B:G:H1	1:5:A:G:H22	2	14.16
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	12	14.16
(1,191)	1:17:B:A:N7	1:4:A:A:H62	19	14.15
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	9	14.15
(1,191)	1:17:B:A:N7	1:4:A:A:H62	11	14.14
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	14	14.14
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	4	14.1
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	4	14.1
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	2	14.1
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	3	14.09
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	7	14.09
(1,191)	1:17:B:A:N7	1:4:A:A:H62	6	14.07
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	12	14.07
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	17	14.07
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	13	14.07
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	16	14.06
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	15	14.05
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	20	14.04
(1,176)	1:18:B:G:H1	1:5:A:G:H22	4	14.03
(1,191)	1:17:B:A:N7	1:4:A:A:H62	17	14.02
(1,191)	1:17:B:A:N7	1:4:A:A:H62	9	14.0
(1,176)	1:18:B:G:H1	1:5:A:G:H22	6	14.0
(1,176)	1:18:B:G:H1	1:5:A:G:H22	16	13.99
(1,166)	1:1:A:G:H5''	1:20:B:A:H8	5	13.99
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	20	13.99
(1,191)	1:17:B:A:N7	1:4:A:A:H62	7	13.98
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	8	13.98
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	20	13.97
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	4	13.96
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	1	13.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	15	13.94
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	17	13.94
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	14	13.92
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	10	13.92
(1,191)	1:17:B:A:N7	1:4:A:A:H62	5	13.89
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	6	13.89
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	17	13.87
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	16	13.86
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	10	13.86
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	5	13.85
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	11	13.84
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	11	13.84
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	19	13.84
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	2	13.83
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	2	13.83
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	4	13.82
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	18	13.82
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	14	13.82
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	13	13.79
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	4	13.78
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	11	13.78
(1,191)	1:17:B:A:N7	1:4:A:A:H62	14	13.75
(1,136)	1:22:B:C:H6	1:10:A:U:H5	15	13.75
(1,191)	1:17:B:A:N7	1:4:A:A:H62	20	13.74
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	20	13.74
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	19	13.74
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	19	13.74
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	10	13.73
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	18	13.71
(1,191)	1:17:B:A:N7	1:4:A:A:H62	12	13.7
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	8	13.7
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	8	13.7
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	1	13.7
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	17	13.7
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	18	13.7
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	18	13.7
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	9	13.69
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	7	13.68
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	16	13.66
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	12	13.64
(1,136)	1:22:B:C:H6	1:10:A:U:H5	3	13.64
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	7	13.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	7	13.62
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	10	13.62
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	14	13.62
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	1	13.61
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	8	13.61
