Full wwPDB NMR Structure Validation Report (i)

Oct 27, 2026 – 04:27 PM JST

PDB ID	:	25NZ / pdb_000025nz
BMRB ID	:	36843
Title	:	Solution structure of the DNA-binding domain of Escherichia coli H-NS in complex with DNA
Authors	:	Wang, J.Y.; Xia, B.
Deposited on	:	2026-04-10

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

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

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

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

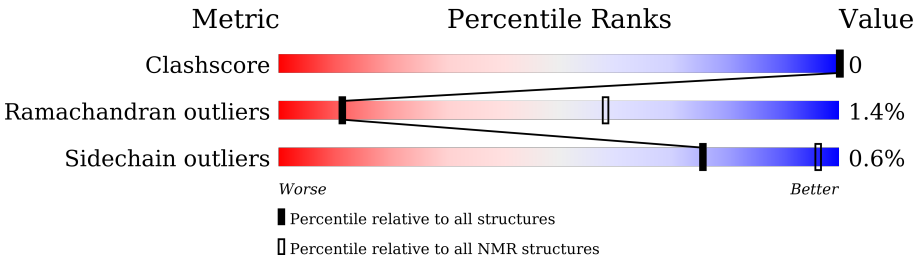
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.3.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 54%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	62	73% . 24%
2	B	12	92% 8%
2	C	12	83% 17%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:89-A:135 (47)	0.48	7

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18
2	15, 20
Single-model clusters	3; 6; 19

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1762 atoms, of which 774 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-binding protein H-NS.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	62	1000	311	498	97	92	2	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	MET	-	initiating methionine	UNP P0ACF8
A	138	LEU	-	expression tag	UNP P0ACF8
A	139	GLU	-	expression tag	UNP P0ACF8
A	140	HIS	-	expression tag	UNP P0ACF8
A	141	HIS	-	expression tag	UNP P0ACF8
A	142	HIS	-	expression tag	UNP P0ACF8
A	143	HIS	-	expression tag	UNP P0ACF8
A	144	HIS	-	expression tag	UNP P0ACF8
A	145	HIS	-	expression tag	UNP P0ACF8

- Molecule 2 is a DNA chain called Top1-DNA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	12	381	118	138	44	70	11	0
			Total	C	H	N	O	P	
2	C	12	381	118	138	44	70	11	0

4 Residue-property plots

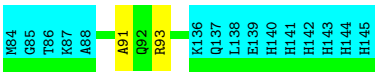
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: DNA-binding protein H-NS

Chain A:

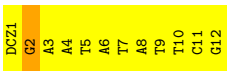




• Molecule 2: Top1-DNA

Chain B:

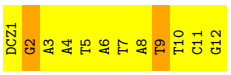




• Molecule 2: Top1-DNA

Chain C:





4.2 Scores per residue for each member of the ensemble

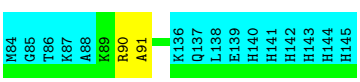
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DNA-binding protein H-NS

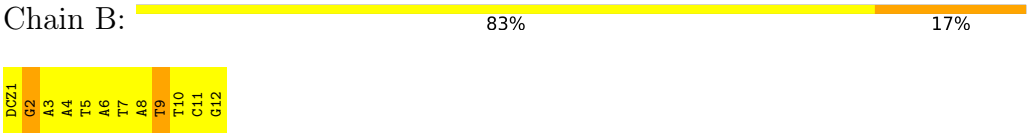
Chain A:





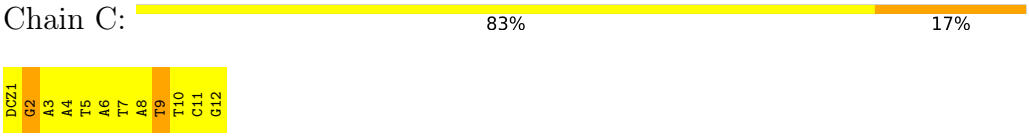
• Molecule 2: Top1-DNA

Chain B:



• Molecule 2: Top1-DNA

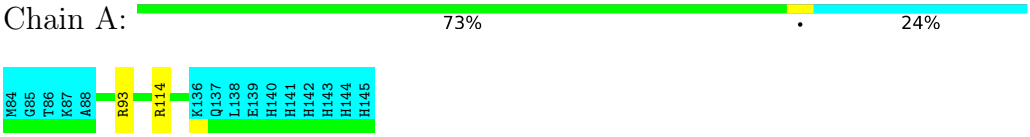
Chain C:



4.2.2 Score per residue for model 2

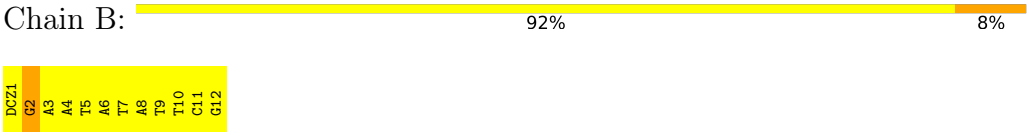
• Molecule 1: DNA-binding protein H-NS

Chain A:



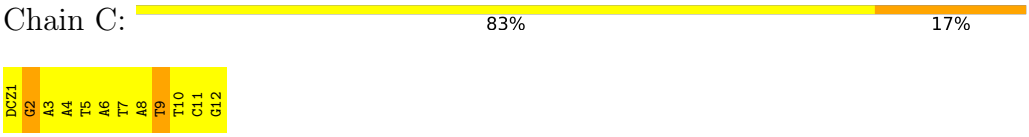
• Molecule 2: Top1-DNA

Chain B:



• Molecule 2: Top1-DNA

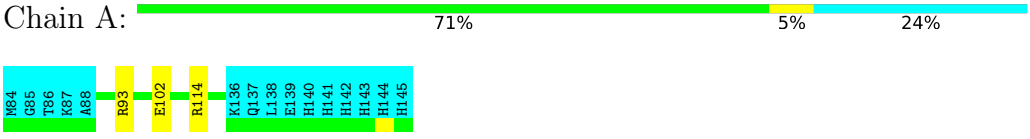
Chain C:



4.2.3 Score per residue for model 3

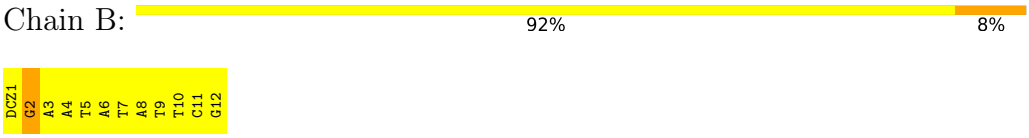
• Molecule 1: DNA-binding protein H-NS

Chain A:



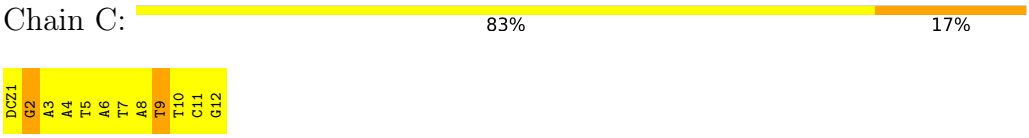
• Molecule 2: Top1-DNA

Chain B:



• Molecule 2: Top1-DNA

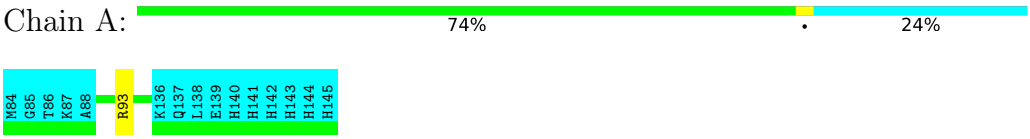
Chain C:



4.2.4 Score per residue for model 4

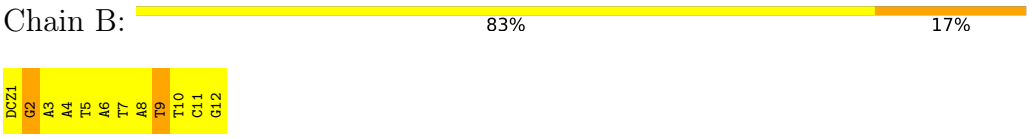
• Molecule 1: DNA-binding protein H-NS

Chain A:



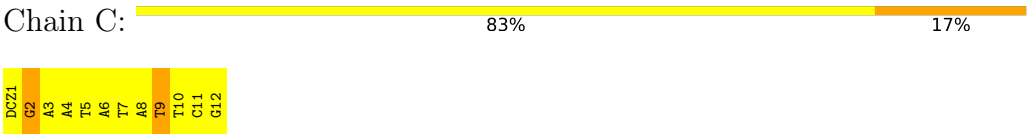
• Molecule 2: Top1-DNA

Chain B:



• Molecule 2: Top1-DNA

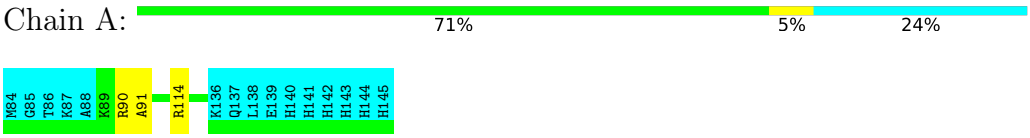
Chain C:



4.2.5 Score per residue for model 5

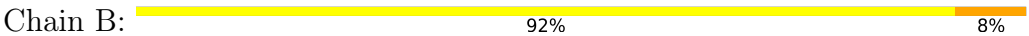
• Molecule 1: DNA-binding protein H-NS

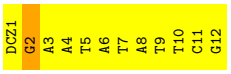
Chain A:



• Molecule 2: Top1-DNA

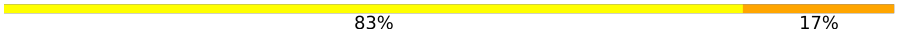
Chain B:

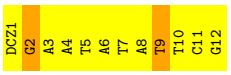




• Molecule 2: Top1-DNA

Chain C:



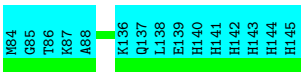


4.2.6 Score per residue for model 6

• Molecule 1: DNA-binding protein H-NS

Chain A:

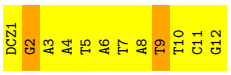




• Molecule 2: Top1-DNA

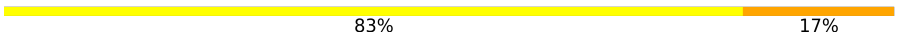
Chain B:

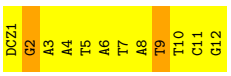




• Molecule 2: Top1-DNA

Chain C:



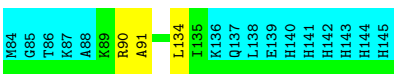


4.2.7 Score per residue for model 7 (medoid)

• Molecule 1: DNA-binding protein H-NS

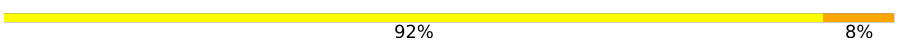
Chain A:

