



Full wwPDB NMR Structure Validation Report ⓘ

Nov 30, 2023 – 03:27 pm GMT

PDB ID : 8Q7J
BMRB ID : 34846
Title : Conformations of macrocyclic peptides sampled by exact NOEs: models for cell-permeability
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Deposited on : 2023-08-16

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

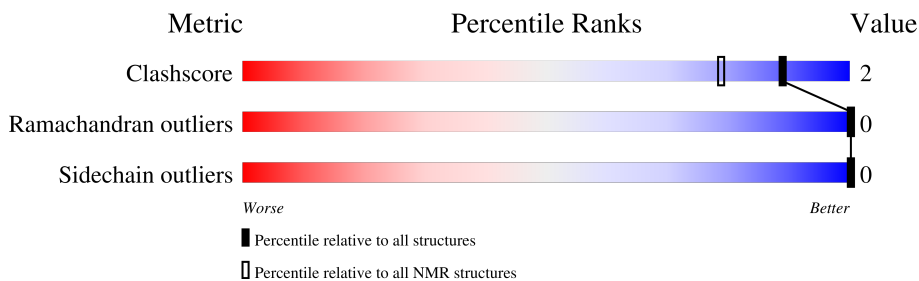
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 58%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	Z	11	

2 Ensemble composition and analysis

This entry contains 20 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (2) was below the domain threshold value (8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 196 atoms, of which 111 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYCLOSPORIN A.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	Z	11	196	62	111	11	12	0

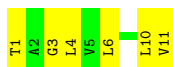
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: CYCLOSPORIN A

Chain Z: 



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: CYCLOSPORIN A

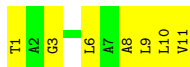
Chain Z: 



4.2.2 Score per residue for model 2

- Molecule 1: CYCLOSPORIN A

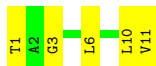
Chain Z: 



4.2.3 Score per residue for model 3

- Molecule 1: CYCLOSPORIN A

Chain Z:  55% 45%



4.2.4 Score per residue for model 4

- Molecule 1: CYCLOSPORIN A

Chain Z:  55% 45%



4.2.5 Score per residue for model 5

- Molecule 1: CYCLOSPORIN A

Chain Z:  55% 45%



4.2.6 Score per residue for model 6

- Molecule 1: CYCLOSPORIN A

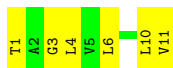
Chain Z:  55% 45%



4.2.7 Score per residue for model 7

- Molecule 1: CYCLOSPORIN A

Chain Z:  45% 55%



4.2.8 Score per residue for model 8

- Molecule 1: CYCLOSPORIN A

Chain Z:  55% 45%



4.2.9 Score per residue for model 9

- Molecule 1: CYCLOSPORIN A

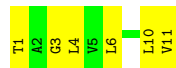
Chain Z:  55% 45%



4.2.10 Score per residue for model 10

- Molecule 1: CYCLOSPORIN A

Chain Z:  45% 55%



4.2.11 Score per residue for model 11

- Molecule 1: CYCLOSPORIN A

Chain Z:  55% 45%



4.2.12 Score per residue for model 12

- Molecule 1: CYCLOSPORIN A

Chain Z:  55% 45%



4.2.13 Score per residue for model 13

- Molecule 1: CYCLOSPORIN A

Chain Z:  55% 27% 18%



4.2.14 Score per residue for model 14

- Molecule 1: CYCLOSPORIN A

Chain Z:  55% 45%



4.2.15 Score per residue for model 15

- Molecule 1: CYCLOSPORIN A

Chain Z:  45% 45% 9%



4.2.16 Score per residue for model 16

- Molecule 1: CYCLOSPORIN A

Chain Z:  45% 45% 9%



4.2.17 Score per residue for model 17

- Molecule 1: CYCLOSPORIN A

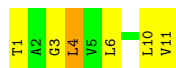
Chain Z:  27% 73%



4.2.18 Score per residue for model 18

- Molecule 1: CYCLOSPORIN A

Chain Z:  45% 45% 9%



4.2.19 Score per residue for model 19

- Molecule 1: CYCLOSPORIN A

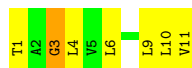
Chain Z:  55% 45%



4.2.20 Score per residue for model 20

- Molecule 1: CYCLOSPORIN A

Chain Z:  36% 55% 9%



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
CYANA	structure calculation	3.98.15
Amber	refinement	22

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	102
Number of shifts mapped to atoms	102
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	58%

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: BMT, SAR, ABA, MVA, MLE, DAL

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	Z	85	111	109	0±0
All	All	1700	2220	2180	7

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:Z:4:MLE:HG	1:Z:4:MLE:HN2	0.48	1.85	15	3
1:Z:3:SAR:N	1:Z:4:MLE:HN1	0.44	2.27	20	1
1:Z:10:MLE:HA	1:Z:11:MVA:HN1	0.41	1.77	13	1
1:Z:8:DAL:HA	1:Z:9:MLE:HN1	0.40	1.83	2	2

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	2/11 (18%)	1±0 (50±0%)	1±0 (50±0%)	0±0 (0±0%)	100	100
All	All	40/220 (18%)	20 (50%)	20 (50%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	1/1 (100%)	1±0 (100±0%)	0±0 (0±0%)	100	100
All	All	20/20 (100%)	20 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	ABA	Z	2	1	4,5,6	0.62±0.08	0±0 (0±0%)
1	MLE	Z	9	1	7,8,9	0.93±0.04	0±0 (0±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	SAR	Z	3	1	4,4,5	1.93±0.13	1±0 (25±0%)
1	MVA	Z	11	1	6,7,8	1.20±0.05	1±0 (16±0%)
1	BMT	Z	1	1	11,12,13	0.94±0.02	1±0 (9±0%)
1	MLE	Z	6	1	7,8,9	1.12±0.04	1±0 (13±3%)
1	MLE	Z	4	1	7,8,9	0.97±0.07	0±0 (3±6%)
1	MLE	Z	10	1	7,8,9	0.96±0.04	0±0 (0±3%)

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
1	ABA	Z	2	1	1,5,7	0.28±0.29	0±0 (0±0%)
1	MLE	Z	9	1	6,9,11	0.88±0.05	0±0 (0±0%)
1	SAR	Z	3	1	1,3,5	2.46±0.14	1±0 (95±21%)
1	MVA	Z	11	1	7,8,10	2.59±0.08	4±0 (57±0%)
1	BMT	Z	1	1	12,14,16	2.15±0.03	4±0 (34±2%)
1	MLE	Z	6	1	6,9,11	1.85±0.20	1±0 (19±7%)
1	MLE	Z	4	1	6,9,11	0.87±0.12	0±0 (0±3%)
1	MLE	Z	10	1	6,9,11	1.39±0.07	1±0 (17±3%)

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
1	SAR	Z	3	1	-	0±0,1,2,3	-
1	MLE	Z	9	1	-	0±0,5,8,10	-
1	BMT	Z	1	1	-	0±0,13,16,18	-
1	MLE	Z	4	1	-	0±0,5,8,10	-
1	MVA	Z	11	1	-	0±0,6,8,10	-
1	ABA	Z	2	1	-	0±0,3,4,6	-
1	MLE	Z	6	1	-	0±0,5,8,10	-
1	MLE	Z	10	1	-	0±0,5,8,10	-