(1,176)	1:18:B:G:H1	1:5:A:G:H22	3	13.6
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	4	13.58
(1,136)	1:22:B:C:H6	1:10:A:U:H5	2	13.58
(1,191)	1:17:B:A:N7	1:4:A:A:H62	4	13.57
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	17	13.57
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	11	13.57
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	14	13.56
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	20	13.55
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	10	13.55
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	9	13.53
(1,191)	1:17:B:A:N7	1:4:A:A:H62	10	13.52
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	8	13.5
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	11	13.48
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	15	13.48
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	4	13.47
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	3	13.47
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	15	13.44
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	19	13.44
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	2	13.41
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	19	13.41
(1,191)	1:17:B:A:N7	1:4:A:A:H62	16	13.37
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	13	13.37
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	3	13.36
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	3	13.36
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	3	13.36
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	13	13.35
(1,167)	1:1:A:G:H5'	1:21:B:G:H1'	14	13.32
(1,167)	1:1:A:G:H5''	1:21:B:G:H1'	14	13.32
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	2	13.32
(1,136)	1:22:B:C:H6	1:10:A:U:H5	8	13.31
(1,136)	1:22:B:C:H6	1:10:A:U:H5	18	13.31
(1,136)	1:22:B:C:H6	1:10:A:U:H5	19	13.31
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	9	13.31
(1,136)	1:22:B:C:H6	1:10:A:U:H5	12	13.3
(1,117)	1:19:B:C:H6	1:5:A:G:H1'	6	13.29
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	3	13.28
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	18	13.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:22:B:C:H6	1:10:A:U:H5	1	13.27
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	16	13.27
(1,136)	1:22:B:C:H6	1:10:A:U:H5	11	13.26
(1,113)	1:19:B:C:H1'	1:5:A:G:H2'	6	13.26
(1,136)	1:22:B:C:H6	1:10:A:U:H5	4	13.18
(1,136)	1:22:B:C:H6	1:10:A:U:H5	20	13.17
(1,141)	1:23:B:U:H6	1:9:A:C:H1'	6	13.16
(1,115)	1:19:B:C:H1'	1:6:A:C:H3'	3	13.15
(1,136)	1:22:B:C:H6	1:10:A:U:H5	5	13.12
(1,136)	1:22:B:C:H6	1:10:A:U:H5	6	13.12
(1,136)	1:22:B:C:H6	1:10:A:U:H5	17	13.12
(1,136)	1:22:B:C:H6	1:10:A:U:H5	14	13.09
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	2	13.08
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	6	13.05
(1,136)	1:22:B:C:H6	1:10:A:U:H5	13	13.04
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	13	13.02
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	6	12.89
(1,136)	1:22:B:C:H6	1:10:A:U:H5	7	12.88
(1,136)	1:22:B:C:H6	1:10:A:U:H5	10	12.81
(1,136)	1:22:B:C:H6	1:10:A:U:H5	16	12.8
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	16	12.77
(1,136)	1:22:B:C:H6	1:10:A:U:H5	9	12.76
(1,118)	1:19:B:C:H6	1:6:A:C:H1'	3	12.34
(1,114)	1:19:B:C:H1'	1:6:A:C:H2'	3	12.28
(1,185)	1:22:B:C:H5	1:9:A:C:H42	15	12.15
(1,185)	1:22:B:C:H5	1:9:A:C:H42	2	11.96
(1,185)	1:22:B:C:H5	1:9:A:C:H42	3	11.96
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	15	11.93
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	15	11.88
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	12	11.68
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	14	11.68
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	4	11.63
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	8	11.63
(1,185)	1:22:B:C:H5	1:9:A:C:H42	8	11.62
(1,185)	1:22:B:C:H5	1:9:A:C:H42	13	11.62
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	2	11.61
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	20	11.59
(1,185)	1:22:B:C:H5	1:9:A:C:H42	11	11.58
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	16	11.57
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	8	11.56
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	2	11.55
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	19	11.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	5	11.55
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	5	11.51
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	3	11.51