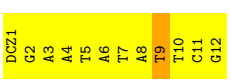




• Molecule 2: Top1-DNA

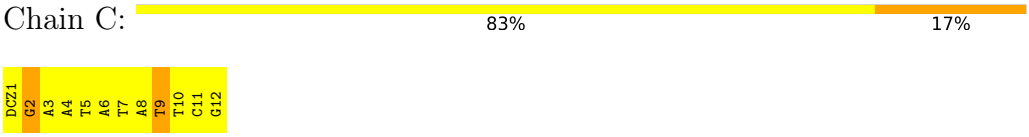
Chain B:





• Molecule 2: Top1-DNA

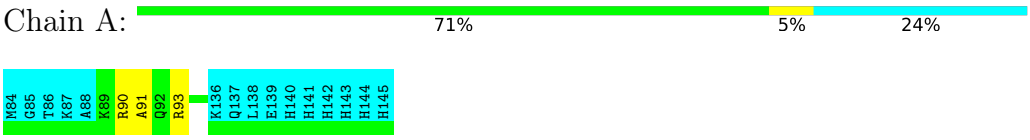
Chain C:



4.2.8 Score per residue for model 8

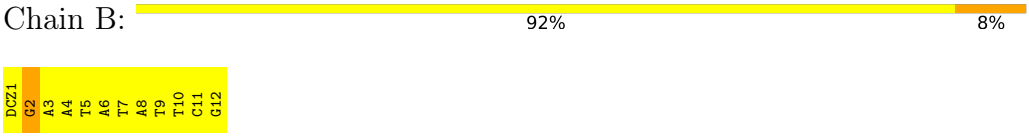
• Molecule 1: DNA-binding protein H-NS

Chain A:



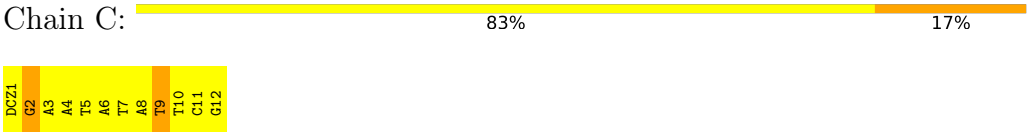
• Molecule 2: Top1-DNA

Chain B:



• Molecule 2: Top1-DNA

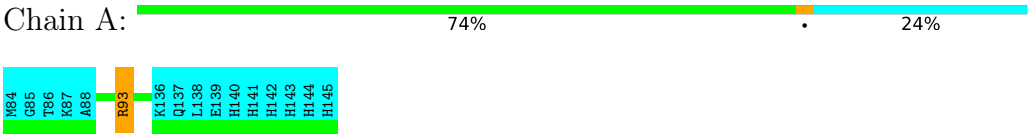
Chain C:



4.2.9 Score per residue for model 9

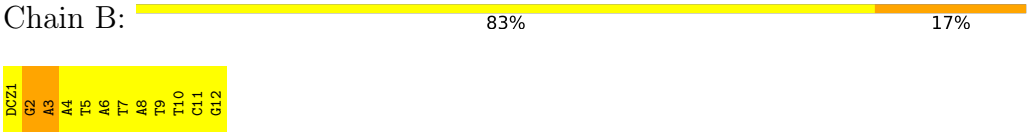
• Molecule 1: DNA-binding protein H-NS

Chain A:



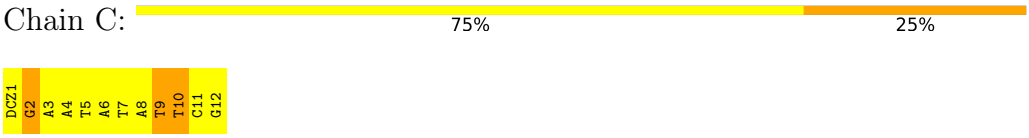
• Molecule 2: Top1-DNA

Chain B:



• Molecule 2: Top1-DNA

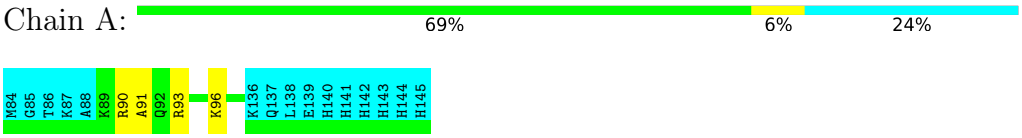
Chain C:



4.2.10 Score per residue for model 10

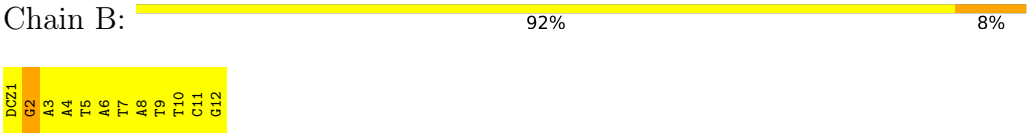
- Molecule 1: DNA-binding protein H-NS

Chain A:



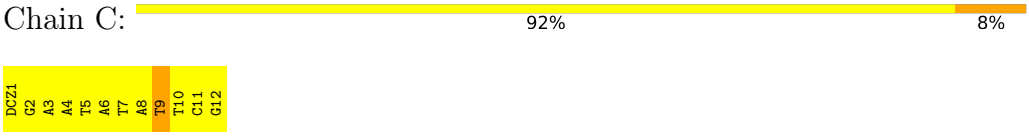
- Molecule 2: Top1-DNA

Chain B:



- Molecule 2: Top1-DNA

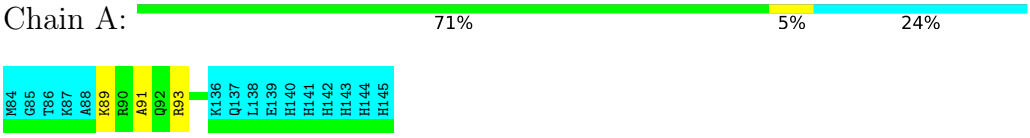
Chain C:



4.2.11 Score per residue for model 11

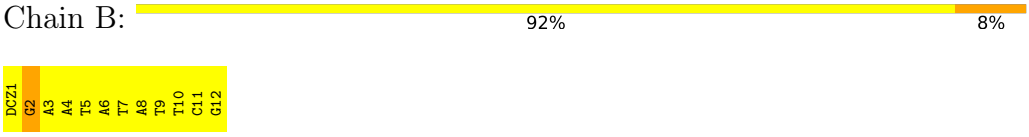
- Molecule 1: DNA-binding protein H-NS

Chain A:



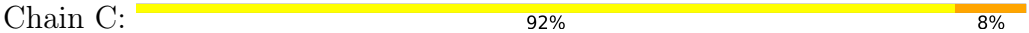
- Molecule 2: Top1-DNA

Chain B:



- Molecule 2: Top1-DNA

Chain C:



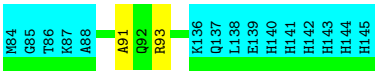


4.2.12 Score per residue for model 12

• Molecule 1: DNA-binding protein H-NS

Chain A:

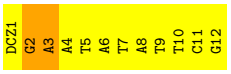




• Molecule 2: Top1-DNA

Chain B:

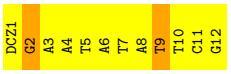




• Molecule 2: Top1-DNA

Chain C:



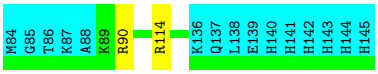


4.2.13 Score per residue for model 13

• Molecule 1: DNA-binding protein H-NS

Chain A:

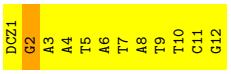




• Molecule 2: Top1-DNA

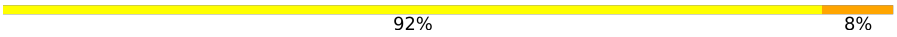
Chain B:





• Molecule 2: Top1-DNA

Chain C:



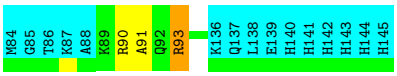


4.2.14 Score per residue for model 14

• Molecule 1: DNA-binding protein H-NS

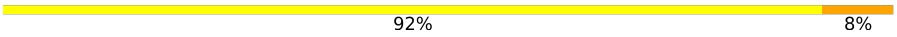
Chain A:

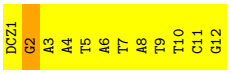




• Molecule 2: Top1-DNA

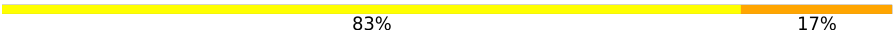
Chain B:





• Molecule 2: Top1-DNA

Chain C:



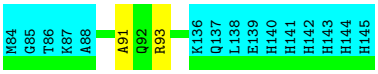


4.2.15 Score per residue for model 15

• Molecule 1: DNA-binding protein H-NS

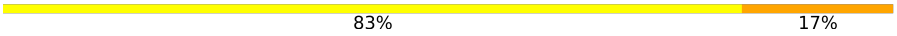
Chain A:





• Molecule 2: Top1-DNA

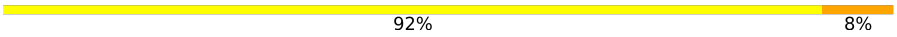
Chain B:

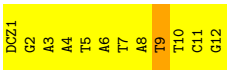




• Molecule 2: Top1-DNA

Chain C:



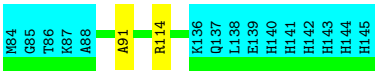


4.2.16 Score per residue for model 16

• Molecule 1: DNA-binding protein H-NS

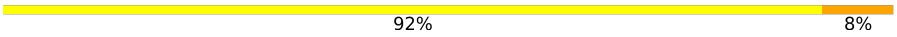
Chain A:

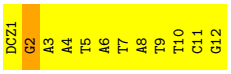




• Molecule 2: Top1-DNA

Chain B:





• Molecule 2: Top1-DNA

Chain C:



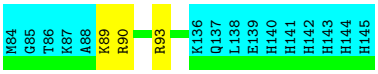


4.2.17 Score per residue for model 17

• Molecule 1: DNA-binding protein H-NS

Chain A:

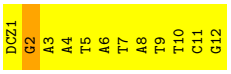




• Molecule 2: Top1-DNA

Chain B:

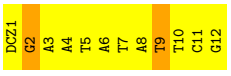




• Molecule 2: Top1-DNA

Chain C:



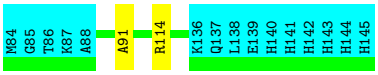


4.2.18 Score per residue for model 18

• Molecule 1: DNA-binding protein H-NS

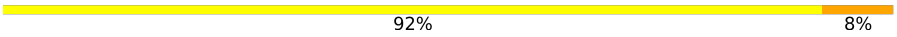
Chain A:

