



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 03:43 AM UTC

PDB ID : 5UY2 / pdb_00005uy2
BMRB ID : 30248
Title : peptide 38146 derived from fragment 41-60 of Plasmodium falciparum Thrombospondin-Related Sporozoite Protein (TRSP)
Authors : Bermudez, A.; Patarroyo, M.E.
Deposited on : 2017-02-23

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

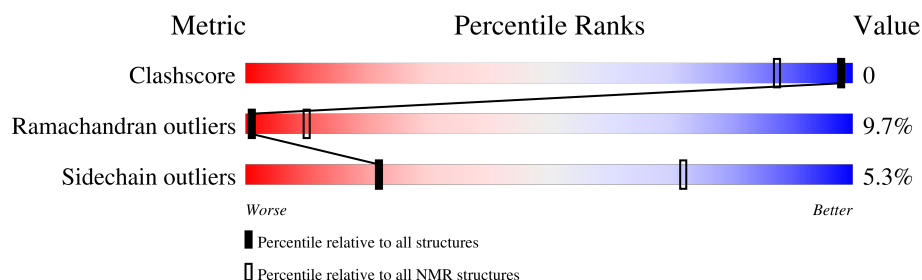
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 49%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	20	45% 55%

2 Ensemble composition and analysis ⓘ

This entry contains 24 models.

Cyrange was unable to find well-defined residues.

Error message: Only domains with < 8 residues could be identified.

NmrClust was unable to cluster the ensemble.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 335 atoms, of which 161 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 20-mer Peptide 38146.

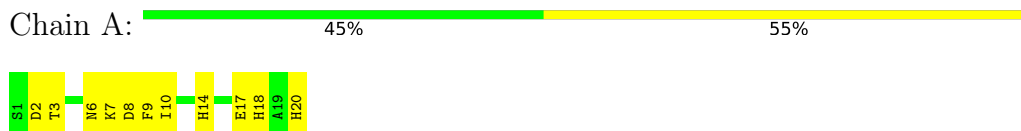
Mol	Chain	Residues	Atoms					Trace
1	A	20	Total	C	H	N	O	0
			335	105	161	35	34	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: 20-mer Peptide 38146