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	7	11.49
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	9	11.48
(1,185)	1:22:B:C:H5	1:9:A:C:H42	6	11.47
(1,185)	1:22:B:C:H5	1:9:A:C:H42	14	11.47
(1,185)	1:22:B:C:H5	1:9:A:C:H42	18	11.47
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	11	11.46
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	17	11.46
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	16	11.46
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	19	11.45
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	14	11.44
(1,185)	1:22:B:C:H5	1:9:A:C:H42	19	11.42
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	3	11.41
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	10	11.38
(1,185)	1:22:B:C:H5	1:9:A:C:H42	17	11.36
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	17	11.35
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	1	11.34
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	4	11.34
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	11	11.32
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	12	11.31
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	1	11.3
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	13	11.29
(1,185)	1:22:B:C:H5	1:9:A:C:H42	4	11.28
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	12	11.28
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	20	11.27
(1,185)	1:22:B:C:H5	1:9:A:C:H42	1	11.25
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	9	11.25
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	11	11.25
(1,185)	1:22:B:C:H5	1:9:A:C:H42	7	11.23
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	7	11.23
(1,185)	1:22:B:C:H5	1:9:A:C:H42	20	11.21
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	18	11.21
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	7	11.2
(1,185)	1:22:B:C:H5	1:9:A:C:H42	16	11.19
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	5	11.18
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	8	11.16
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	6	11.14
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	6	11.13
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	18	11.12
(1,135)	1:22:B:C:H6	1:9:A:C:H1'	13	11.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	1	11.07
(1,185)	1:22:B:C:H5	1:9:A:C:H42	12	11.03
(1,185)	1:22:B:C:H5	1:9:A:C:H42	10	11.01
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	20	10.99
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	14	10.96
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	13	10.95
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	2	10.93
(1,134)	1:22:B:C:H5	1:9:A:C:H2'	10	10.9
(1,185)	1:22:B:C:H5	1:9:A:C:H42	9	10.83
(1,185)	1:22:B:C:H5	1:9:A:C:H42	5	10.8
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	17	10.79
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	4	10.77
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	6	10.71
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	15	10.71
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	9	10.7
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	18	10.69
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	13	10.67
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	19	10.65
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	4	10.63
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	10	10.57
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	7	10.53
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	16	10.39
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	11	10.36
(1,126)	1:20:B:A:H8	1:6:A:C:H6	5	10.34
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	1	10.32
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	5	10.3
(1,126)	1:20:B:A:H8	1:6:A:C:H6	4	10.26
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	8	10.26
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	10	10.25
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	2	10.24
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	14	10.21
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	17	10.21
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	3	10.16
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	16	10.13
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	18	10.11
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	20	10.1
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	4	10.1
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	5	10.09