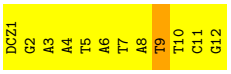




• Molecule 2: Top1-DNA

Chain B:





• Molecule 2: Top1-DNA

Chain C:



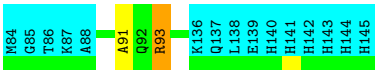


4.2.19 Score per residue for model 19

• Molecule 1: DNA-binding protein H-NS

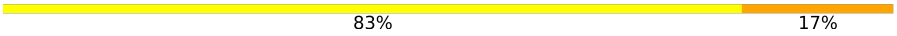
Chain A:





• Molecule 2: Top1-DNA

Chain B:

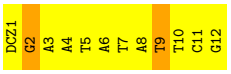




• Molecule 2: Top1-DNA

Chain C:



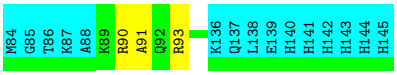


4.2.20 Score per residue for model 20

• Molecule 1: DNA-binding protein H-NS

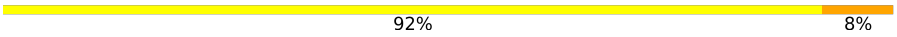
Chain A:

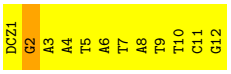




• Molecule 2: Top1-DNA

Chain B:





• Molecule 2: Top1-DNA

Chain C:





5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	structure calculation	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	806
Number of shifts mapped to atoms	728
Number of unparsed shifts	0
Number of shifts with mapping errors	78
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

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: DCZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.88±0.01	0±0/381 (0.0± 0.0%)	1.35±0.03	1±0/512 (0.1± 0.1%)
2	B	1.75±0.01	0±0/254 (0.0± 0.0%)	2.62±0.02	30±1/390 (7.6± 0.2%)
2	C	1.75±0.01	0±0/254 (0.0± 0.0%)	2.61±0.01	31±1/390 (8.0± 0.3%)
All	All	1.44	0/17780 (0.0%)	2.20	1228/25840 (4.8%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.7
2	B	0.0±0.0	1.4±0.5
2	C	0.0±0.0	1.7±0.6
All	All	0	80

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	8	DA	N1-C6-N6	-10.50	112.30	118.60	1	20
2	B	4	DA	N1-C6-N6	-10.40	112.36	118.60	8	20
2	B	8	DA	N1-C6-N6	-9.75	112.75	118.60	3	20
2	C	6	DA	N1-C6-N6	-9.23	113.06	118.60	3	20
2	B	6	DA	N1-C6-N6	-9.20	113.08	118.60	13	20
2	B	9	DT	O5'-C5'-C4'	8.83	116.46	109.40	3	20
2	B	6	DA	O5'-C5'-C4'	8.78	116.42	109.40	12	20
2	C	8	DA	O5'-C5'-C4'	8.43	116.14	109.40	13	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	4	DA	C5-C6-N1	8.36	121.88	117.70	18	20
2	B	3	DA	N1-C6-N6	-8.32	113.61	118.60	4	20
2	C	3	DA	C5-C6-N1	8.28	121.84	117.70	2	20
2	C	4	DA	N1-C6-N6	-8.11	113.73	118.60	11	20
2	B	8	DA	C5-C6-N1	7.93	121.67	117.70	4	20
2	B	3	DA	C5-C6-N1	7.81	121.61	117.70	11	20
2	C	11	DC	O5'-C5'-C4'	7.77	115.61	109.40	9	20
2	C	6	DA	C5-C6-N1	7.75	121.57	117.70	12	20
2	C	11	DC	N3-C2-O2	-7.71	116.50	121.90	4	20
2	B	4	DA	C4-C5-C6	-7.67	113.17	117.00	9	20
2	B	11	DC	N3-C2-O2	-7.63	116.56	121.90	12	20
2	C	3	DA	N1-C6-N6	-7.61	114.03	118.60	20	20
2	B	6	DA	C4-C5-C6	-7.59	113.21	117.00	12	20
2	B	6	DA	C5-C6-N1	7.52	121.46	117.70	19	20
2	B	4	DA	C5-C6-N1	7.39	121.39	117.70	1	20
2	B	4	DA	O5'-C5'-C4'	7.35	115.28	109.40	12	20
2	C	8	DA	C5-C6-N1	7.34	121.37	117.70	9	20
2	B	5	DT	O5'-C5'-C4'	7.33	115.26	109.40	14	20
2	C	6	DA	C4-C5-C6	-7.17	113.42	117.00	18	20
2	C	8	DA	C4-C5-C6	-7.13	113.43	117.00	10	20
2	B	8	DA	C4-C5-C6	-7.08	113.46	117.00	17	20
2	C	11	DC	O4'-C1'-N1	7.02	112.92	108.00	17	14
2	C	4	DA	C4-C5-C6	-7.01	113.50	117.00	5	20
2	B	3	DA	O5'-C5'-C4'	6.99	114.99	109.40	18	20
2	B	3	DA	C4-C5-C6	-6.94	113.53	117.00	4	20
2	C	3	DA	C4-C5-C6	-6.93	113.53	117.00	6	20
2	C	12	DG	O5'-C5'-C4'	6.89	114.91	109.40	11	18
2	B	9	DT	N3-C2-O2	-6.87	118.18	122.30	15	19
2	B	5	DT	N3-C2-O2	-6.61	118.33	122.30	15	20
2	C	10	DT	N3-C2-O2	-6.60	118.34	122.30	11	20
2	C	3	DA	O5'-C5'-C4'	6.48	114.59	109.40	1	20
2	C	10	DT	O5'-C5'-C4'	6.43	114.55	109.40	2	11
2	B	11	DC	O5'-C5'-C4'	6.39	114.52	109.40	7	20
2	C	9	DT	O4'-C4'-C3'	6.39	109.83	106.00	6	19
2	B	12	DG	O5'-C5'-C4'	6.38	114.50	109.40	11	20
1	A	93	ARG	NE-CZ-NH2	6.33	124.90	119.20	15	11
2	B	2	DG	N1-C6-O6	-6.29	116.13	119.90	8	20
2	C	4	DA	O5'-C5'-C4'	6.13	114.30	109.40	17	20
2	B	7	DT	N3-C2-O2	-6.10	118.64	122.30	1	20
2	B	11	DC	N1-C2-O2	6.05	122.53	118.90	1	20
2	B	2	DG	O5'-C5'-C4'	5.98	114.18	109.40	9	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	9	DT	N3-C2-O2	-5.95	118.73	122.30	12	19
2	C	9	DT	O5'-C5'-C4'	5.95	114.16	109.40	3	12
2	C	6	DA	O5'-C5'-C4'	5.94	114.15	109.40	15	16
2	B	10	DT	N3-C2-O2	-5.89	118.77	122.30	19	20
2	C	2	DG	O5'-C5'-C4'	5.84	114.08	109.40	6	20
2	C	5	DT	O5'-C5'-C4'	5.81	114.05	109.40	15	18
2	C	11	DC	N1-C2-O2	5.81	122.38	118.90	4	20
2	C	7	DT	O5'-C5'-C4'	5.69	113.95	109.40	19	18
2	C	7	DT	N3-C2-O2	-5.66	118.90	122.30	8	19
2	C	2	DG	N1-C6-O6	-5.63	116.52	119.90	13	20
2	C	12	DG	N1-C6-O6	-5.61	116.53	119.90	9	18
2	B	12	DG	N1-C6-O6	-5.58	116.55	119.90	2	18
2	C	5	DT	O4'-C1'-N1	5.56	111.89	108.00	18	1
2	C	11	DC	N3-C4-C5	5.48	124.09	121.90	19	3
2	B	7	DT	O4'-C4'-C3'	5.47	109.28	106.00	6	8
2	C	5	DT	N3-C2-O2	-5.43	119.04	122.30	5	16
2	B	10	DT	O5'-C5'-C4'	5.42	113.74	109.40	5	1
2	B	7	DT	O5'-C5'-C4'	5.29	113.63	109.40	3	7
2	C	7	DT	O4'-C1'-N1	5.25	111.68	108.00	18	2
2	B	6	DA	C1'-O4'-C4'	-5.23	104.87	110.10	15	2
2	B	10	DT	O4'-C1'-N1	5.22	111.66	108.00	18	3
1	A	114	ARG	NE-CZ-NH2	5.20	123.88	119.20	18	1
2	B	5	DT	C5-C6-N1	-5.19	120.59	123.70	9	3
2	B	8	DA	O5'-C5'-C4'	5.12	113.50	109.40	11	3
2	B	8	DA	O4'-C4'-C3'	5.09	109.05	106.00	3	1
2	B	11	DC	N3-C4-C5	5.08	123.93	121.90	18	5
2	C	4	DA	O4'-C4'-C3'	5.08	109.05	106.00	9	1
2	C	6	DA	O4'-C4'-C3'	5.01	109.01	106.00	18	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	C	9	DT	Sidechain	20
2	B	2	DG	Sidechain	18
2	C	2	DG	Sidechain	13
1	A	90	ARG	Sidechain	9
2	B	9	DT	Sidechain	7
1	A	93	ARG	Sidechain	5
1	A	114	ARG	Sidechain	5

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Mol	Chain	Res	Type	Group	Models (Total)
2	B	3	DA	Sidechain	2
2	C	10	DT	Sidechain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	17200	12980	12980	-

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is -.

There are no clashes.