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	Z	3	SAR	CA-N	4.28	1.51	1.46	20	20
1	Z	6	MLE	CA-N	2.66	1.52	1.47	5	19
1	Z	1	BMT	CA-N	2.63	1.52	1.47	15	20
1	Z	11	MVA	CA-N	2.51	1.51	1.47	8	20
1	Z	4	MLE	CA-N	2.19	1.51	1.47	18	5
1	Z	9	MLE	CA-N	2.11	1.51	1.47	20	1
1	Z	10	MLE	CA-N	2.11	1.51	1.47	1	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	Z	11	MVA	CB-CA-C	5.24	106.46	113.04	14	20
1	Z	1	BMT	CB-CA-N	4.18	119.72	111.41	5	20
1	Z	6	MLE	CG-CB-CA	4.01	125.34	115.34	1	18
1	Z	1	BMT	CD2-CG2-CB	3.91	118.00	110.39	6	20
1	Z	1	BMT	OG1-CB-CA	3.63	117.03	109.32	14	20
1	Z	1	BMT	C-CA-N	3.21	121.64	110.88	20	20
1	Z	10	MLE	CG-CB-CA	3.10	123.06	115.34	5	20
1	Z	11	MVA	C-CA-N	2.93	120.69	110.88	15	19
1	Z	11	MVA	CG2-CB-CA	2.87	115.60	111.21	7	20
1	Z	11	MVA	CB-CA-N	2.81	114.82	111.17	19	1
1	Z	3	SAR	O-C-CA	2.61	117.86	125.42	4	19
1	Z	11	MVA	O-C-CA	2.59	117.61	124.83	18	20
1	Z	1	BMT	OG1-CB-CG2	2.19	113.94	109.83	2	2
1	Z	6	MLE	O-C-CA	2.15	119.14	124.78	2	5
1	Z	10	MLE	O-C-CA	2.04	119.44	124.78	19	1
1	Z	4	MLE	CG-CB-CA	2.03	120.40	115.34	15	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 58% for the well-defined parts and 58% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	102
Number of shifts mapped to atoms	102
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 [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 58%, i.e. 14 atoms were assigned a chemical shift out of a possible 24. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	4/10 (40%)	4/4 (100%)	0/4 (0%)	0/2 (0%)
Sidechain	10/14 (71%)	10/10 (100%)	0/4 (0%)	0/0 (—%)
Overall	14/24 (58%)	14/14 (100%)	0/8 (0%)	0/2 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 58%, i.e. 14 atoms were assigned a chemical shift out of a possible 24. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	4/10 (40%)	4/4 (100%)	0/4 (0%)	0/2 (0%)
Sidechain	10/14 (71%)	10/10 (100%)	0/4 (0%)	0/0 (—%)
Overall	14/24 (58%)	14/14 (100%)	0/8 (0%)	0/2 (0%)

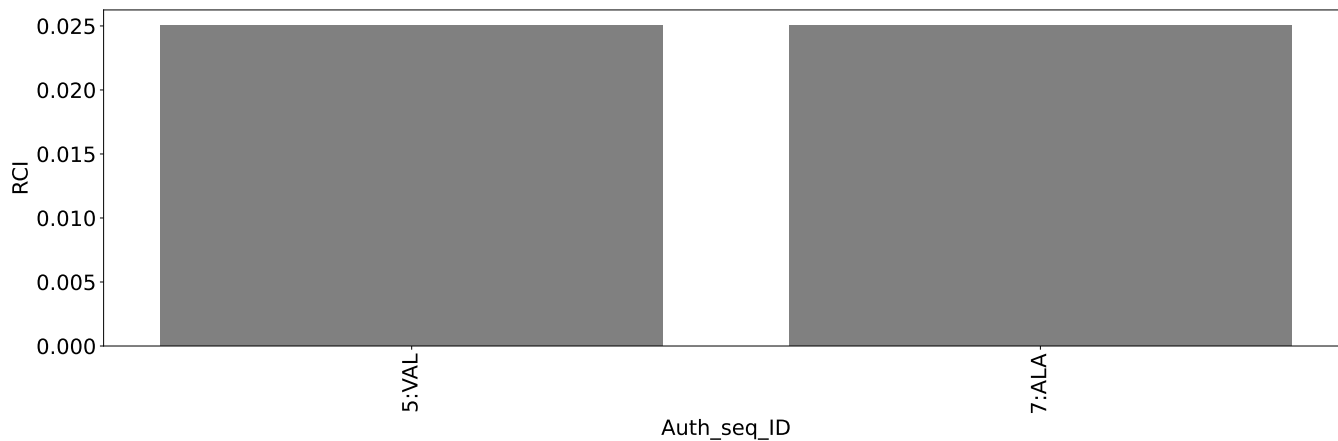
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain Z:



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	167
Intra-residue ($ i-j =0$)	81
Sequential ($ i-j =1$)	42
Medium range ($ i-j >1$ and $ i-j <5$)	18
Long range ($ i-j \geq 5$)	20
Inter-chain	0
Hydrogen bond restraints	6
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	15.2
Number of long range restraints per residue ¹	1.8

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)	17.8	0.2
0.2-0.5 (Medium)	7.8	0.44
>0.5 (Large)	3.0	0.99

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis

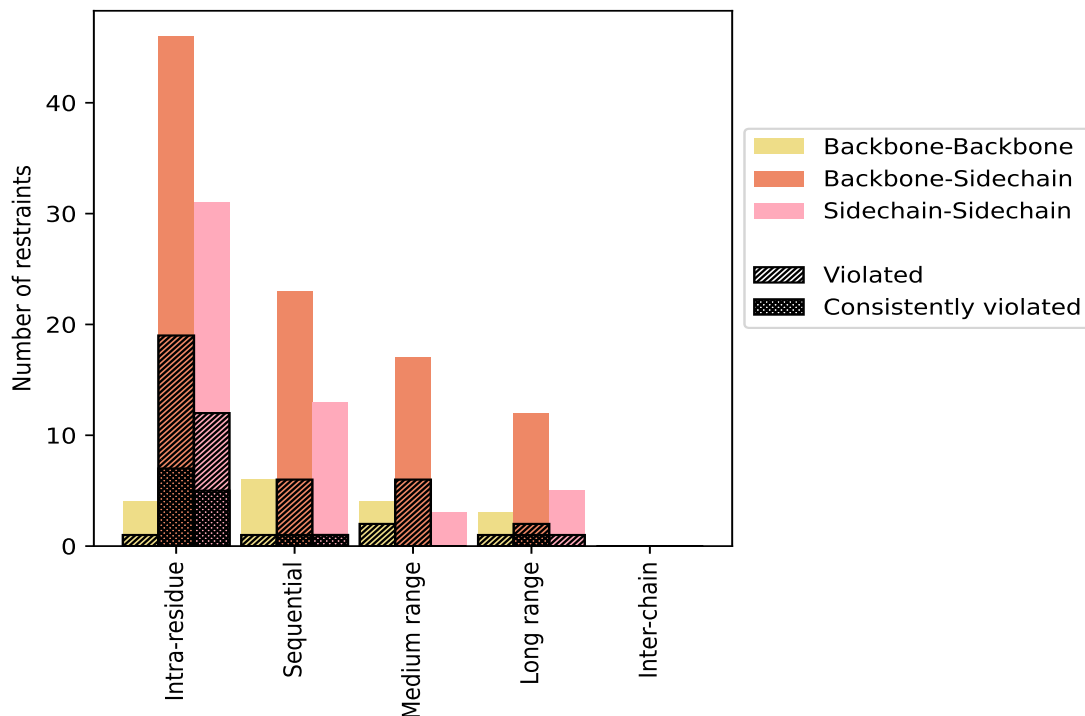
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	81	48.5	32	39.5	19.2	12	14.8	7.2
Backbone-Backbone	4	2.4	1	25.0	0.6	0	0.0	0.0
Backbone-Sidechain	46	27.5	19	41.3	11.4	7	15.2	4.2
Sidechain-Sidechain	31	18.6	12	38.7	7.2	5	16.1	3.0
Sequential ($i-j =1$)	42	25.1	8	19.0	4.8	2	4.8	1.2
Backbone-Backbone	6	3.6	1	16.7	0.6	0	0.0	0.0
Backbone-Sidechain	23	13.8	6	26.1	3.6	1	4.3	0.6
Sidechain-Sidechain	13	7.8	1	7.7	0.6	1	7.7	0.6
Medium range ($i-j >1$ & $i-j <5$)	18	10.8	6	33.3	3.6	0	0.0	0.0
Backbone-Backbone	4	2.4	2	50.0	1.2	0	0.0	0.0
Backbone-Sidechain	11	6.6	4	36.4	2.4	0	0.0	0.0
Sidechain-Sidechain	3	1.8	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	20	12.0	4	20.0	2.4	1	5.0	0.6
Backbone-Backbone	3	1.8	1	33.3	0.6	0	0.0	0.0
Backbone-Sidechain	12	7.2	2	16.7	1.2	1	8.3	0.6
Sidechain-Sidechain	5	3.0	1	20.0	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	6	3.6	2	33.3	1.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	167	100.0	52	31.1	31.1	15	9.0	9.0
Backbone-Backbone	17	10.2	5	29.4	3.0	0	0.0	0.0
Backbone-Sidechain	98	58.7	33	33.7	19.8	9	9.2	5.4
Sidechain-Sidechain	52	31.1	14	26.9	8.4	6	11.5	3.6