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	19	10.08
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	7	10.02
(1,126)	1:20:B:A:H8	1:6:A:C:H6	11	9.99
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	4	9.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	9	9.98
(1,126)	1:20:B:A:H8	1:6:A:C:H6	7	9.97
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	12	9.96
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	7	9.95
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	3	9.94
(1,126)	1:20:B:A:H8	1:6:A:C:H6	10	9.93
(1,116)	1:19:B:C:H5	1:5:A:G:H2'	6	9.92
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	1	9.91
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	13	9.9
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	10	9.89
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	18	9.89
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	2	9.88
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	11	9.88
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	1	9.85
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	5	9.85
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	6	9.85
(1,126)	1:20:B:A:H8	1:6:A:C:H6	1	9.84
(1,121)	1:20:B:A:H1'	1:7:A:A:H3'	15	9.83
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	3	9.82
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	16	9.81
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	4	9.8
(1,126)	1:20:B:A:H8	1:6:A:C:H6	12	9.78
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	9	9.78
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	10	9.77
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	16	9.77
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	19	9.77
(1,126)	1:20:B:A:H8	1:6:A:C:H6	16	9.76
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	5	9.76
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	12	9.76
(1,126)	1:20:B:A:H8	1:6:A:C:H6	14	9.75
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	11	9.75
(1,126)	1:20:B:A:H8	1:6:A:C:H6	9	9.73
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	14	9.73
(1,126)	1:20:B:A:H8	1:6:A:C:H6	3	9.72
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	17	9.72
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	17	9.72
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	9	9.71
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	8	9.7
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	20	9.7
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	10	9.69
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	18	9.68
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	19	9.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	20	9.66
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	2	9.62
(1,126)	1:20:B:A:H8	1:6:A:C:H6	2	9.61
(1,126)	1:20:B:A:H8	1:6:A:C:H6	8	9.61
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	12	9.59
(1,126)	1:20:B:A:H8	1:6:A:C:H6	17	9.58
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	12	9.57
(1,120)	1:20:B:A:H1'	1:7:A:A:H2'	15	9.57
(1,126)	1:20:B:A:H8	1:6:A:C:H6	19	9.56
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	6	9.56
(1,126)	1:20:B:A:H8	1:6:A:C:H6	18	9.51
(1,126)	1:20:B:A:H8	1:6:A:C:H6	20	9.51
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	7	9.5
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	14	9.48
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	14	9.47
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	8	9.46
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	11	9.4
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	13	9.39
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	19	9.38
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	17	9.38
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	1	9.36
(1,126)	1:20:B:A:H8	1:6:A:C:H6	13	9.35
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	18	9.33
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	9	9.28
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	20	9.27
(1,126)	1:20:B:A:H8	1:6:A:C:H6	6	9.25
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	16	9.24
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	9	9.23
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	20	9.22
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	19	9.21
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	15	9.19
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	1	9.18
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	16	9.17