6.3 Torsion angles

6.3.1 Protein backbone

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	A	47/62 (76%)	45±1 (96±1%)	1±1 (2±2%)	1±0 (1±1%)	11	58
All	All	940/1240 (76%)	907 (96%)	20 (2%)	13 (1%)	11	58

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	91	ALA	13

6.3.2 Protein sidechains

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	A	39/52 (75%)	39±0 (99±1%)	0±0 (1±1%)	76 96
All	All	780/1040 (75%)	775 (99%)	5 (1%)	76 96

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	89	LYS	2
1	A	102	GLU	1
1	A	134	LEU	1
1	A	96	LYS	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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
2	DCZ	B	1	2	17,17,17	0.59±0.01	0±0 (0±0%)
2	DCZ	C	1	2	17,17,17	0.59±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	DCZ	B	1	2	24,24,24	1.12±0.02	1±0 (4±0%)
2	DCZ	C	1	2	24,24,24	1.13±0.01	1±0 (4±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DCZ	B	1	2	-	0±0,6,18,18	0±0,2,2,2
2	DCZ	C	1	2	-	0±0,6,18,18	0±0,2,2,2

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	1	DCZ	O2-C2-N3	3.61	116.46	122.33	19	20
2	B	1	DCZ	O2-C2-N3	3.57	116.52	122.33	14	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no oligosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 54% for the well-defined parts and 57% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_ output*

7.1.1 Bookkeeping

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	806
Number of shifts mapped to atoms	728
Number of unparsed shifts	0
Number of shifts with mapping errors	78
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 78 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	DC	H5’	3.704	.	1
1	A	146	DC	H5”	3.665	.	1
1	A	146	DC	H4’	4.023	.	1
1	A	146	DC	H3’	4.637	.	1
1	A	146	DC	H2’	1.729	.	1
1	A	146	DC	H2”	2.278	.	1
1	A	146	DC	H1’	5.657	.	1
1	A	146	DC	HN1	7.922	.	2
1	A	146	DC	HN2	6.996	.	2
1	A	146	DC	H5	5.832	.	4
1	A	146	DC	H6	7.543	.	4
1	A	147	DG	H5’	4.042	.	1
1	A	147	DG	H5”	3.924	.	1
1	A	147	DG	H4’	4.263	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	DG	H3'	4.96	.	1
1	A	147	DG	H2'	2.653	.	1
1	A	147	DG	H2"	2.726	.	1
1	A	147	DG	H1'	5.304	.	1
1	A	147	DG	H8	7.896	.	1
1	A	147	DG	H1	12.835	.	1
1	A	148	DA	H5'	4.125	.	1
1	A	148	DA	H5"	4.201	.	1
1	A	148	DA	H4'	4.45	.	1
1	A	148	DA	H3'	5.074	.	1
1	A	148	DA	H2'	2.732	.	1
1	A	148	DA	H2"	2.921	.	1
1	A	148	DA	H1'	6.006	.	1
1	A	148	DA	H8	8.155	.	4
1	A	148	DA	H2	7.351	.	4
1	A	150	DT	H5'	4.265	.	1
1	A	150	DT	H5"	4.149	.	1
1	A	150	DT	H4'	4.149	.	1
1	A	150	DT	H3'	4.843	.	1
1	A	150	DT	H2'	2.027	.	1
1	A	150	DT	H2"	2.463	.	1
1	A	150	DT	H1'	5.653	.	1
1	A	150	DT	H3	13.098	.	1
1	A	150	DT	H5M	1.358	.	1
1	A	150	DT	H6	7.032	.	1
1	?	.	DT	H5'	4.159	.	1
1	?	.	DT	H5"	4.095	.	1
1	?	.	DT	H4'	4.22	.	1
1	?	.	DT	H3'	4.871	.	1
1	?	.	DT	H2'	2.118	.	1
1	?	.	DT	H2"	2.47	.	1
1	?	.	DT	H1'	6.062	.	1
1	?	.	DT	H3	13.806	.	4
1	?	.	DT	H5M	1.574	.	1
1	?	.	DT	H6	7.381	.	4
1	?	.	DC	H5'	4.076	.	1
1	?	.	DC	H5"	4.076	.	1
1	?	.	DC	H4'	4.127	.	1
1	?	.	DC	H3'	4.839	.	1
1	?	.	DC	H2'	2.027	.	1
1	?	.	DC	H2"	2.355	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	.	DC	H1'	5.682	.	1
1	?	.	DC	HN1	8.569	.	2
1	?	.	DC	HN2	7.016	.	2
1	?	.	DC	H5	5.708	.	4
1	?	.	DC	H6	7.487	.	4
1	?	.	DG	H5'	4.084	.	1
1	?	.	DG	H5"	4.084	.	1
1	?	.	DG	H4'	4.179	.	1
1	?	.	DG	H3'	4.684	.	1
1	?	.	DG	H2'	2.618	.	1
1	?	.	DG	H2"	2.364	.	1
1	?	.	DG	H1'	6.136	.	1
1	?	.	DG	H8	7.923	.	1
1	?	.	DG	H1	12.835	.	1
1	?	.	DA	H5'	4.125	.	1
1	?	.	DA	H5"	4.201	.	1
1	?	.	DA	H4'	4.45	.	1
1	?	.	DA	H3'	5.074	.	1
1	?	.	DA	H2'	2.732	.	1
1	?	.	DA	H2"	2.921	.	1
1	?	.	DA	H1'	6.006	.	1
1	?	.	DA	H8	8.155	.	1
1	?	.	DA	H2	7.351	.	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	61	0.15 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	56	-0.08 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	56	-0.07 ± 0.32	None needed (< 0.5 ppm)
^{15}N	57	-0.85 ± 0.33	Should be applied

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 54%, i.e. 581 atoms were assigned a chemical shift out of a possible 1067. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	225/235 (96%)	91/96 (95%)	90/94 (96%)	44/45 (98%)
Sidechain	318/364 (87%)	210/232 (91%)	101/113 (89%)	7/19 (37%)
Aromatic	38/40 (95%)	19/19 (100%)	18/20 (90%)	1/1 (100%)
Sugar	0/264 (0%)	0/154 (0%)	0/110 (0%)	0/0 (—%)
Base	0/164 (0%)	0/98 (0%)	0/40 (0%)	0/26 (0%)
Overall	581/1067 (54%)	320/599 (53%)	209/377 (55%)	52/91 (57%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 57%, i.e. 727 atoms were assigned a chemical shift out of a possible 1285. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	292/311 (94%)	118/127 (93%)	117/124 (94%)	57/60 (95%)
Sidechain	397/458 (87%)	262/293 (89%)	127/143 (89%)	8/22 (36%)
Aromatic	38/88 (43%)	19/43 (44%)	18/32 (56%)	1/13 (8%)
Sugar	0/264 (0%)	0/154 (0%)	0/110 (0%)	0/0 (—%)
Base	0/164 (0%)	0/98 (0%)	0/40 (0%)	0/26 (0%)
Overall	727/1285 (57%)	399/715 (56%)	262/449 (58%)	66/121 (55%)

7.1.4 Statistically unusual chemical shifts (i)

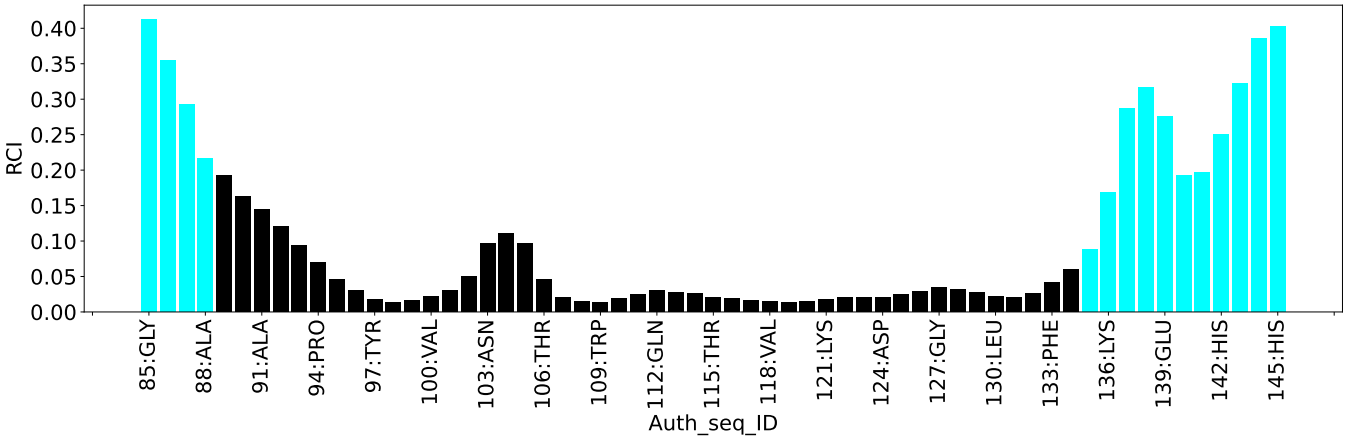
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	116	PRO	HD2	1.57	1.93 – 5.38	-6.0
1	A	116	PRO	HD3	1.59	1.76 – 5.48	-5.5

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 A:


RCI
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
85:GLY
88:ALA
91:ALA
94:PRO
97:TYR
100:VAL
103:ASN
106:THR
109:TRP
112:GLN
115:THR
118:VAL
121:LYS
124:ASP
127:GLY
130:LEU
133:PHE
136:LYS
139:GLU
142:HIS
145:HIS
Auth_seq_ID

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	3730
Intra-residue (|i-j|=0)	1632
Sequential (|i-j|=1)	1056
Medium range (|i-j|>1 and |i-j|<5)	363
Long range (|i-j|≥5)	364
Inter-chain	229
Hydrogen bond restraints	86
Disulfide bond restraints	0
Total dihedral-angle restraints	547
Number of unmapped restraints	0
Number of restraints per residue	49.7
Number of long range restraints per residue[1]	4.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	3.0	0.15
0.2-0.5 (Medium)	0.9	0.28
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.1	2.46
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