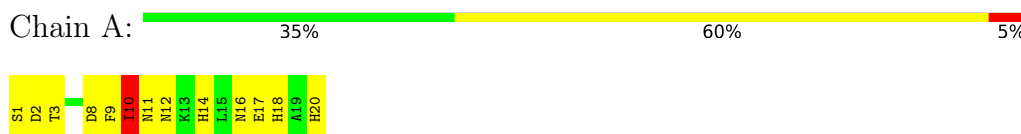


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

- Molecule 1: 20-mer Peptide 38146



4.2.2 Score per residue for model 2

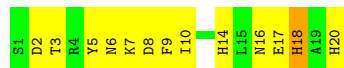
- Molecule 1: 20-mer Peptide 38146



4.2.3 Score per residue for model 3

- Molecule 1: 20-mer Peptide 38146

Chain A:  35% 60% 5%



4.2.4 Score per residue for model 4

- Molecule 1: 20-mer Peptide 38146

Chain A:  50% 45% 5%



4.2.5 Score per residue for model 5

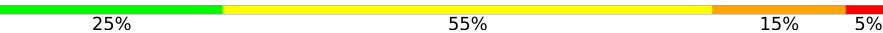
- Molecule 1: 20-mer Peptide 38146

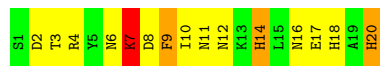
Chain A:  55% 45%



4.2.6 Score per residue for model 6

- Molecule 1: 20-mer Peptide 38146

Chain A:  25% 55% 15% 5%



4.2.7 Score per residue for model 7

- Molecule 1: 20-mer Peptide 38146

Chain A:  55% 45%



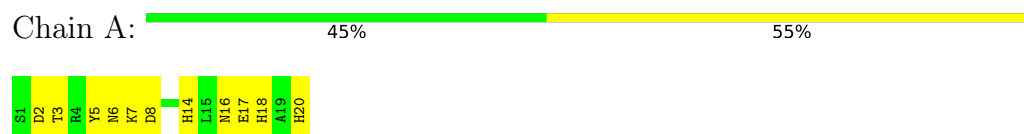
4.2.8 Score per residue for model 8

- Molecule 1: 20-mer Peptide 38146



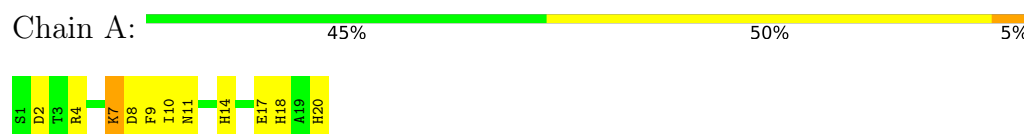
4.2.9 Score per residue for model 9

- Molecule 1: 20-mer Peptide 38146



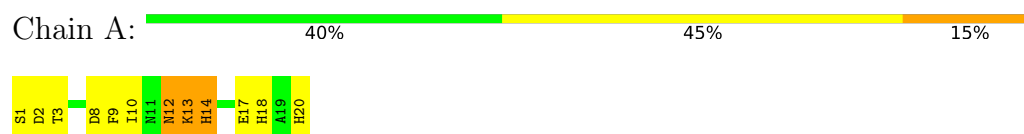
4.2.10 Score per residue for model 10

- Molecule 1: 20-mer Peptide 38146



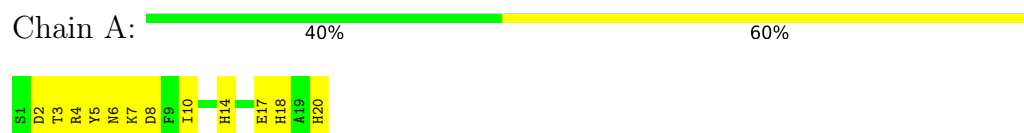
4.2.11 Score per residue for model 11

- Molecule 1: 20-mer Peptide 38146



4.2.12 Score per residue for model 12

- Molecule 1: 20-mer Peptide 38146



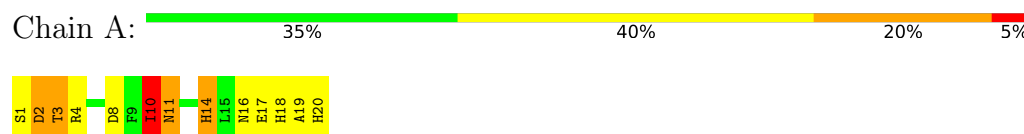
4.2.13 Score per residue for model 13

- Molecule 1: 20-mer Peptide 38146



4.2.14 Score per residue for model 14

- Molecule 1: 20-mer Peptide 38146



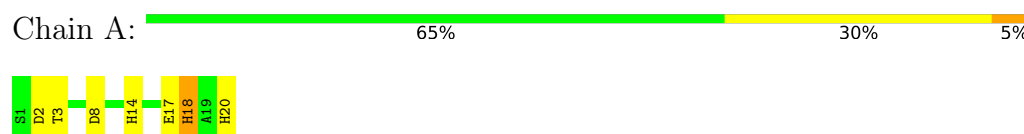
4.2.15 Score per residue for model 15

- Molecule 1: 20-mer Peptide 38146



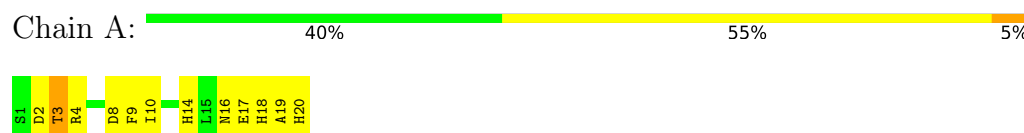
4.2.16 Score per residue for model 16

- Molecule 1: 20-mer Peptide 38146



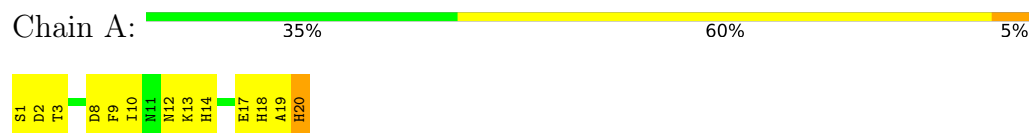
4.2.17 Score per residue for model 17

- Molecule 1: 20-mer Peptide 38146



4.2.18 Score per residue for model 18

- Molecule 1: 20-mer Peptide 38146



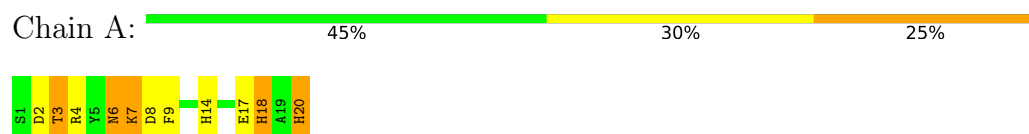
4.2.19 Score per residue for model 19