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 disulfid 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	20	3	4	2	0	29	0.25	0.98	0.21	0.19
2	20	4	4	3	0	31	0.25	0.94	0.2	0.18
3	20	3	5	2	0	30	0.25	0.98	0.21	0.17
4	20	3	5	2	0	30	0.25	0.98	0.2	0.18
5	22	3	4	2	0	31	0.24	0.94	0.2	0.19
6	20	3	5	3	0	31	0.25	0.98	0.2	0.17
7	20	3	3	3	0	29	0.25	0.98	0.21	0.17
8	19	3	4	3	0	29	0.25	0.98	0.21	0.16
9	20	3	4	2	0	29	0.25	0.98	0.21	0.17
10	21	3	3	2	0	29	0.25	0.98	0.21	0.17
11	21	3	5	3	0	32	0.23	0.98	0.2	0.16

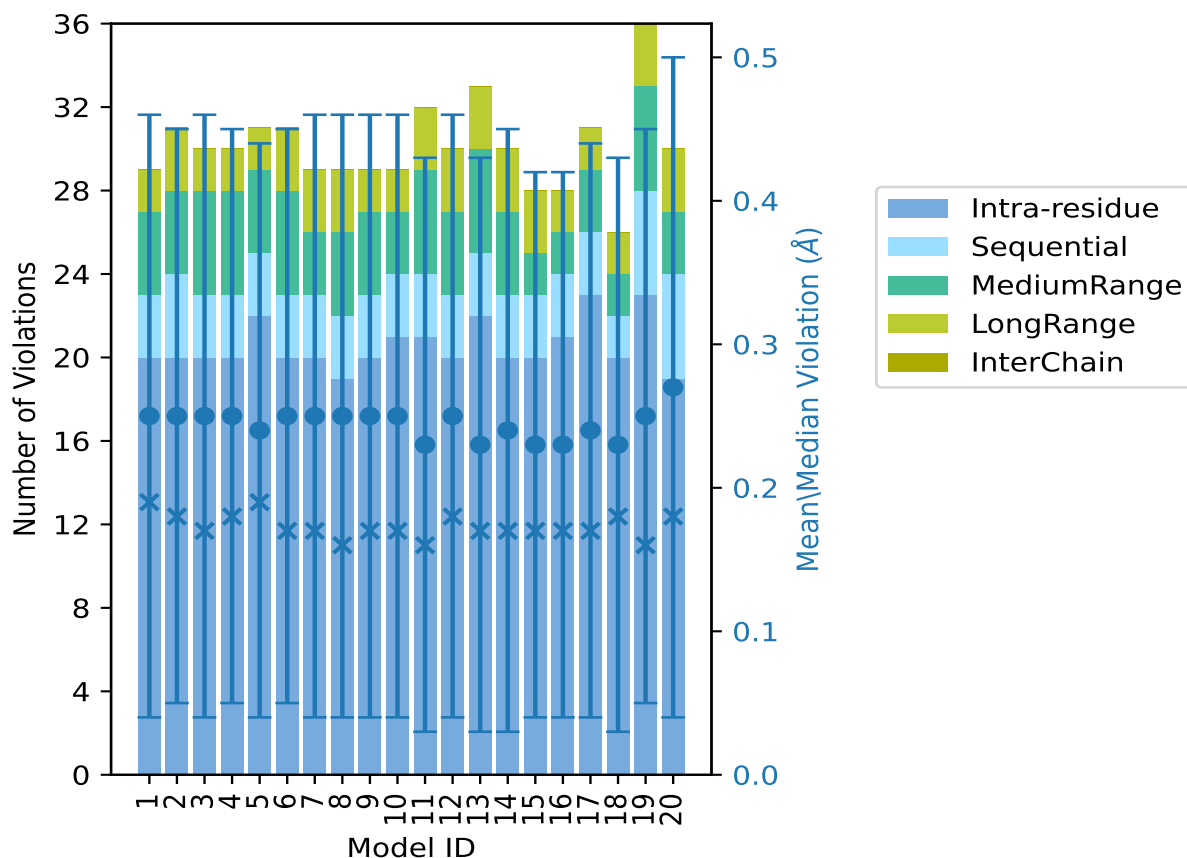
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
12	20	3	4	3	0	30	0.25	0.98	0.21	0.18
13	22	3	5	3	0	33	0.23	0.99	0.2	0.17
14	20	3	4	3	0	30	0.24	0.99	0.21	0.17
15	20	3	2	3	0	28	0.23	0.99	0.19	0.17
16	21	3	2	2	0	28	0.23	0.99	0.19	0.17
17	23	3	3	2	0	31	0.24	0.97	0.2	0.17
18	20	2	2	2	0	26	0.23	0.99	0.2	0.18
19	23	5	5	3	0	36	0.25	0.97	0.2	0.16
20	19	5	3	3	0	30	0.27	0.98	0.23	0.18

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

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



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

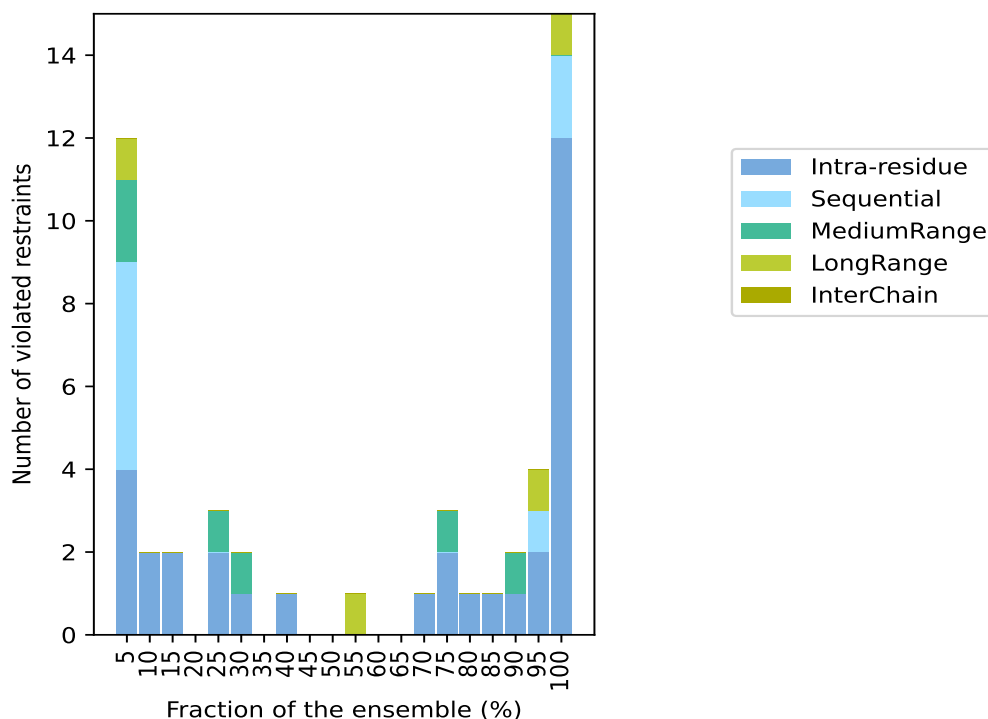
9.3 Distance violation statistics for the ensemble

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, 111(IR:49, SQ:34, MR:12, LR:16, IC:0) restraints are not violated in the ensemble.