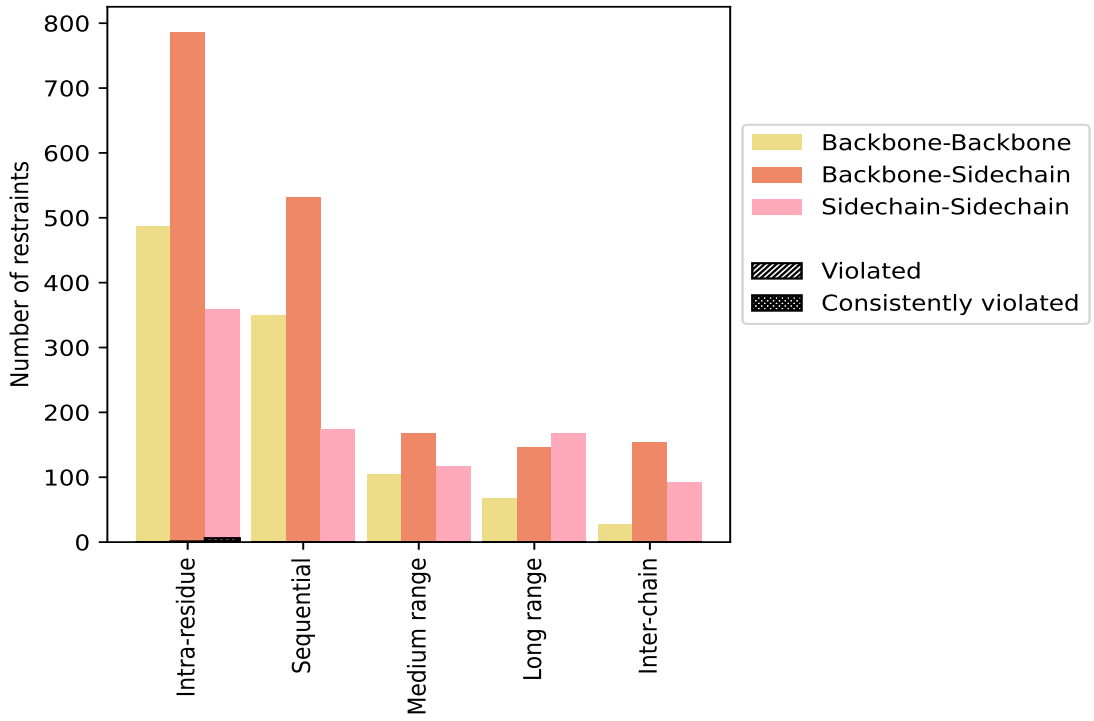
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	1632	43.8	7	0.4	0.2	2	0.1	0.1
Backbone-Backbone	487	13.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	786	21.1	1	0.1	0.0	0	0.0	0.0
Sidechain-Sidechain	359	9.6	6	1.7	0.2	2	0.6	0.1
Sequential (|i-j|=1)	1056	28.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	350	9.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	532	14.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	174	4.7	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	363	9.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	84	2.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	163	4.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	116	3.1	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	364	9.8	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	52	1.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	144	3.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	168	4.5	0	0.0	0.0	0	0.0	0.0
Inter-chain	229	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	28	0.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	153	4.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	48	1.3	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	86	2.3	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3730	100.0	7	0.2	0.2	2	0.1	0.1
Backbone-Backbone	1037	27.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1784	47.8	1	0.1	0.0	0	0.0	0.0
Sidechain-Sidechain	909	24.4	6	0.7	0.2	2	0.2	0.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	4	0	0	0	0	4	0.16	0.28	0.07	0.12
2	3	0	0	0	0	3	0.18	0.27	0.07	0.15
3	5	0	0	0	0	5	0.15	0.27	0.06	0.12
4	2	0	0	0	0	2	0.19	0.27	0.08	0.19
5	3	0	0	0	0	3	0.18	0.27	0.07	0.15
6	6	0	0	0	0	6	0.14	0.25	0.05	0.12
7	5	0	0	0	0	5	0.12	0.14	0.01	0.11
8	4	0	0	0	0	4	0.16	0.27	0.06	0.13
9	5	0	0	0	0	5	0.14	0.26	0.06	0.11
10	4	0	0	0	0	4	0.16	0.26	0.06	0.13

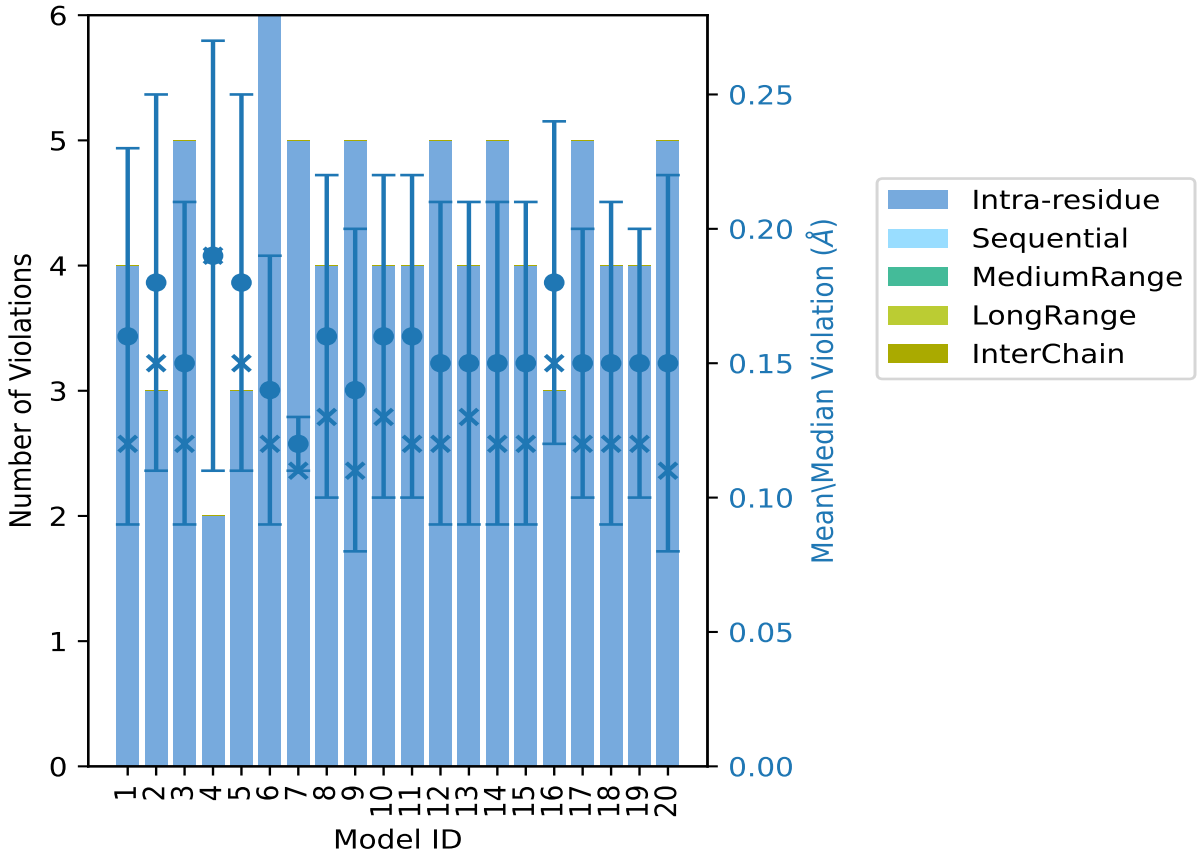
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	4	0	0	0	0	4	0.16	0.26	0.06	0.12
12	5	0	0	0	0	5	0.15	0.26	0.06	0.12
13	4	0	0	0	0	4	0.15	0.25	0.06	0.13
14	5	0	0	0	0	5	0.15	0.26	0.06	0.12
15	4	0	0	0	0	4	0.15	0.26	0.06	0.12
16	3	0	0	0	0	3	0.18	0.27	0.06	0.15
17	5	0	0	0	0	5	0.15	0.25	0.05	0.12
18	4	0	0	0	0	4	0.15	0.26	0.06	0.12
19	4	0	0	0	0	4	0.15	0.23	0.05	0.12
20	5	0	0	0	0	5	0.15	0.28	0.07	0.11

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

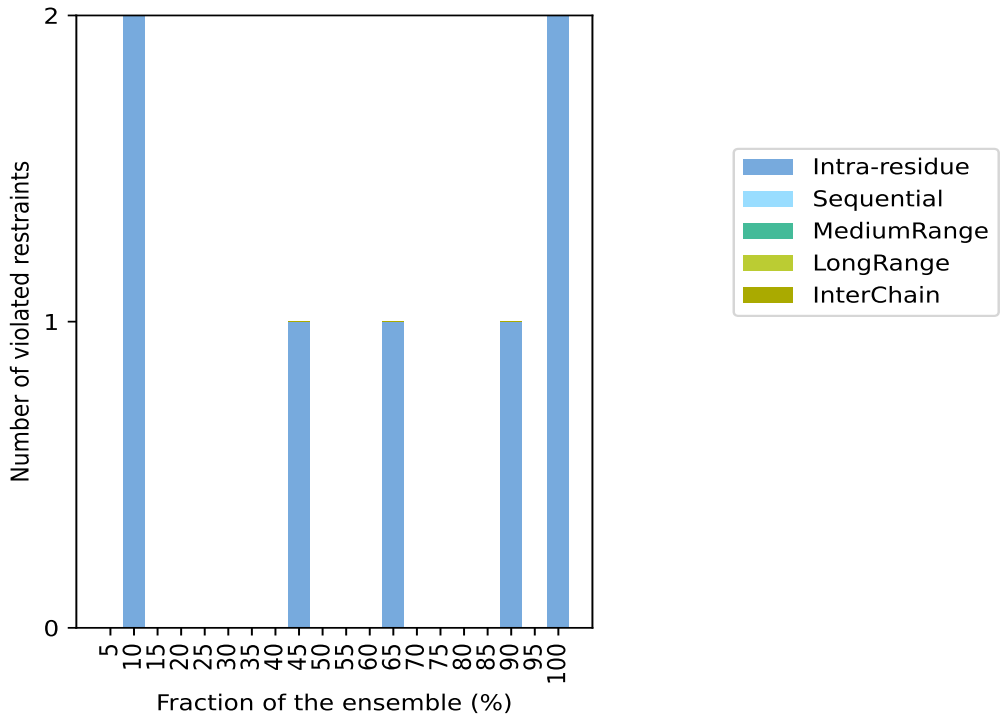
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3637(IR:1625, SQ:1056, MR:363, LR:364, IC:229) restraints are not violated in the ensemble.

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

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

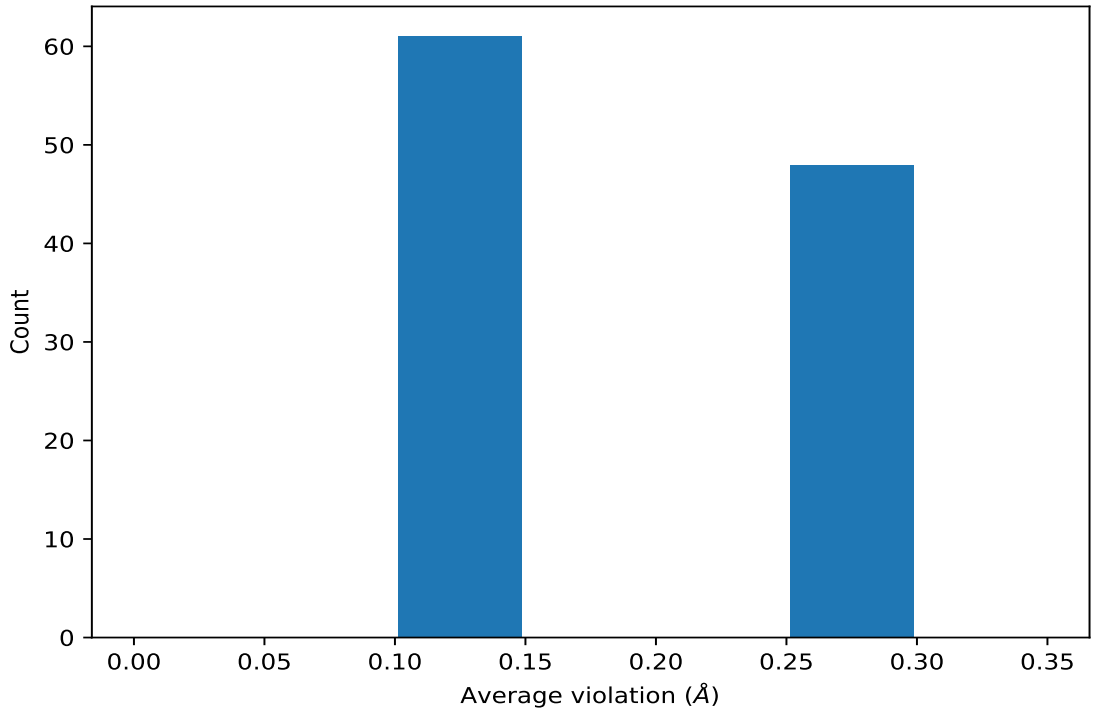
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of theviolation 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)
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	20	0.26	0.03	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	20	0.26	0.03	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	20	0.26	0.03	0.26
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	20	0.11	0.0	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	20	0.11	0.0	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	20	0.11	0.0	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	20	0.11	0.0	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	20	0.11	0.0	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	20	0.11	0.0	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	20	0.11	0.0	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	20	0.11	0.0	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	20	0.11	0.0	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	20	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	20	0.11	0.0	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	20	0.11	0.0	0.11
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	18	0.14	0.01	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	18	0.14	0.01	0.14
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	13	0.12	0.01	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	13	0.12	0.01	0.12
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	9	0.1	0.0	0.1
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD2	2	0.12	0.01	0.12
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD3	2	0.12	0.01	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD2	2	0.12	0.01	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD3	2	0.12	0.01	0.12