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	17	9.17
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	18	9.16
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	10	9.15
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	3	9.15
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	2	9.14
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	8	9.14
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	12	9.13
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	11	9.11
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	4	9.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	5	9.1
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	7	9.08
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	3	9.08
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	6	9.06
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	6	9.05
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	14	9.03
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	8	9.0
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	2	8.96
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	13	8.93
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	13	8.91
(1,125)	1:20:B:A:H8	1:7:A:A:H1'	3	8.89
(1,124)	1:20:B:A:H8	1:6:A:C:H1'	15	8.84
(1,126)	1:20:B:A:H8	1:6:A:C:H6	15	8.8
(1,119)	1:20:B:A:H1'	1:6:A:C:H2'	15	8.64
(1,184)	1:19:B:C:H5	1:6:A:C:H42	5	8.59
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	16	8.59
(1,177)	1:21:B:G:H1	1:8:A:G:H22	5	8.52
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	2	8.48
(1,177)	1:21:B:G:H1	1:8:A:G:H22	15	8.44
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	15	8.43
(1,177)	1:21:B:G:H1	1:8:A:G:H22	12	8.39
(1,184)	1:19:B:C:H5	1:6:A:C:H42	1	8.37
(1,184)	1:19:B:C:H5	1:6:A:C:H42	12	8.34
(1,177)	1:21:B:G:H1	1:8:A:G:H22	17	8.31
(1,184)	1:19:B:C:H5	1:6:A:C:H42	11	8.27
(1,177)	1:21:B:G:H1	1:8:A:G:H22	10	8.23
(1,177)	1:21:B:G:H1	1:8:A:G:H22	18	8.23
(1,177)	1:21:B:G:H1	1:8:A:G:H22	1	8.22
(1,177)	1:21:B:G:H1	1:8:A:G:H22	20	8.22
(1,177)	1:21:B:G:H1	1:8:A:G:H22	9	8.2
(1,177)	1:21:B:G:H1	1:8:A:G:H22	11	8.18
(1,184)	1:19:B:C:H5	1:6:A:C:H42	13	8.17
(1,184)	1:19:B:C:H5	1:6:A:C:H42	8	8.16
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	3	8.16
(1,177)	1:21:B:G:H1	1:8:A:G:H22	19	8.15
(1,177)	1:21:B:G:H1	1:8:A:G:H22	16	8.14
(1,184)	1:19:B:C:H5	1:6:A:C:H42	7	8.12
(1,184)	1:19:B:C:H5	1:6:A:C:H42	20	8.09
(1,177)	1:21:B:G:H1	1:8:A:G:H22	8	8.09
(1,184)	1:19:B:C:H5	1:6:A:C:H42	14	8.08
(1,177)	1:21:B:G:H1	1:8:A:G:H22	4	8.03
(1,177)	1:21:B:G:H1	1:8:A:G:H22	14	8.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	8	8.0
(1,177)	1:21:B:G:H1	1:8:A:G:H22	2	7.98
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	11	7.98
(1,177)	1:21:B:G:H1	1:8:A:G:H22	13	7.96
(1,184)	1:19:B:C:H5	1:6:A:C:H42	2	7.95
(1,184)	1:19:B:C:H5	1:6:A:C:H42	17	7.95
(1,184)	1:19:B:C:H5	1:6:A:C:H42	4	7.94
(1,177)	1:21:B:G:H1	1:8:A:G:H22	7	7.94
(1,131)	1:21:B:G:H8	1:9:A:C:H5	3	7.93
(1,184)	1:19:B:C:H5	1:6:A:C:H42	15	7.92
(1,184)	1:19:B:C:H5	1:6:A:C:H42	18	7.91
(1,177)	1:21:B:G:H1	1:8:A:G:H22	3	7.9
(1,184)	1:19:B:C:H5	1:6:A:C:H42	19	7.89
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	14	7.87
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	7	7.85
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	6	7.84
(1,184)	1:19:B:C:H5	1:6:A:C:H42	9	7.79
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	9	7.77
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	19	7.75
(1,184)	1:19:B:C:H5	1:6:A:C:H42	10	7.74
(1,177)	1:21:B:G:H1	1:8:A:G:H22	6	7.71
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	20	7.7
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	13	7.65
(1,131)	1:21:B:G:H8	1:9:A:C:H5	15	7.65
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	4	7.63
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	1	7.56
(1,131)	1:21:B:G:H8	1:9:A:C:H5	2	7.54
(1,184)	1:19:B:C:H5	1:6:A:C:H42	16	7.52
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	17	7.49
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	5	7.46
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	10	7.45
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	12	7.36
(1,133)	1:22:B:C:H5	1:8:A:G:H2'	18	7.32
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	15	7.24
(1,184)	1:19:B:C:H5	1:6:A:C:H42	3	7.16
(1,131)	1:21:B:G:H8	1:9:A:C:H5	14	7.1
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	2	7.06
(1,184)	1:19:B:C:H5	1:6:A:C:H42	6	7.04