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

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

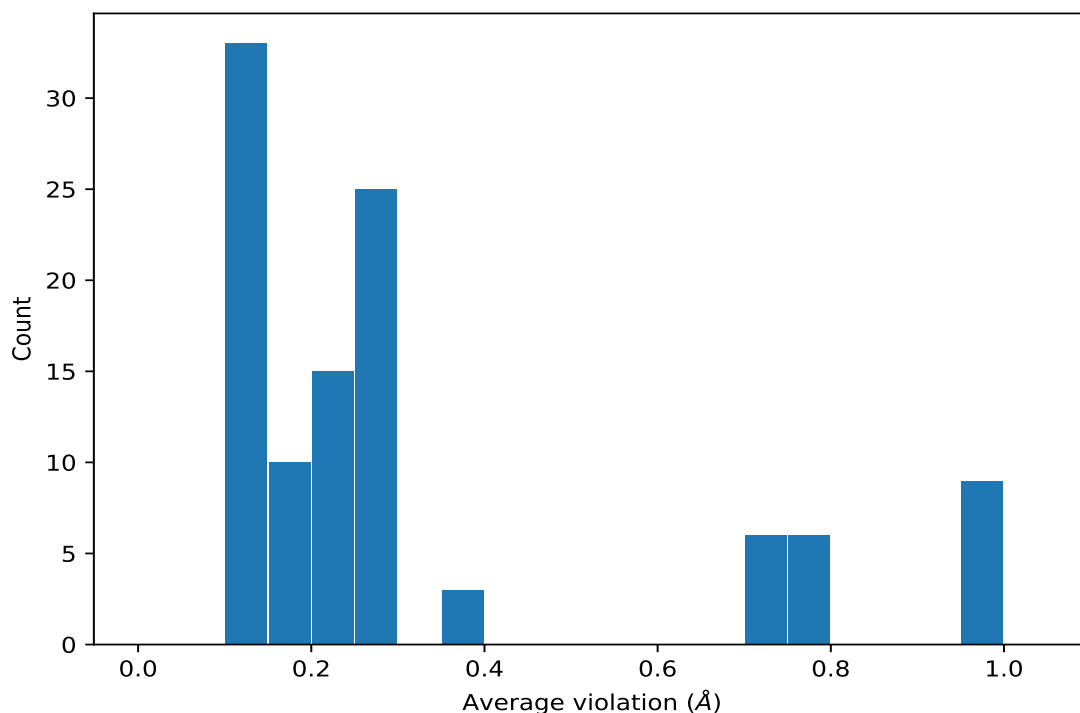
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	20	0.98	0.01	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	20	0.98	0.01	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	20	0.98	0.01	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	20	0.98	0.01	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	20	0.98	0.01	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	20	0.98	0.01	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	20	0.98	0.01	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	20	0.98	0.01	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	20	0.98	0.01	0.98
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	20	0.76	0.03	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	20	0.76	0.03	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	20	0.76	0.03	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	20	0.76	0.03	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	20	0.76	0.03	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	20	0.76	0.03	0.77
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	20	0.36	0.01	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	20	0.36	0.01	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	20	0.36	0.01	0.36
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	20	0.22	0.01	0.22
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	20	0.22	0.01	0.22
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	20	0.22	0.01	0.22
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	20	0.21	0.02	0.21
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	20	0.21	0.04	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	20	0.2	0.01	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	20	0.2	0.01	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	20	0.2	0.01	0.2
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	20	0.18	0.04	0.18
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	20	0.17	0.01	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	20	0.17	0.01	0.17
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	20	0.16	0.02	0.16
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	20	0.15	0.02	0.15
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	20	0.14	0.01	0.15
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	20	0.13	0.01	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	20	0.13	0.01	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	20	0.13	0.01	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	20	0.13	0.01	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	20	0.13	0.01	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	20	0.13	0.01	0.13
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	19	0.3	0.02	0.3
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	19	0.3	0.02	0.3
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	19	0.3	0.02	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	19	0.3	0.03	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	19	0.3	0.03	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	19	0.3	0.03	0.3
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	19	0.13	0.05	0.12
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	19	0.13	0.02	0.12
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	18	0.27	0.0	0.27
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	18	0.21	0.06	0.22
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	18	0.21	0.06	0.22
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	18	0.21	0.06	0.22
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	17	0.73	0.01	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	17	0.73	0.01	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	17	0.73	0.01	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	17	0.73	0.01	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	17	0.73	0.01	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	17	0.73	0.01	0.73
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	17	0.13	0.02	0.13
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	16	0.24	0.02	0.24
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	16	0.24	0.02	0.24
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	16	0.24	0.02	0.24
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	15	0.17	0.0	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	15	0.17	0.0	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	15	0.17	0.0	0.17
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	15	0.13	0.01	0.13
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	15	0.12	0.05	0.11
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	14	0.1	0.0	0.1
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	13	0.12	0.03	0.11
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	11	0.12	0.02	0.12
(1,84)	1:8:Z:DAL:H	1:8:Z:DAL:HB3	8	0.14	0.02	0.15
(1,25)	1:2:Z:ABA:H	1:5:Z:VAL:H	6	0.12	0.02	0.12
(1,22)	1:2:Z:ABA:H	1:2:Z:ABA:HB2	6	0.11	0.0	0.11
(1,92)	1:9:Z:MLE:HN1	1:9:Z:MLE:HB2	5	0.17	0.03	0.18
(1,92)	1:9:Z:MLE:HN2	1:9:Z:MLE:HB2	5	0.17	0.03	0.18
(1,92)	1:9:Z:MLE:HN3	1:9:Z:MLE:HB2	5	0.17	0.03	0.18
(1,128)	1:6:Z:MLE:HG	1:8:Z:DAL:H	5	0.13	0.03	0.11
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG23	5	0.11	0.01	0.11
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG21	5	0.11	0.01	0.11
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG22	5	0.11	0.01	0.11
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG23	5	0.11	0.01	0.11
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG21	5	0.11	0.01	0.11
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG22	5	0.11	0.01	0.11
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG23	5	0.11	0.01	0.11
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG21	5	0.11	0.01	0.11
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG22	5	0.11	0.01	0.11
(1,44)	1:4:Z:MLE:HA	1:4:Z:MLE:HB3	3	0.2	0.0	0.2

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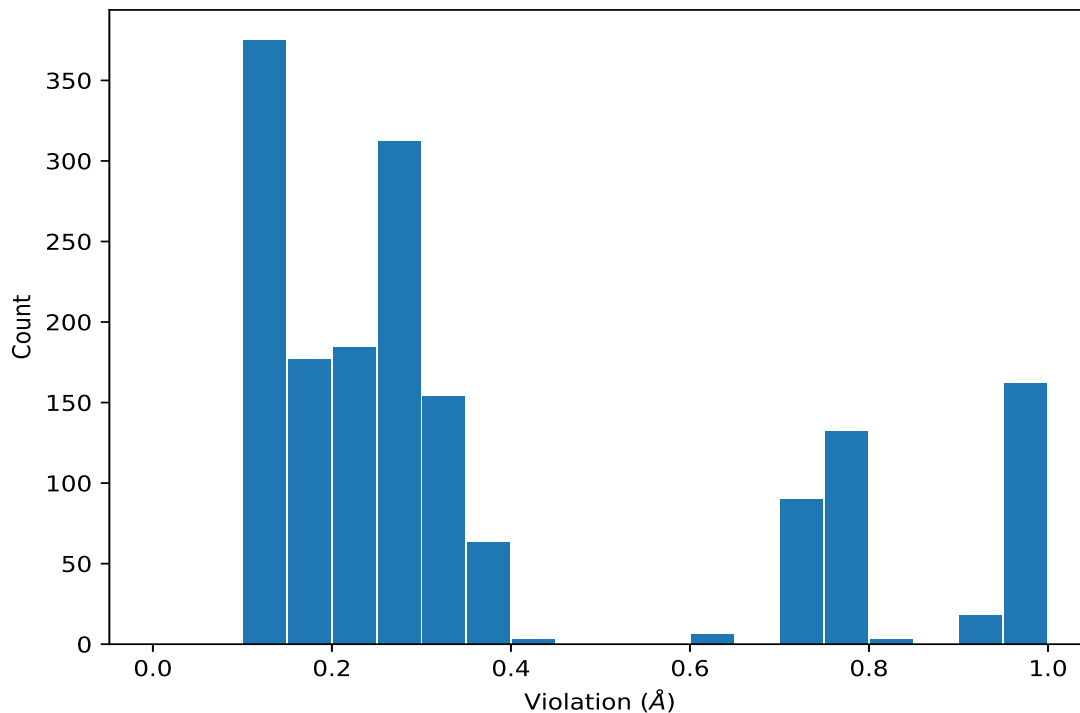
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,23)	1:2:Z:ABA:H	1:2:Z:ABA:HG3	3	0.13	0.0	0.13
(1,76)	1:6:Z:MLE:HG	1:6:Z:MLE:HN3	2	0.27	0.02	0.27
(1,76)	1:6:Z:MLE:HG	1:6:Z:MLE:HN1	2	0.27	0.02	0.27
(1,76)	1:6:Z:MLE:HG	1:6:Z:MLE:HN2	2	0.27	0.02	0.27
(1,102)	1:10:Z:MLE:HN3	1:10:Z:MLE:HB2	2	0.11	0.0	0.11
(1,102)	1:10:Z:MLE:HN1	1:10:Z:MLE:HB2	2	0.11	0.0	0.11
(1,102)	1:10:Z:MLE:HN2	1:10:Z:MLE:HB2	2	0.11	0.0	0.11