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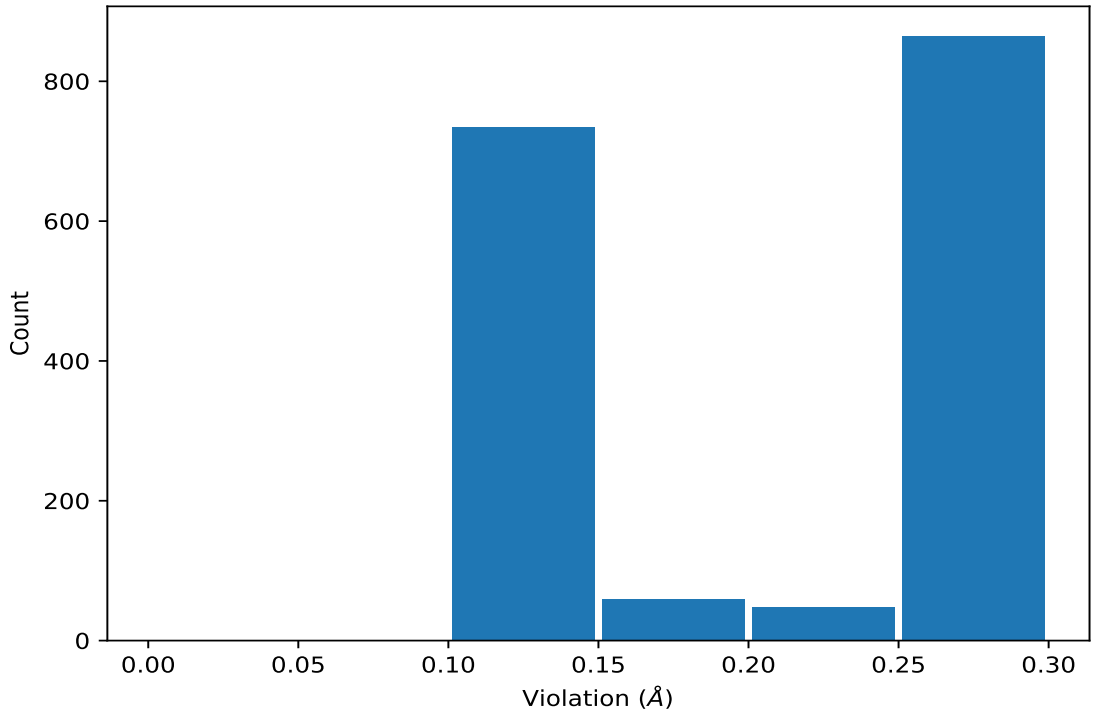
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD2	2	0.12	0.01	0.12
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD3	2	0.12	0.01	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD2	2	0.12	0.01	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD3	2	0.12	0.01	0.12
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD2	2	0.12	0.01	0.12
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD3	2	0.12	0.01	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD2	2	0.12	0.01	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD3	2	0.12	0.01	0.12
(1,2250)	2:11:C:DC:H2”	2:11:C:DC:H6	2	0.11	0.0	0.11

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

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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



9.5.2 Table : All distance violations

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

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	1	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	1	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	20	0.28
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	20	0.28
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	2	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	2	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	3	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	3	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	4	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	4	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	5	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	5	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	8	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	8	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	16	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	16	0.27
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	16	0.27
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	9	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	9	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	10	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	10	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	11	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	11	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	12	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	12	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	12	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	14	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	14	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	15	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	15	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	18	0.26
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	18	0.26
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	6	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	6	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	13	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	13	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	17	0.25
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	17	0.25
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	19	0.23
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	19	0.23
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	19	0.23
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	2	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	2	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	2	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	2	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	2	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	2	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	2	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	2	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	2	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	2	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	2	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	3	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	3	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	3	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	3	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	3	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	3	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	3	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	3	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	3	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	3	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	3	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	3	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	5	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	5	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	5	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	5	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	5	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	5	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	5	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	5	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	5	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	5	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	5	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	5	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	13	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	13	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	13	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	13	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	13	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	13	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	13	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	13	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	13	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	13	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	13	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	13	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	16	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	16	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	16	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	16	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	16	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	16	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	16	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	16	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	16	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	16	0.15
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	16	0.15
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	6	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	6	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	6	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	6	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	6	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	6	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	6	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	6	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	6	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	6	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	6	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	6	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	7	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	7	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	7	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	7	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	7	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	7	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	7	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	7	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	7	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	7	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	7	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	7	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	8	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	8	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	8	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	8	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	8	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	8	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	8	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	8	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	8	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	8	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	8	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	10	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	10	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	10	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	10	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	10	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	10	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	10	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	10	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	10	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	10	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	10	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	10	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	17	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	17	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	17	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	17	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	17	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	17	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	17	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	17	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	17	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	17	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	17	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	17	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	19	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	19	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	19	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	19	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	19	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	19	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	19	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	19	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	19	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	19	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	19	0.14
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	19	0.14
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	15	0.14
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	15	0.14
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	15	0.14
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	15	0.14
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	15	0.14
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	15	0.14
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	15	0.14
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	15	0.14
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	15	0.14
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	15	0.14
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	15	0.14
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD11	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD12	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD21	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD22	1:134:A:LEU:HB3	7	0.14
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB2	7	0.14
(1,298)	1:134:A:LEU:HD23	1:134:A:LEU:HB3	7	0.14
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	1	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	1	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	1	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	1	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	1	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	1	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	1	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	1	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	1	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	1	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	1	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	1	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	9	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	9	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	9	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	9	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	9	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	9	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	9	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	9	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	9	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	9	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	9	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	9	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	11	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	11	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	11	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	11	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	11	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	11	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	11	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	11	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	11	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	11	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	11	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	12	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	12	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	12	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	12	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	12	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	12	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	12	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	12	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	12	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	12	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	12	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	12	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	14	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	14	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	14	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	14	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	14	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	14	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	14	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	14	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	14	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	14	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	14	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	14	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	20	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	20	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	20	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	20	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	20	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	20	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	20	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	20	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	20	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	20	0.13
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	20	0.13
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD2	6	0.13
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD3	6	0.13
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD2	6	0.13
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD3	6	0.13
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD2	6	0.13
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD3	6	0.13
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD2	6	0.13
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD3	6	0.13
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD2	6	0.13
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD3	6	0.13
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD2	6	0.13
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD3	6	0.13
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	18	0.12
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	18	0.12
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	18	0.12
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	18	0.12
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	18	0.12
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	18	0.12
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	18	0.12
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	18	0.12
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB2	18	0.12
(1,1357)	1:114:A:ARG:HG2	1:114:A:ARG:HB3	18	0.12
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB2	18	0.12
(1,1357)	1:114:A:ARG:HG3	1:114:A:ARG:HB3	18	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	8	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	8	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	8	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	8	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	8	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	8	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	8	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	8	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	8	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	8	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	8	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	8	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	10	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	10	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	10	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	10	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	10	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	10	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	10	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	10	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	10	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	10	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	10	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	11	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	11	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	11	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	11	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	11	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	11	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	11	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	11	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	11	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	11	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	11	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	11	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	12	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	12	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	12	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	12	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	12	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	12	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	12	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	12	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	12	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	12	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	12	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	12	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	14	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	14	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	14	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	14	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	14	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	14	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	14	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	14	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	14	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	14	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	14	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	17	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	17	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	17	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	17	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	17	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	17	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	17	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	17	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	17	0.12
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	17	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	17	0.12
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	17	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	16	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	16	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	16	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	16	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	16	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	16	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	16	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	16	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	16	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	16	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	16	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	16	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	17	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	17	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	17	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	17	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	17	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	17	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	17	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	17	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	17	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	17	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	17	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	17	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	18	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	18	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	18	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	18	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	18	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	18	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	18	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	18	0.12
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	18	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	18	0.12
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	18	0.12
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD2	3	0.12
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD3	3	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD2	3	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD3	3	0.12
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD2	3	0.12
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD3	3	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD2	3	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD3	3	0.12
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD2	3	0.12
(1,1153)	1:107:A:LYS:HG2	1:107:A:LYS:HD3	3	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD2	3	0.12
(1,1153)	1:107:A:LYS:HG3	1:107:A:LYS:HD3	3	0.12
(1,2250)	2:11:C:DC:H2”	2:11:C:DC:H6	14	0.11
(1,2250)	2:11:C:DC:H2”	2:11:C:DC:H6	17	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	1	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	1	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	1	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	1	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	1	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	1	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	1	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	1	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	1	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	1	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	1	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	1	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	6	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	6	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	6	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	6	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	6	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	6	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	6	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	6	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	6	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	6	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	6	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	7	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	7	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	7	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	7	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	7	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	7	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	7	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	7	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	7	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	7	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	7	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	7	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	9	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	9	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	9	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	9	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	9	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	9	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	9	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	9	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	9	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	9	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	9	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	9	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	19	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	19	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	19	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	19	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	19	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	19	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	19	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	19	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	19	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	19	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	19	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	19	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	20	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	20	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	20	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	20	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	20	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	20	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	20	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG2	20	0.11
(1,1181)	1:114:A:ARG:HD2	1:114:A:ARG:HG3	20	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	20	0.11
(1,1181)	1:114:A:ARG:HD3	1:114:A:ARG:HG3	20	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	1	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	1	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	1	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	1	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	1	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	1	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	1	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	1	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	1	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	1	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	1	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	1	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	2	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	2	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	2	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	2	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	2	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	2	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	2	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	2	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	2	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	2	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	2	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	2	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	3	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	3	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	3	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	3	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	3	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	3	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	3	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	3	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	3	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	3	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	3	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	4	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	4	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	4	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	4	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	4	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	4	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	4	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	4	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	4	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	4	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	4	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	4	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	5	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	5	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	5	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	5	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	5	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	5	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	5	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	5	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	5	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	5	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	5	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	5	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	6	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	6	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	6	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	6	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	6	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	6	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	6	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	6	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	6	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	6	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	6	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	6	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	7	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	7	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	7	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	7	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	7	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	7	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	7	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	7	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	7	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	7	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	7	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	8	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	8	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	8	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	8	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	8	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	8	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	8	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	8	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	8	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	8	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	8	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	8	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	9	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	9	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	9	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	9	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	9	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	9	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	9	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	9	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	9	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	9	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	9	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	9	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	10	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	10	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	10	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	10	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	10	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	10	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	10	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	10	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	10	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	10	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	10	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	11	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	11	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	11	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	11	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	11	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	11	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	11	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	11	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	11	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	11	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	11	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	11	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	12	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	12	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	12	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	12	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	12	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	12	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	12	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	12	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	12	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	12	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	12	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	12	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	13	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	13	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	13	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	13	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	13	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	13	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	13	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	13	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	13	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	13	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	13	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	13	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	13	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	13	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	13	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	13	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	14	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	14	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	14	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	14	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	14	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	14	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	14	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	14	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	14	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	14	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	14	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	15	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	15	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	15	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	15	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	15	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	15	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	15	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	15	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	15	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	15	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	15	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	15	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	19	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	19	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	19	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	19	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	19	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	19	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	19	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	19	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	19	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	19	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	19	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	19	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	20	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	20	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	20	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	20	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	20	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	20	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	20	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	20	0.11
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG3	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:94:A:PRO:HB2	1:94:A:PRO:HG2	20	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG3	20	0.11
(1,1172)	1:94:A:PRO:HB3	1:94:A:PRO:HG2	20	0.11
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	7	0.11
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	9	0.11
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	12	0.11
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	18	0.11
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	3	0.1
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	6	0.1
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	13	0.1
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	15	0.1
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG11	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG12	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG13	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG21	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG22	1:118:A:VAL:HB	20	0.1
(1,1062)	1:118:A:VAL:HG23	1:118:A:VAL:HB	20	0.1