(1,131)	1:21:B:G:H8	1:9:A:C:H5	8	7.03
(1,131)	1:21:B:G:H8	1:9:A:C:H5	16	7.03
(1,131)	1:21:B:G:H8	1:9:A:C:H5	6	6.99
(1,131)	1:21:B:G:H8	1:9:A:C:H5	13	6.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	16	6.88
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	15	6.85
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	8	6.78
(1,131)	1:21:B:G:H8	1:9:A:C:H5	7	6.75
(1,131)	1:21:B:G:H8	1:9:A:C:H5	19	6.74
(1,131)	1:21:B:G:H8	1:9:A:C:H5	18	6.68
(1,131)	1:21:B:G:H8	1:9:A:C:H5	11	6.62
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	14	6.62
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	6	6.59
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	7	6.59
(1,131)	1:21:B:G:H8	1:9:A:C:H5	1	6.57
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	11	6.56
(1,131)	1:21:B:G:H8	1:9:A:C:H5	17	6.51
(1,131)	1:21:B:G:H8	1:9:A:C:H5	20	6.48
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	1	6.46
(1,131)	1:21:B:G:H8	1:9:A:C:H5	4	6.44
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	20	6.38
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	3	6.36
(1,131)	1:21:B:G:H8	1:9:A:C:H5	12	6.35
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	2	6.34
(1,131)	1:21:B:G:H8	1:9:A:C:H5	9	6.32
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	5	6.3
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	12	6.3
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	9	6.25
(1,131)	1:21:B:G:H8	1:9:A:C:H5	10	6.23
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	10	6.23
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	19	6.22
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	20	6.22
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	13	6.2
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	8	6.18
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	19	6.17
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	14	6.16
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	17	6.13
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	4	6.11
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	13	6.07
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	9	6.05
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	17	6.03
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	6	5.99
(1,131)	1:21:B:G:H8	1:9:A:C:H5	5	5.97
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	16	5.87
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	11	5.83
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	18	5.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	12	5.77
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	15	5.64
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	10	5.64
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	1	5.61
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	2	5.58
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	7	5.56
(1,128)	1:21:B:G:H1'	1:8:A:G:H2'	18	5.51
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	16	5.42
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	5	5.41
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	3	5.34
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	3	5.28
(1,129)	1:21:B:G:H8	1:7:A:A:H1'	4	5.14
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	14	5.09
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	8	4.97
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	13	4.97
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	11	4.96
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	6	4.75
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	20	4.75
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	9	4.74
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	19	4.74
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	7	4.59
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	1	4.58
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	3	4.58
(1,127)	1:20:B:A:H8	1:8:A:G:H8	3	4.53
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	18	4.45
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	19	4.43
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	17	4.4
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	17	4.38
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	20	4.37
(1,127)	1:20:B:A:H8	1:8:A:G:H8	4	4.36
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	9	4.36
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	10	4.33
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	4	4.29