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)
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	13	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	13	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	13	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	13	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	13	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	13	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	13	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	13	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	13	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	14	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	14	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	14	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	14	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	14	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	14	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	14	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	14	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	14	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	15	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	15	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	15	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	15	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	15	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	15	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	15	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	15	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	15	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	16	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	16	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	16	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	16	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	16	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	16	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	16	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	16	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	16	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	18	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	18	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	18	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	18	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	18	0.99
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	18	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	18	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	18	0.99
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	18	0.99
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	1	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	1	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	1	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	1	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	1	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	1	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	1	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	1	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	1	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	3	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	3	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	3	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	3	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	3	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	3	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	3	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	3	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	3	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	4	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	4	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	4	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	4	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	4	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	4	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	4	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	4	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	4	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	6	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	6	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	6	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	6	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	6	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	6	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	6	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	6	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	6	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	7	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	7	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	7	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	7	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	7	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	7	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	7	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	7	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	7	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	8	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	8	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	8	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	8	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	8	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	8	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	8	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	8	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	8	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	9	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	9	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	9	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	9	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	9	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	9	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	9	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	9	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	9	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	10	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	10	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	10	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	10	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	10	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	10	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	10	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	10	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	10	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	11	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	11	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	11	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	11	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	11	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	11	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	11	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	11	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	11	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	12	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	12	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	12	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	12	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	12	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	12	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	12	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	12	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	12	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	20	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	20	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	20	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	20	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	20	0.98
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	20	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	20	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	20	0.98
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	20	0.98
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	17	0.97
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	17	0.97
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	17	0.97
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	17	0.97
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	17	0.97
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	17	0.97
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	17	0.97
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	17	0.97
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	17	0.97
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	19	0.97
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	19	0.97
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	19	0.97
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	19	0.97
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	19	0.97
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	19	0.97
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	19	0.97
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	19	0.97
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	19	0.97
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	2	0.94
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	2	0.94
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	2	0.94
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	2	0.94
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	2	0.94
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	2	0.94
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	2	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	2	0.94
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	2	0.94
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN3	5	0.94
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN1	5	0.94
(1,60)	1:5:Z:VAL:HG11	1:6:Z:MLE:HN2	5	0.94
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN3	5	0.94
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN1	5	0.94
(1,60)	1:5:Z:VAL:HG12	1:6:Z:MLE:HN2	5	0.94
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN3	5	0.94
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN1	5	0.94
(1,60)	1:5:Z:VAL:HG13	1:6:Z:MLE:HN2	5	0.94
(1,37)	1:4:Z:MLE:HN1	1:4:Z:MLE:HA	20	0.83
(1,37)	1:4:Z:MLE:HN2	1:4:Z:MLE:HA	20	0.83
(1,37)	1:4:Z:MLE:HN3	1:4:Z:MLE:HA	20	0.83
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	2	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	2	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	2	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	2	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	2	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	2	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	3	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	3	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	3	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	3	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	3	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	3	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	5	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	5	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	5	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	5	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	5	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	5	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	7	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	7	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	7	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	7	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	7	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	7	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	8	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	8	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	8	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	8	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	8	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	8	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	9	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	9	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	9	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	9	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	9	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	9	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	10	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	10	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	10	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	10	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	10	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	10	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	11	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	11	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	11	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	11	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	11	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	11	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	12	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	12	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	12	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	12	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	12	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	12	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	15	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	15	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	15	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	15	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	15	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	15	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	17	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	17	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	17	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	17	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	17	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	17	0.77
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	1	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	1	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	1	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	1	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	1	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	4	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	4	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	4	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	4	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	4	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	4	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	14	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	14	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	14	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	14	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	14	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	14	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	18	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	18	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	18	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	18	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	18	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	18	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	20	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	20	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	20	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	20	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	20	0.76
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	20	0.76
(1,99)	1:9:Z:MLE:HA	1:10:Z:MLE:HD11	19	0.75
(1,99)	1:9:Z:MLE:HA	1:10:Z:MLE:HD12	19	0.75
(1,99)	1:9:Z:MLE:HA	1:10:Z:MLE:HD13	19	0.75
(1,99)	1:9:Z:MLE:HA	1:10:Z:MLE:HD21	19	0.75
(1,99)	1:9:Z:MLE:HA	1:10:Z:MLE:HD22	19	0.75
(1,99)	1:9:Z:MLE:HA	1:10:Z:MLE:HD23	19	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	6	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	6	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	6	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	6	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	6	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	6	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	13	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	13	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	13	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	13	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	13	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	13	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	16	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	16	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	16	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	16	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	16	0.75
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	16	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	12	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	12	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	12	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	12	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	12	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	12	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	20	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	20	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	20	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	20	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	20	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	20	0.75
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	13	0.74
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	13	0.74
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	13	0.74
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	13	0.74
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	13	0.74
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	13	0.74
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	3	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	3	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	3	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	3	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	3	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	3	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	7	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	7	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	7	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	7	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	7	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	7	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	11	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	11	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	11	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	11	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	11	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	11	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	14	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	14	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	14	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	14	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	14	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	14	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	17	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	17	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	17	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	17	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	17	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	17	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	19	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	19	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	19	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	19	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	19	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	19	0.73
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	1	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	1	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	1	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	1	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	1	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	1	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	2	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	2	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	2	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	2	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	2	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	2	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	5	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	5	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	5	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	5	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	5	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	5	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	6	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	6	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	6	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	6	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	6	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	6	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	8	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	8	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	8	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	8	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	8	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	8	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	9	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	9	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	9	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	9	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	9	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	9	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	10	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	10	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	10	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	10	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	10	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	10	0.72
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD12	4	0.71
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD13	4	0.71
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD21	4	0.71
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD22	4	0.71
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD23	4	0.71
(1,46)	1:4:Z:MLE:HA	1:4:Z:MLE:HD11	4	0.71
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD11	19	0.63
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD12	19	0.63
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD13	19	0.63
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	19	0.63
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	19	0.63
(1,95)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	19	0.63
(1,103)	1:10:Z:MLE:HN3	1:10:Z:MLE:HB3	19	0.44
(1,103)	1:10:Z:MLE:HN1	1:10:Z:MLE:HB3	19	0.44
(1,103)	1:10:Z:MLE:HN2	1:10:Z:MLE:HB3	19	0.44
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	5	0.39
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	5	0.39
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	5	0.39
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	1	0.38