10 Dihedral-angle violation analysis (i)

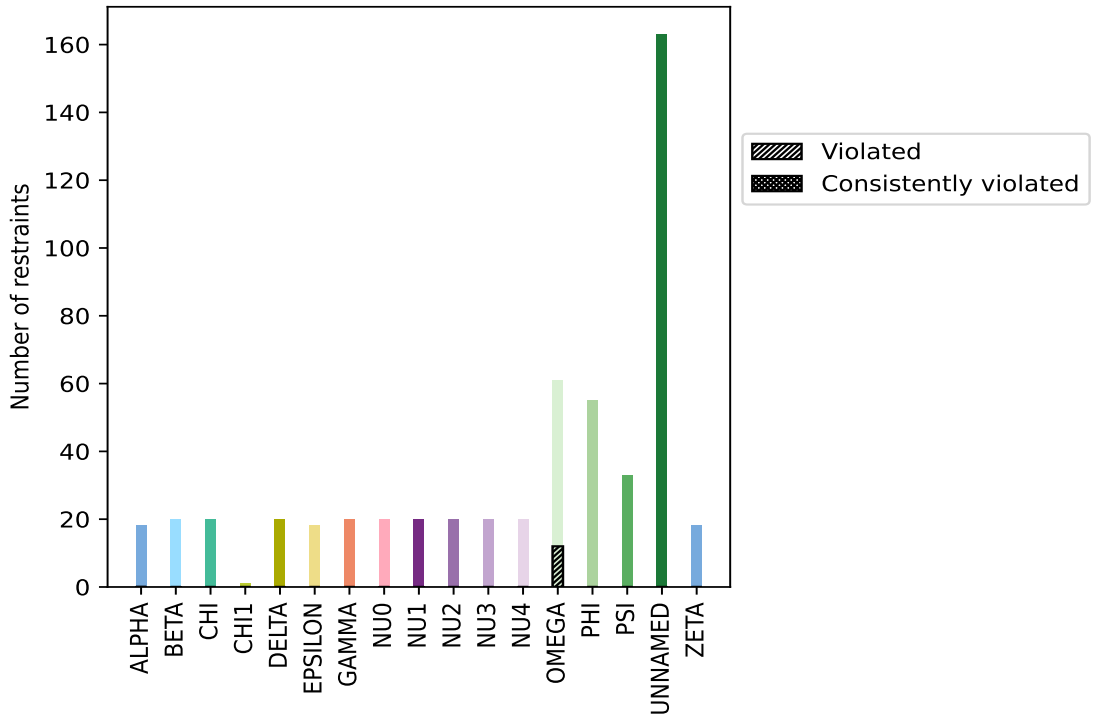
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
ALPHA	18	3.3	0	0.0	0.0	0	0.0	0.0
BETA	20	3.7	0	0.0	0.0	0	0.0	0.0
CHI	20	3.7	0	0.0	0.0	0	0.0	0.0
CHI1	1	0.2	0	0.0	0.0	0	0.0	0.0
DELTA	20	3.7	0	0.0	0.0	0	0.0	0.0
EPSILON	18	3.3	0	0.0	0.0	0	0.0	0.0
GAMMA	20	3.7	0	0.0	0.0	0	0.0	0.0
NU0	20	3.7	0	0.0	0.0	0	0.0	0.0
NU1	20	3.7	0	0.0	0.0	0	0.0	0.0
NU2	20	3.7	0	0.0	0.0	0	0.0	0.0
NU3	20	3.7	0	0.0	0.0	0	0.0	0.0
NU4	20	3.7	0	0.0	0.0	0	0.0	0.0
OMEGA	61	11.2	12	19.7	2.2	0	0.0	0.0
PHI	55	10.1	0	0.0	0.0	0	0.0	0.0
PSI	33	6.0	0	0.0	0.0	0	0.0	0.0
UNNAMED	163	29.8	0	0.0	0.0	0	0.0	0.0
ZETA	18	3.3	0	0.0	0.0	0	0.0	0.0
Total	547	100.0	12	2.2	2.2	0	0.0	0.0

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

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



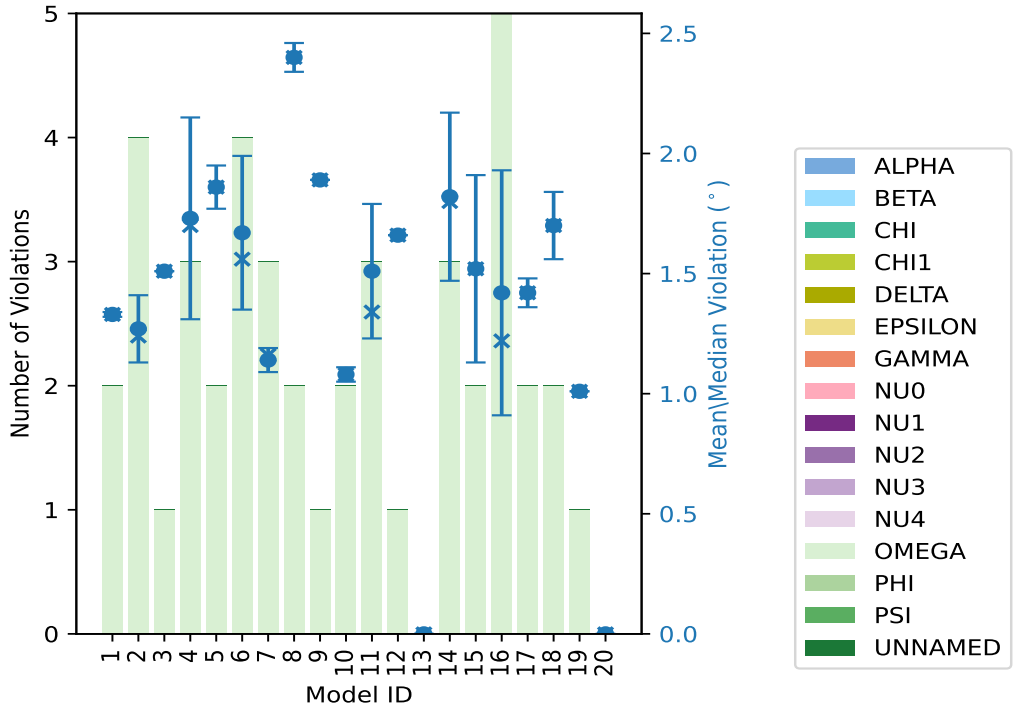
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations															
	ALPHA	BETA	CHI	CHI1	DELTA	EPSILON	GAMMA	NU0	NU1	NU2	NU3	NU4	OMEGA	PHI	PSI	UNNAME
1	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0
5	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
6	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0
8	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
9	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
10	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0
12	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0
15	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
16	0	0	0	0	0	0	0	0	0	0	0	0	5	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
18	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
19	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

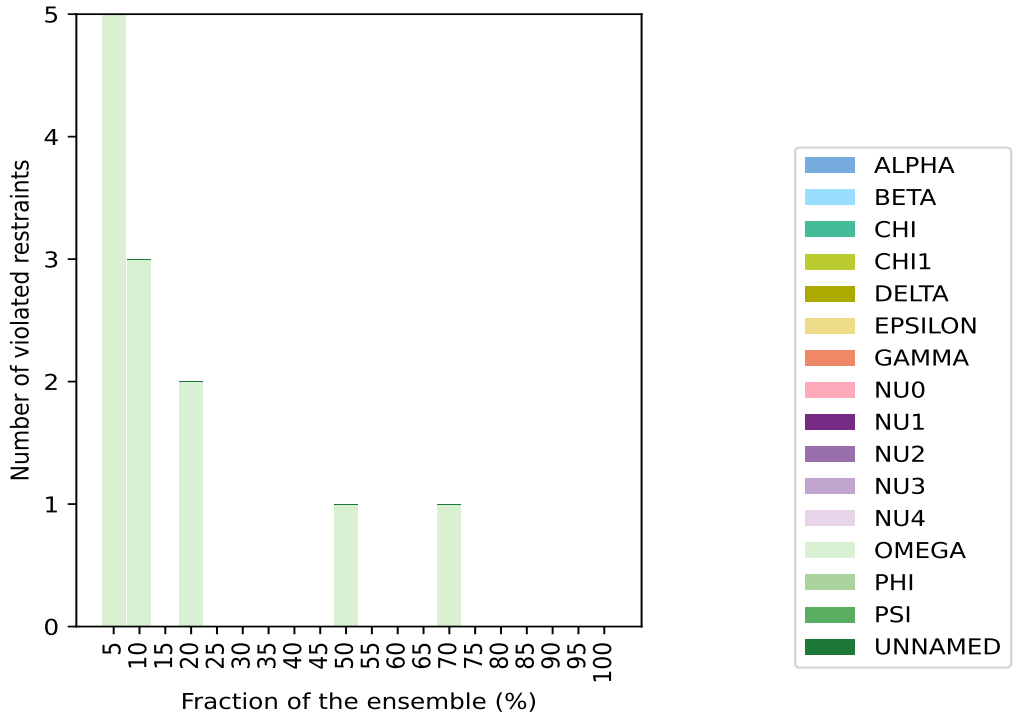
Number of violated restraints													
ALPHA	BETA	CHI	CHI1	DELTA	EPSILON	GAMMA	NU0	NU1	NU2	NU3	NU4	OMEGA	PHI
0	0	0	0	0	0	0	0	0	0	0	0	5	0
0	0	0	0	0	0	0	0	0	0	0	0	3	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	2	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