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	12	4.26
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	1	4.26
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	2	4.26
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	10	4.25
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	12	4.25
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	14	4.25
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	15	4.24
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	16	4.24
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	5	4.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:20:B:A:H8	1:8:A:G:H8	16	4.22
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	11	4.21
(1,127)	1:20:B:A:H8	1:8:A:G:H8	2	4.2
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	13	4.15
(1,127)	1:20:B:A:H8	1:8:A:G:H8	14	4.14
(1,127)	1:20:B:A:H8	1:8:A:G:H8	11	4.13
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	8	4.12
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	7	4.11
(1,130)	1:21:B:G:H8	1:8:A:G:H1'	18	4.09
(1,127)	1:20:B:A:H8	1:8:A:G:H8	7	4.09
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	6	4.05
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	4	4.04
(1,127)	1:20:B:A:H8	1:8:A:G:H8	6	4.02
(1,127)	1:20:B:A:H8	1:8:A:G:H8	10	3.98
(1,122)	1:20:B:A:H2	1:7:A:A:H1'	5	3.94
(1,127)	1:20:B:A:H8	1:8:A:G:H8	1	3.93
(1,127)	1:20:B:A:H8	1:8:A:G:H8	13	3.92
(1,127)	1:20:B:A:H8	1:8:A:G:H8	5	3.89
(1,127)	1:20:B:A:H8	1:8:A:G:H8	8	3.81
(1,127)	1:20:B:A:H8	1:8:A:G:H8	18	3.75
(1,127)	1:20:B:A:H8	1:8:A:G:H8	9	3.71
(1,127)	1:20:B:A:H8	1:8:A:G:H8	17	3.7
(1,127)	1:20:B:A:H8	1:8:A:G:H8	19	3.7
(1,127)	1:20:B:A:H8	1:8:A:G:H8	20	3.6
(1,127)	1:20:B:A:H8	1:8:A:G:H8	12	3.57
(1,192)	1:20:B:A:N7	1:7:A:A:H62	10	3.55
(1,192)	1:20:B:A:N7	1:7:A:A:H62	17	3.46
(1,192)	1:20:B:A:N7	1:7:A:A:H62	19	3.46
(1,192)	1:20:B:A:N7	1:7:A:A:H62	5	3.44
(1,192)	1:20:B:A:N7	1:7:A:A:H62	14	3.41
(1,127)	1:20:B:A:H8	1:8:A:G:H8	15	3.38
(1,192)	1:20:B:A:N7	1:7:A:A:H62	12	3.37
(1,192)	1:20:B:A:N7	1:7:A:A:H62	15	3.37
(1,192)	1:20:B:A:N7	1:7:A:A:H62	20	3.37
(1,192)	1:20:B:A:N7	1:7:A:A:H62	6	3.35
(1,192)	1:20:B:A:N7	1:7:A:A:H62	9	3.32
(1,192)	1:20:B:A:N7	1:7:A:A:H62	11	3.32
(1,192)	1:20:B:A:N7	1:7:A:A:H62	8	3.3
(1,192)	1:20:B:A:N7	1:7:A:A:H62	18	3.3
(1,192)	1:20:B:A:N7	1:7:A:A:H62	1	3.23
(1,192)	1:20:B:A:N7	1:7:A:A:H62	2	3.19
(1,192)	1:20:B:A:N7	1:7:A:A:H62	7	3.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:20:B:A:N7	1:7:A:A:H62	4	3.09
(1,192)	1:20:B:A:N7	1:7:A:A:H62	13	3.05
(1,192)	1:20:B:A:N7	1:7:A:A:H62	16	3.02
(1,192)	1:20:B:A:N7	1:7:A:A:H62	3	2.83
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	14	2.81
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	16	2.81
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	2	2.8
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	3	2.77
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	11	2.72
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	4	2.69
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	10	2.57
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	13	2.56
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	1	2.54
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	7	2.52
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	8	2.48
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	6	2.42
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	15	2.41
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	9	2.4
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	5	2.37
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	19	2.33
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	20	2.33
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	17	2.29
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	18	2.25
(1,123)	1:20:B:A:H2	1:8:A:G:H1'	12	2.22

10 Dihedral-angle violation analysis [i](#)

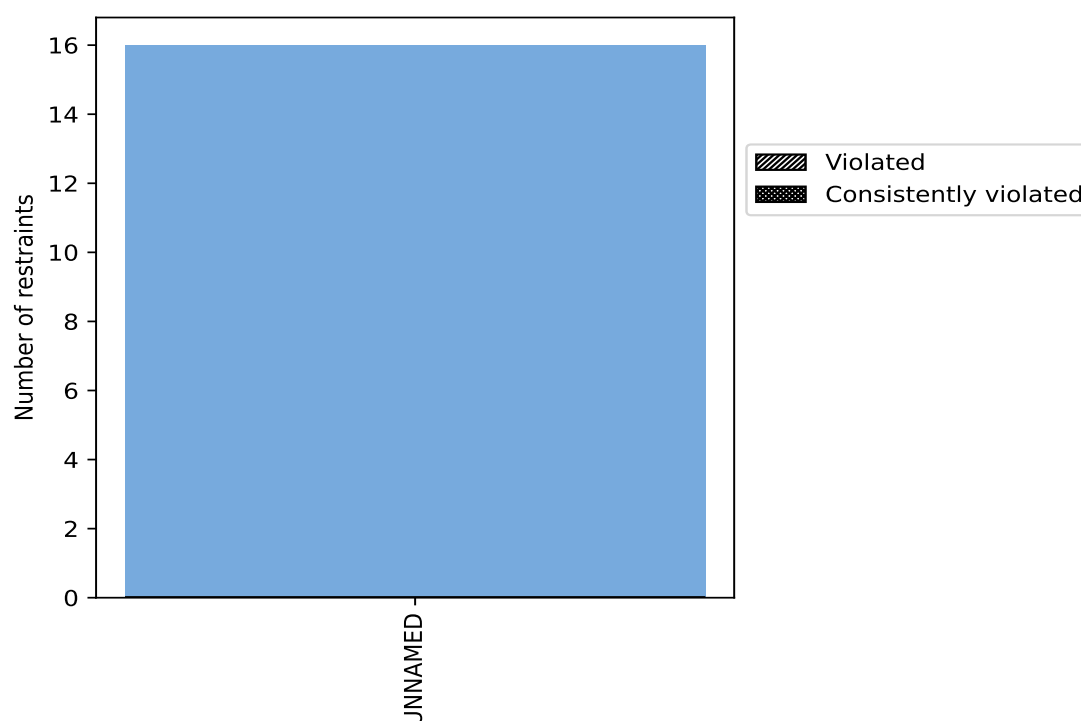
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
UNNAMED	16	100.0	0	0.0	0.0	0	0.0	0.0
Total	16	100.0	0	0.0	0.0	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



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

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

No violations found

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

No violations found

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

No violations found

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

No violations found