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	1	0.38
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	1	0.38
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	2	0.38
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	2	0.38
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	6	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	6	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	6	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	7	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	7	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	7	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	9	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	9	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	9	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	12	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	12	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	12	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	13	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	13	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	13	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	14	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	14	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	14	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	19	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	19	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	19	0.37
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	3	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	3	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	3	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	4	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	4	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	4	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	15	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	15	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	15	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	16	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	16	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	16	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	17	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	17	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	17	0.36
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	2	0.36
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	2	0.36
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	2	0.36
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	2	0.36
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	2	0.36
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	2	0.36
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	2	0.36
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	2	0.36
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	2	0.36
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	2	0.36
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	2	0.36
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	2	0.36
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	2	0.36
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	2	0.36
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	2	0.36
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	2	0.36
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	2	0.36
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	8	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	8	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	8	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	10	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	10	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	10	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	11	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	11	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	11	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	18	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	18	0.35
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	18	0.35
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	3	0.34
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	3	0.34
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	3	0.34
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	3	0.34
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	3	0.34
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	3	0.34
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	3	0.34
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	3	0.34
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	3	0.34
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	3	0.34
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	3	0.34
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	3	0.34
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	3	0.34
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	3	0.34
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	3	0.34
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	3	0.34
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	3	0.34
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	3	0.33
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	3	0.33
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	3	0.33
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	19	0.32
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	6	0.32
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	6	0.32
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	6	0.32
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	14	0.32
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	14	0.32
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	14	0.32
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD11	20	0.32
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD12	20	0.32
(1,14)	1:1:Z:BMT:HB	1:1:Z:BMT:HD13	20	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	12	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	12	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	12	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	12	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	12	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	12	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	12	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	12	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	12	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	12	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	12	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	12	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	12	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	12	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	12	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	12	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	12	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	12	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	16	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	16	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	16	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	16	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	16	0.32
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	16	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	16	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	16	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	16	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	16	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	16	0.32
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	16	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	16	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	16	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	16	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	16	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	16	0.32
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	16	0.32
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	4	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	4	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	4	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	7	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	7	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	7	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	9	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	9	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	9	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	12	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	12	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	12	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	16	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	16	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	16	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	17	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	17	0.31
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	17	0.31
(1,41)	1:4:Z:MLE:HN1	1:5:Z:VAL:H	20	0.31
(1,41)	1:4:Z:MLE:HN2	1:5:Z:VAL:H	20	0.31
(1,41)	1:4:Z:MLE:HN3	1:5:Z:VAL:H	20	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	6	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	6	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	6	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	6	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	6	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	6	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	6	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	6	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	6	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	6	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	6	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	6	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	6	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	6	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	6	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	6	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	6	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	7	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	7	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	7	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	7	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	7	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	7	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	7	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	7	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	7	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	7	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	7	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	7	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	7	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	7	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	7	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	7	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	7	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	7	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	13	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	13	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	13	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	13	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	13	0.31
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	13	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	13	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	13	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	13	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	13	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	13	0.31
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	13	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	13	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	13	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	13	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	13	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	13	0.31
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	5	0.3
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	4	0.3
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	4	0.3
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	4	0.3
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	6	0.3
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	6	0.3
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	6	0.3
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	8	0.3
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	8	0.3
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	8	0.3
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	19	0.3
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	19	0.3
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	19	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	1	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	1	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	1	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	1	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	1	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	1	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	1	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	1	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	1	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	1	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	1	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	1	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	1	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	1	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	1	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	1	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	1	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	1	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	4	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	4	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	4	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	4	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	4	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	4	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	4	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	4	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	4	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	4	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	4	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	4	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	4	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	4	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	4	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	4	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	4	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	9	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	9	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	9	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	9	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	9	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	9	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	9	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	9	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	9	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	9	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	9	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	9	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	9	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	9	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	9	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	9	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	9	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	9	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	10	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	10	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	10	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	10	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	10	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	10	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	10	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	10	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	10	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	10	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	10	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	10	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	10	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	10	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	10	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	10	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	10	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	17	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	17	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	17	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	17	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	17	0.3
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	17	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	17	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	17	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	17	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	17	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	17	0.3
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	17	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	17	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	17	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	17	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	17	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	17	0.3
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	17	0.3
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	2	0.29
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	19	0.29
(1,76)	1:6:Z:MLE:HG	1:6:Z:MLE:HN3	2	0.29
(1,76)	1:6:Z:MLE:HG	1:6:Z:MLE:HN1	2	0.29
(1,76)	1:6:Z:MLE:HG	1:6:Z:MLE:HN2	2	0.29
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	2	0.29
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	2	0.29
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	2	0.29
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	10	0.29
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	10	0.29
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	10	0.29
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	20	0.29
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	9	0.29
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	9	0.29
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	9	0.29
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	1	0.28
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	3	0.28
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	4	0.28
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	6	0.28
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	11	0.28
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	13	0.28
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	1	0.28
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	1	0.28
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	13	0.28
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	13	0.28
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	13	0.28
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	15	0.28
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	15	0.28
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	15	0.28
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	3	0.28
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	3	0.28
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	3	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	5	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	5	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	5	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	5	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	5	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	5	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	5	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	5	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	5	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	5	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	5	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	5	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	5	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	5	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	5	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	5	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	5	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	5	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	8	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	8	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	8	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	8	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	8	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	8	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	8	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	8	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	8	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	8	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	8	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	8	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	8	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	8	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	8	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	8	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	8	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	11	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	11	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	11	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	11	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	11	0.28
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	11	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	11	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	11	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	11	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	11	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	11	0.28
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	11	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	11	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	11	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	11	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	11	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	11	0.28
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	11	0.28
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	7	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	8	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	9	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	10	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	12	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	14	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	15	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	16	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	17	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	18	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	19	0.27
(1,74)	1:6:Z:MLE:HB3	1:6:Z:MLE:HG	20	0.27
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	5	0.27
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	5	0.27
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	5	0.27
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	11	0.27
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	11	0.27
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	11	0.27
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG22	18	0.27