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Number of violated restraints													
ALPHA	BETA	CHI	CHI1	DELTA	EPSILON	GAMMA	NU0	NU1	NU2	NU3	NU4	OMEGA	PHI
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

[1] Number of models with violations

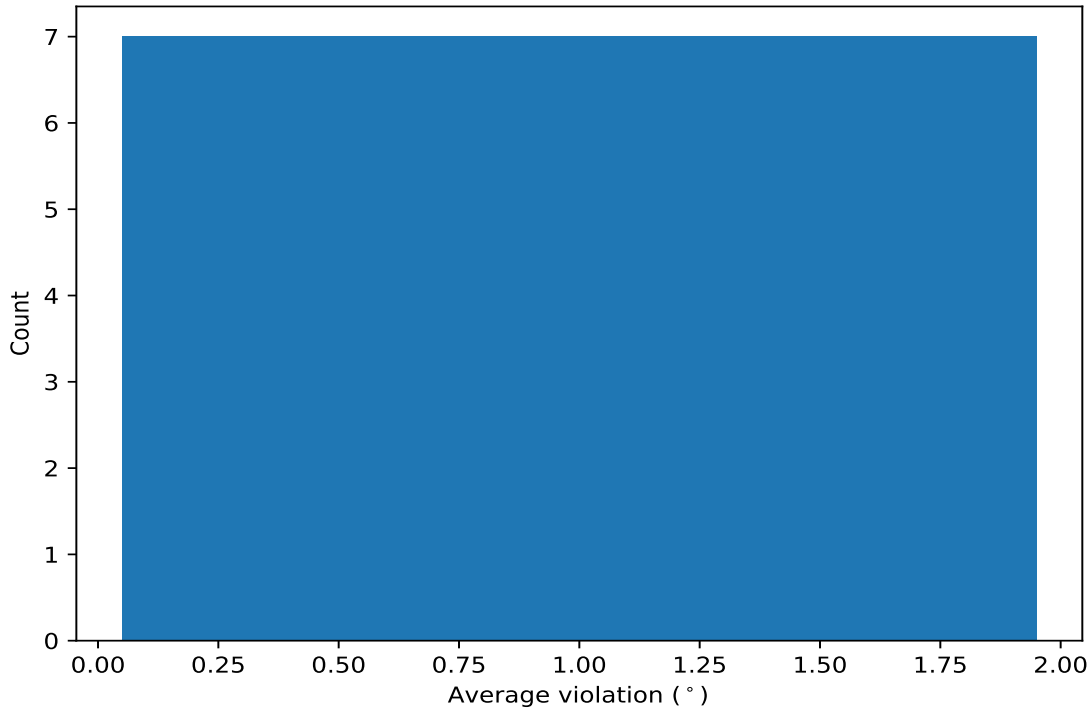
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

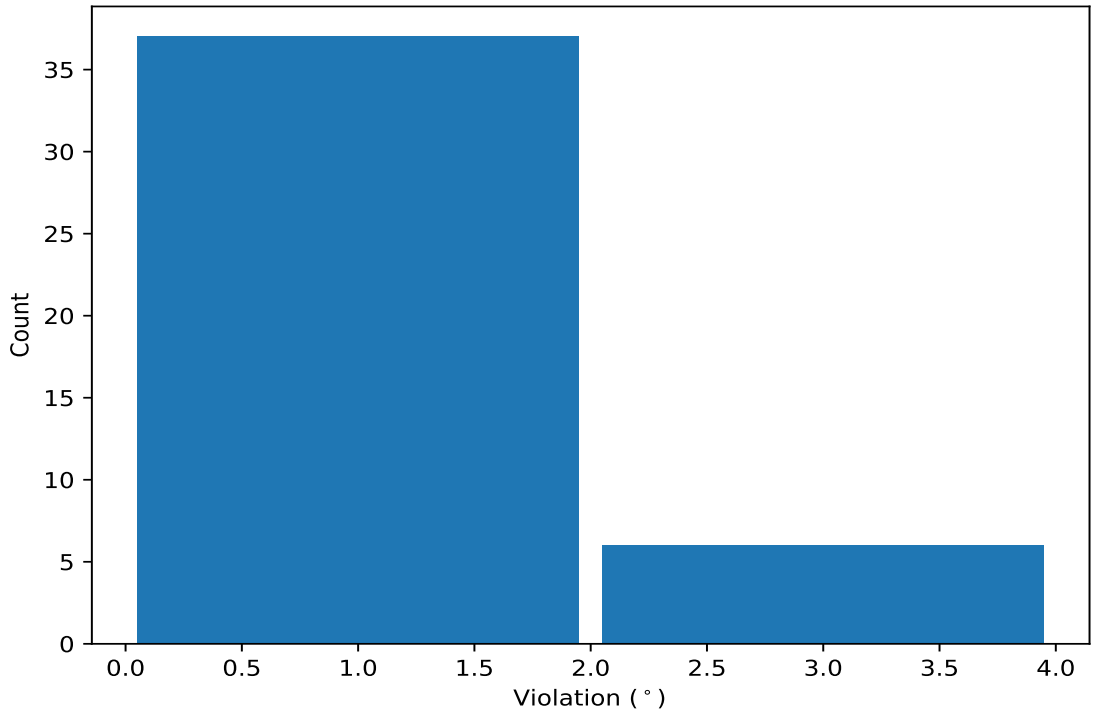
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	14	1.8	0.44	1.86
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	10	1.45	0.33	1.34
(1,279)	1:111:A:GLY:CA	1:111:A:GLY:N	1:110:A:THR:C	1:110:A:THR:CA	4	1.42	0.19	1.38
(1,297)	1:129:A:SER:CA	1:129:A:SER:N	1:128:A:LYS:C	1:128:A:LYS:CA	4	1.4	0.32	1.28
(1,268)	1:100:A:VAL:CA	1:100:A:VAL:N	1:99:A:TYR:C	1:99:A:TYR:CA	2	1.39	0.24	1.39
(1,285)	1:117:A:ALA:CA	1:117:A:ALA:N	1:116:A:PRO:C	1:116:A:PRO:CA	2	1.32	0.19	1.32
(1,313)	1:145:A:HIS:CA	1:145:A:HIS:N	1:144:A:HIS:C	1:144:A:HIS:CA	2	1.22	0.15	1.22

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	8	2.46
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	16	2.43
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	8	2.33
(1,293)	1:125:A:GLU:CA	1:125:A:GLU:N	1:124:A:ASP:C	1:124:A:ASP:CA	14	2.26
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	4	2.26
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	6	2.2
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	5	1.95
(1,297)	1:129:A:SER:CA	1:129:A:SER:N	1:128:A:LYS:C	1:128:A:LYS:CA	15	1.91
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	11	1.9
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	9	1.89
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	18	1.84
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	14	1.8
(1,306)	1:138:A:LEU:CA	1:138:A:LEU:N	1:137:A:GLN:C	1:137:A:GLN:CA	5	1.76
(1,279)	1:111:A:GLY:CA	1:111:A:GLY:N	1:110:A:THR:C	1:110:A:THR:CA	4	1.7
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	12	1.66
(1,268)	1:100:A:VAL:CA	1:100:A:VAL:N	1:99:A:TYR:C	1:99:A:TYR:CA	6	1.63
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	18	1.57
(1,285)	1:117:A:ALA:CA	1:117:A:ALA:N	1:116:A:PRO:C	1:116:A:PRO:CA	3	1.51
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	17	1.49
(1,279)	1:111:A:GLY:CA	1:111:A:GLY:N	1:110:A:THR:C	1:110:A:THR:CA	6	1.48
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	2	1.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,297)	1:129:A:SER:CA	1:129:A:SER:N	1:128:A:LYS:C	1:128:A:LYS:CA	14	1.41
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	6	1.38
(1,313)	1:145:A:HIS:CA	1:145:A:HIS:N	1:144:A:HIS:C	1:144:A:HIS:CA	17	1.36
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	11	1.34
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	1	1.34
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	2	1.33
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	1	1.32
(1,279)	1:111:A:GLY:CA	1:111:A:GLY:N	1:110:A:THR:C	1:110:A:THR:CA	11	1.28
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	16	1.26
(1,279)	1:111:A:GLY:CA	1:111:A:GLY:N	1:110:A:THR:C	1:110:A:THR:CA	16	1.22
(1,260)	1:92:A:GLN:CA	1:92:A:GLN:N	1:91:A:ALA:C	1:91:A:ALA:CA	4	1.22
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	7	1.18
(1,297)	1:129:A:SER:CA	1:129:A:SER:N	1:128:A:LYS:C	1:128:A:LYS:CA	7	1.16
(1,268)	1:100:A:VAL:CA	1:100:A:VAL:N	1:99:A:TYR:C	1:99:A:TYR:CA	2	1.15
(1,285)	1:117:A:ALA:CA	1:117:A:ALA:N	1:116:A:PRO:C	1:116:A:PRO:CA	2	1.13
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	15	1.13
(1,298)	1:130:A:LEU:CA	1:130:A:LEU:N	1:129:A:SER:C	1:129:A:SER:CA	10	1.11
(1,297)	1:129:A:SER:CA	1:129:A:SER:N	1:128:A:LYS:C	1:128:A:LYS:CA	16	1.1
(1,313)	1:145:A:HIS:CA	1:145:A:HIS:N	1:144:A:HIS:C	1:144:A:HIS:CA	16	1.07
(1,257)	1:89:A:LYS:CA	1:89:A:LYS:N	1:88:A:ALA:C	1:88:A:ALA:CA	7	1.07
(1,303)	1:135:A:ILE:CA	1:135:A:ILE:N	1:134:A:LEU:C	1:134:A:LEU:CA	10	1.05
(1,263)	1:95:A:ALA:CA	1:95:A:ALA:N	1:94:A:PRO:C	1:94:A:PRO:CA	19	1.01