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG23	18	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:5:Z:VAL:HA	1:5:Z:VAL:HG21	18	0.27
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	2	0.27
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	2	0.27
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	2	0.27
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	3	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	3	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	3	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	8	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	8	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	8	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	12	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	12	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	12	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	19	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	19	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	19	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	20	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	20	0.26
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	20	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	18	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	18	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	18	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	18	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	18	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	18	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	18	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	18	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	18	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	18	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	18	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	18	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	18	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	18	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	18	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	18	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	18	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	18	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	20	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	20	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	20	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	20	0.26
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	20	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	20	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	20	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	20	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	20	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	20	0.26
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	20	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	20	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	20	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	20	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	20	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	20	0.26
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	20	0.26
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	13	0.25
(1,76)	1:6:Z:MLE:HG	1:6:Z:MLE:HN3	5	0.25
(1,76)	1:6:Z:MLE:HG	1:6:Z:MLE:HN1	5	0.25
(1,76)	1:6:Z:MLE:HG	1:6:Z:MLE:HN2	5	0.25
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	6	0.25
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	5	0.25
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	5	0.25
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	5	0.25
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	11	0.25
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	11	0.25
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	11	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	14	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	14	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	14	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	14	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	14	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	14	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	14	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	14	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	14	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	14	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	14	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	14	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	14	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	14	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	14	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	14	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	14	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG23	15	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG11	15	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG12	15	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG13	15	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG21	15	0.25
(1,4)	1:1:Z:BMT:HN1	1:11:Z:MVA:HG22	15	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG23	15	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG11	15	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG12	15	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG13	15	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG21	15	0.25
(1,4)	1:1:Z:BMT:HN2	1:11:Z:MVA:HG22	15	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG23	15	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG11	15	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG12	15	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG13	15	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG21	15	0.25
(1,4)	1:1:Z:BMT:HN3	1:11:Z:MVA:HG22	15	0.25
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	1	0.24
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	15	0.24
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	13	0.24
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	13	0.24
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	13	0.24
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	3	0.24
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	1	0.24
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	1	0.24
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	1	0.24
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	15	0.24
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	15	0.24
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	15	0.24
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	8	0.24
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	8	0.24
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	8	0.24
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	10	0.24
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	10	0.24
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	10	0.24
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	12	0.24
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	12	0.24
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	12	0.24
(1,35)	1:3:Z:SAR:HA2	1:4:Z:MLE:HN1	20	0.24
(1,35)	1:3:Z:SAR:HA2	1:4:Z:MLE:HN2	20	0.24
(1,35)	1:3:Z:SAR:HA2	1:4:Z:MLE:HN3	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	2	0.24
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	18	0.23
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	7	0.23
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	5	0.23
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	5	0.23
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	5	0.23
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	10	0.23
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	10	0.23
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	10	0.23
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	14	0.23
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	14	0.23
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	14	0.23
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	20	0.23
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	20	0.23
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	20	0.23
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	4	0.23
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	4	0.23
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	4	0.23
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	6	0.23
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	6	0.23
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	6	0.23
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	13	0.23
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	13	0.23
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	13	0.23
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	14	0.23
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	14	0.23
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	14	0.23
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	17	0.23
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	17	0.23
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	17	0.23
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	11	0.22
(1,88)	1:8:Z:DAL:HA	1:11:Z:MVA:HN1	19	0.22
(1,88)	1:8:Z:DAL:HA	1:11:Z:MVA:HN2	19	0.22
(1,88)	1:8:Z:DAL:HA	1:11:Z:MVA:HN3	19	0.22
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	9	0.22
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	9	0.22
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	9	0.22
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	14	0.22
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	14	0.22
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	14	0.22
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	4	0.22
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	12	0.22
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	19	0.22
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	2	0.22
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	2	0.22
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	2	0.22
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	3	0.22
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	3	0.22
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	3	0.22
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	6	0.22
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	6	0.22
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	6	0.22
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	8	0.22
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	8	0.22
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	8	0.22
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	9	0.22
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	9	0.22
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	9	0.22
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	11	0.22
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	11	0.22
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	11	0.22
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	12	0.22
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	12	0.22
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	12	0.22
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	13	0.22
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	13	0.22
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	13	0.22
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	18	0.22
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	18	0.22
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	18	0.22
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	1	0.22
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	1	0.22
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	1	0.22
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	7	0.22
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	7	0.22
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	7	0.22
(1,39)	1:4:Z:MLE:HN1	1:4:Z:MLE:HB3	19	0.22
(1,39)	1:4:Z:MLE:HN2	1:4:Z:MLE:HB3	19	0.22
(1,39)	1:4:Z:MLE:HN3	1:4:Z:MLE:HB3	19	0.22
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	2	0.22
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	4	0.21
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	4	0.21
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	7	0.21
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	7	0.21
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	7	0.21
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	20	0.21
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	20	0.21
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	20	0.21
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	10	0.21
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	1	0.21
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	2	0.21
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	9	0.21
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	10	0.21
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	13	0.21
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	17	0.21
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	7	0.21
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	7	0.21
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	7	0.21
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	16	0.21
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	16	0.21
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	16	0.21
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	17	0.21
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	17	0.21
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	17	0.21
(1,44)	1:4:Z:MLE:HA	1:4:Z:MLE:HB3	15	0.21
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	5	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	2	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	2	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	2	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	3	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	3	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	3	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	5	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	5	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	5	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	6	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	6	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	6	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	9	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	9	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	9	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	11	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	11	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	15	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	15	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	15	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	16	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	16	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	16	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	17	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	17	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	17	0.2
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	4	0.2
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	8	0.2
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	14	0.2
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	16	0.2
(1,92)	1:9:Z:MLE:HN1	1:9:Z:MLE:HB2	6	0.2
(1,92)	1:9:Z:MLE:HN2	1:9:Z:MLE:HB2	6	0.2
(1,92)	1:9:Z:MLE:HN3	1:9:Z:MLE:HB2	6	0.2
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	18	0.2
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	18	0.2
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	18	0.2
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	5	0.2
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	11	0.2
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	15	0.2
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	18	0.2
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	4	0.2
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	4	0.2
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	4	0.2
(1,64)	1:6:Z:MLE:HN3	1:6:Z:MLE:HB3	19	0.2
(1,64)	1:6:Z:MLE:HN1	1:6:Z:MLE:HB3	19	0.2
(1,64)	1:6:Z:MLE:HN2	1:6:Z:MLE:HB3	19	0.2
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	4	0.2
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	10	0.2
(1,44)	1:4:Z:MLE:HA	1:4:Z:MLE:HB3	16	0.2
(1,44)	1:4:Z:MLE:HA	1:4:Z:MLE:HB3	18	0.2
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	11	0.2
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	1	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	1	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	1	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	8	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	8	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	8	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	10	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	10	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	12	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	12	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	12	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	13	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	13	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	13	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	14	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	14	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	14	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	18	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	18	0.19
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	18	0.19
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	12	0.19
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	17	0.19
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	20	0.19
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	2	0.19
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	5	0.19
(1,92)	1:9:Z:MLE:HN1	1:9:Z:MLE:HB2	1	0.19
(1,92)	1:9:Z:MLE:HN2	1:9:Z:MLE:HB2	1	0.19
(1,92)	1:9:Z:MLE:HN3	1:9:Z:MLE:HB2	1	0.19
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	1	0.19
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	1	0.19
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	1	0.19
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	15	0.19
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	15	0.19
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	15	0.19
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	14	0.19
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	16	0.19
(1,68)	1:6:Z:MLE:HA	1:6:Z:MLE:HG	20	0.19
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	5	0.19
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	6	0.19
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	8	0.19
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	11	0.19
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	12	0.19
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	14	0.19
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	19	0.19
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	1	0.19
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	13	0.19
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	5	0.19
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	2	0.18
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:6:Z:MLE:HG	1:8:Z:DAL:H	2	0.18
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG23	19	0.18
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG21	19	0.18
(1,112)	1:11:Z:MVA:HB	1:11:Z:MVA:HG22	19	0.18
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	7	0.18
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	9	0.18
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	1	0.18
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	3	0.18
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	4	0.18
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	12	0.18
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	15	0.18
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	17	0.18
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	18	0.18
(1,92)	1:9:Z:MLE:HN1	1:9:Z:MLE:HB2	13	0.18
(1,92)	1:9:Z:MLE:HN2	1:9:Z:MLE:HB2	13	0.18
(1,92)	1:9:Z:MLE:HN3	1:9:Z:MLE:HB2	13	0.18
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	1	0.18
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	2	0.18
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	3	0.18
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	7	0.18
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	13	0.18
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	17	0.18
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	5	0.18
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	6	0.18
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	19	0.17
(1,128)	1:6:Z:MLE:HG	1:8:Z:DAL:H	5	0.17
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	6	0.17
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	7	0.17
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	9	0.17
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	10	0.17
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	11	0.17
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	13	0.17
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	14	0.17
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	16	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	2	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	2	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	2	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	3	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	3	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	3	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	7	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	7	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	9	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	9	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	9	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	10	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	10	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	10	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	11	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	11	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	11	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	12	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	12	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	12	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	15	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	15	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	15	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	17	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	17	0.17
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	17	0.17
(1,92)	1:9:Z:MLE:HN1	1:9:Z:MLE:HB2	16	0.17
(1,92)	1:9:Z:MLE:HN2	1:9:Z:MLE:HB2	16	0.17
(1,92)	1:9:Z:MLE:HN3	1:9:Z:MLE:HB2	16	0.17
(1,84)	1:8:Z:DAL:H	1:8:Z:DAL:HB3	17	0.17
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	15	0.17
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	16	0.17
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	18	0.17
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	9	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	2	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	4	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	6	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	7	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	10	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	14	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	15	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	16	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	18	0.17
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	20	0.17
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	3	0.17
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	7	0.17
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	9	0.17
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	12	0.17
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	3	0.16
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	6	0.16
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	8	0.16
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	20	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	4	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	4	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	4	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	5	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	5	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	5	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	8	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	8	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	8	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	14	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	14	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	14	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	18	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	18	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	18	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD21	20	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD22	20	0.16
(1,96)	1:9:Z:MLE:HA	1:9:Z:MLE:HD23	20	0.16
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	17	0.16
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	17	0.16
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	17	0.16
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	13	0.16
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	16	0.16
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	18	0.16
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	20	0.16
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	3	0.16
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	8	0.16
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	9	0.16
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	12	0.16
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	17	0.16
(1,30)	1:2:Z:ABA:HA	1:2:Z:ABA:HB2	19	0.16
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	2	0.16
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	4	0.16
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	5	0.16
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	6	0.16
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	8	0.16
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	19	0.16
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	19	0.16
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	6	0.15
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	13	0.15
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	16	0.15
(1,84)	1:8:Z:DAL:H	1:8:Z:DAL:HB3	7	0.15
(1,84)	1:8:Z:DAL:H	1:8:Z:DAL:HB3	10	0.15
(1,84)	1:8:Z:DAL:H	1:8:Z:DAL:HB3	11	0.15
(1,84)	1:8:Z:DAL:H	1:8:Z:DAL:HB3	16	0.15
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	1	0.15
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	7	0.15
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	10	0.15
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	11	0.15
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	14	0.15
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	15	0.15
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	17	0.15
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	19	0.15
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	19	0.15
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	19	0.15
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	20	0.15
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	20	0.15
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	20	0.15
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	8	0.15
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	1	0.15
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	10	0.15
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	14	0.15
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	17	0.15
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	1	0.15
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	4	0.15
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	9	0.15
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	13	0.15
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	1	0.14
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	7	0.14
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	7	0.14
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	7	0.14
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	3	0.14
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	4	0.14
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	6	0.14
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	12	0.14
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	19	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	4	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	4	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	6	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	6	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	6	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	8	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	8	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	8	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	9	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	9	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	9	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	12	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	12	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	12	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	14	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	14	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	14	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	17	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	17	0.14
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	17	0.14
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	15	0.14
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	15	0.14
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	15	0.14
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	16	0.14
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	16	0.14
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	16	0.14
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	18	0.14
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	18	0.14
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	18	0.14
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	12	0.14
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	17	0.14
(1,25)	1:2:Z:ABA:H	1:5:Z:VAL:H	15	0.14
(1,25)	1:2:Z:ABA:H	1:5:Z:VAL:H	18	0.14
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	11	0.14
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	16	0.14
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	20	0.14
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	7	0.14
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	8	0.14
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	10	0.14
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	11	0.14
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	15	0.14
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	1	0.13
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	2	0.13
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	5	0.13
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	7	0.13
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	10	0.13
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	12	0.13
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	14	0.13
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	19	0.13
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	6	0.13
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	2	0.13
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	9	0.13
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	20	0.13
(1,84)	1:8:Z:DAL:H	1:8:Z:DAL:HB3	2	0.13
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	8	0.13
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	9	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	1	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	1	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	1	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	2	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	2	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	2	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	3	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	3	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	3	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	7	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	7	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	7	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	10	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	10	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	10	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	11	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	11	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	11	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	13	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	13	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	13	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	15	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	15	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	15	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	16	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	16	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	16	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	20	0.13
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	20	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	1	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	1	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	1	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	2	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	2	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	2	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	3	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	3	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	3	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	6	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	6	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	6	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	10	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	10	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	10	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	11	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	11	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	11	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	17	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	17	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	17	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	19	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	19	0.13
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	19	0.13
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	4	0.13
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	9	0.13
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	10	0.13
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	3	0.13
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	4	0.13
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	6	0.13
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	7	0.13
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	10	0.13
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	14	0.13
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	19	0.13
(1,23)	1:2:Z:ABA:H	1:2:Z:ABA:HG3	1	0.13
(1,23)	1:2:Z:ABA:H	1:2:Z:ABA:HG3	13	0.13
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	15	0.13
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	14	0.13
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	16	0.13
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	17	0.13
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:1:Z:BMT:HA	1:1:Z:BMT:HD23	20	0.13
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	3	0.12
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	4	0.12
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	12	0.12
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	1	0.12
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	6	0.12
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	8	0.12
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	9	0.12
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	13	0.12
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	17	0.12
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	2	0.12
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	8	0.12
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	11	0.12
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	15	0.12
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG23	4	0.12
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG21	4	0.12
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG22	4	0.12
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG23	4	0.12
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG21	4	0.12
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG22	4	0.12
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG23	4	0.12
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG21	4	0.12
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG22	4	0.12
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG23	19	0.12
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG21	19	0.12
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG22	19	0.12
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG23	19	0.12
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG21	19	0.12
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG22	19	0.12
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG23	19	0.12
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG21	19	0.12
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG22	19	0.12
(1,106)	1:10:Z:MLE:HA	1:10:Z:MLE:HB3	19	0.12
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	5	0.12
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	3	0.12
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	5	0.12
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	8	0.12
(1,92)	1:9:Z:MLE:HN1	1:9:Z:MLE:HB2	19	0.12
(1,92)	1:9:Z:MLE:HN2	1:9:Z:MLE:HB2	19	0.12
(1,92)	1:9:Z:MLE:HN3	1:9:Z:MLE:HB2	19	0.12
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	10	0.12
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	10	0.12
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	5	0.12
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	5	0.12
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	5	0.12
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG22	18	0.12
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG23	18	0.12
(1,58)	1:5:Z:VAL:HB	1:5:Z:VAL:HG21	18	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	4	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	4	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	4	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	5	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	5	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	5	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	7	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	7	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	7	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	8	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	8	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	8	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	9	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	9	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	9	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	12	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	12	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	12	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	13	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	13	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	13	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG11	14	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG12	14	0.12
(1,57)	1:5:Z:VAL:HB	1:5:Z:VAL:HG13	14	0.12
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	1	0.12
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	2	0.12
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	3	0.12
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	8	0.12
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	12	0.12
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	13	0.12
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	14	0.12
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	1	0.12
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	9	0.12
(1,25)	1:2:Z:ABA:H	1:5:Z:VAL:H	16	0.12
(1,23)	1:2:Z:ABA:H	1:2:Z:ABA:HG3	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:2:Z:ABA:H	1:2:Z:ABA:HB2	9	0.12
(1,22)	1:2:Z:ABA:H	1:2:Z:ABA:HB2	18	0.12
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	13	0.12
(1,19)	1:1:Z:BMT:HD22	1:6:Z:MLE:HA	18	0.12
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	8	0.11
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	13	0.11
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	14	0.11
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	20	0.11
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	4	0.11
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	7	0.11
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	12	0.11
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	13	0.11
(1,128)	1:6:Z:MLE:HG	1:8:Z:DAL:H	4	0.11
(1,128)	1:6:Z:MLE:HG	1:8:Z:DAL:H	6	0.11
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG23	3	0.11
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG21	3	0.11
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG22	3	0.11
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG23	3	0.11
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG21	3	0.11
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG22	3	0.11
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG23	3	0.11
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG21	3	0.11
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG22	3	0.11
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG23	6	0.11
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG21	6	0.11
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG22	6	0.11
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG23	6	0.11
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG21	6	0.11
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG22	6	0.11
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG23	6	0.11
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG21	6	0.11
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG22	6	0.11
(1,107)	1:10:Z:MLE:HA	1:10:Z:MLE:HG	19	0.11
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	1	0.11
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	2	0.11
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	10	0.11
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	11	0.11
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	12	0.11
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	13	0.11
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	14	0.11
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	15	0.11
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:10:Z:MLE:HN3	1:10:Z:MLE:HB2	5	0.11
(1,102)	1:10:Z:MLE:HN1	1:10:Z:MLE:HB2	5	0.11
(1,102)	1:10:Z:MLE:HN2	1:10:Z:MLE:HB2	5	0.11
(1,102)	1:10:Z:MLE:HN3	1:10:Z:MLE:HB2	13	0.11
(1,102)	1:10:Z:MLE:HN1	1:10:Z:MLE:HB2	13	0.11
(1,102)	1:10:Z:MLE:HN2	1:10:Z:MLE:HB2	13	0.11
(1,98)	1:9:Z:MLE:HA	1:10:Z:MLE:HG	19	0.11
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	4	0.11
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	7	0.11
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	10	0.11
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	11	0.11
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	12	0.11
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	14	0.11
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	15	0.11
(1,97)	1:9:Z:MLE:HA	1:10:Z:MLE:HB2	17	0.11
(1,93)	1:9:Z:MLE:HA	1:9:Z:MLE:HB2	19	0.11
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	16	0.11
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	16	0.11
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	16	0.11
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	2	0.11
(1,66)	1:6:Z:MLE:HA	1:6:Z:MLE:HB2	5	0.11
(1,52)	1:5:Z:VAL:HA	1:5:Z:VAL:HB	20	0.11
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	5	0.11
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	6	0.11
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	7	0.11
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	11	0.11
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	17	0.11
(1,50)	1:5:Z:VAL:H	1:5:Z:VAL:HB	19	0.11
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	15	0.11
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	18	0.11
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	11	0.11
(1,26)	1:2:Z:ABA:H	1:5:Z:VAL:HB	13	0.11
(1,25)	1:2:Z:ABA:H	1:5:Z:VAL:H	11	0.11
(1,25)	1:2:Z:ABA:H	1:5:Z:VAL:H	19	0.11
(1,22)	1:2:Z:ABA:H	1:2:Z:ABA:HB2	5	0.11
(1,22)	1:2:Z:ABA:H	1:2:Z:ABA:HB2	15	0.11
(1,22)	1:2:Z:ABA:H	1:2:Z:ABA:HB2	16	0.11
(1,22)	1:2:Z:ABA:H	1:2:Z:ABA:HB2	17	0.11
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	6	0.11
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	15	0.11
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	6	0.1
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:6:Z:MLE:O	1:8:Z:DAL:H	11	0.1
(2,3)	1:2:Z:ABA:O	1:5:Z:VAL:H	11	0.1
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	14	0.1
(1,139)	1:2:Z:ABA:H	1:11:Z:MVA:HB	20	0.1
(1,128)	1:6:Z:MLE:HG	1:8:Z:DAL:H	3	0.1
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG23	17	0.1
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG21	17	0.1
(1,110)	1:11:Z:MVA:HN1	1:11:Z:MVA:HG22	17	0.1
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG23	17	0.1
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG21	17	0.1
(1,110)	1:11:Z:MVA:HN2	1:11:Z:MVA:HG22	17	0.1
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG23	17	0.1
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG21	17	0.1
(1,110)	1:11:Z:MVA:HN3	1:11:Z:MVA:HG22	17	0.1
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	4	0.1
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	7	0.1
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	16	0.1
(1,105)	1:10:Z:MLE:HA	1:10:Z:MLE:HB2	17	0.1
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN1	11	0.1
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN2	11	0.1
(1,85)	1:8:Z:DAL:H	1:11:Z:MVA:HN3	11	0.1
(1,84)	1:8:Z:DAL:H	1:8:Z:DAL:HB3	13	0.1
(1,84)	1:8:Z:DAL:H	1:8:Z:DAL:HB3	20	0.1
(1,70)	1:6:Z:MLE:HA	1:7:Z:ALA:H	2	0.1
(1,48)	1:4:Z:MLE:HB3	1:5:Z:VAL:H	16	0.1
(1,27)	1:2:Z:ABA:H	1:6:Z:MLE:HA	5	0.1
(1,25)	1:2:Z:ABA:H	1:5:Z:VAL:H	13	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	3	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	5	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	8	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	9	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	10	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	12	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	14	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	16	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	17	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	18	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	19	0.1
(1,21)	1:2:Z:ABA:H	1:2:Z:ABA:HA	20	0.1
(1,12)	1:1:Z:BMT:HA	1:7:Z:ALA:H	19	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found