- Molecule 1: 20-mer Peptide 38146



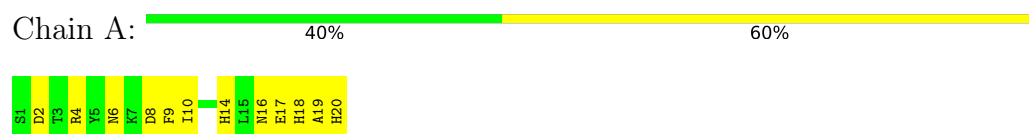
4.2.20 Score per residue for model 20

- Molecule 1: 20-mer Peptide 38146



4.2.21 Score per residue for model 21

- Molecule 1: 20-mer Peptide 38146



4.2.22 Score per residue for model 22

- Molecule 1: 20-mer Peptide 38146



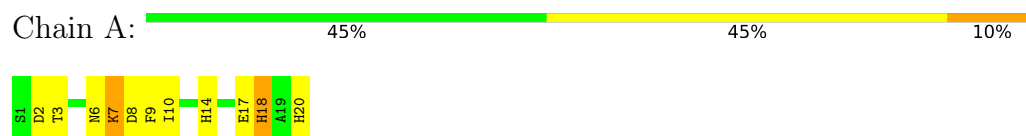
4.2.23 Score per residue for model 23

- Molecule 1: 20-mer Peptide 38146



4.2.24 Score per residue for model 24

- Molecule 1: 20-mer Peptide 38146



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-DISTANCE GEOMETRY SIMULATED A*.

Of the 50 calculated structures, 24 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
TopSpin	refinement	
Insight II	structure solution	

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	139
Number of shifts mapped to atoms	139
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	49%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	2.26±0.04	8±1/178 (4.5± 0.6%)	2.83±0.08	17±2/237 (7.1± 0.9%)
All	All	2.26	192/4272 (4.5%)	2.83	403/5688 (7.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	20	HIS	C-OXT	8.90	1.41	1.23	4	24
1	A	2	ASP	CG-OD2	6.56	1.37	1.25	10	24
1	A	17	GLU	CD-OE2	6.51	1.37	1.25	16	24
1	A	8	ASP	CG-OD2	6.51	1.37	1.25	21	24
1	A	8	ASP	CA-C	6.40	1.61	1.52	1	8
1	A	9	PHE	CA-C	6.01	1.60	1.52	19	2
1	A	20	HIS	ND1-CE1	5.61	1.38	1.32	1	24
1	A	18	HIS	ND1-CE1	5.58	1.38	1.32	1	24
1	A	8	ASP	N-CA	5.56	1.53	1.46	1	2
1	A	5	TYR	CA-C	5.54	1.60	1.52	9	1
1	A	14	HIS	ND1-CE1	5.43	1.38	1.32	17	24
1	A	9	PHE	C-N	5.17	1.40	1.33	10	2
1	A	11	ASN	CA-C	5.16	1.60	1.53	1	4
1	A	18	HIS	CE1-NE2	5.11	1.37	1.32	24	3
1	A	20	HIS	CE1-NE2	5.02	1.37	1.32	23	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	HIS	ND1-CE1-NE2	11.98	120.38	108.40	18	24
1	A	20	HIS	ND1-CE1-NE2	11.95	120.35	108.40	11	24
1	A	18	HIS	ND1-CE1-NE2	11.91	120.31	108.40	22	24
1	A	16	ASN	CA-CB-CG	11.40	124.00	112.60	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	7	LYS	CB-CA-C	10.94	128.52	110.24	10	4
1	A	18	HIS	CE1-NE2-CD2	-9.48	99.52	109.00	17	24
1	A	20	HIS	CE1-NE2-CD2	-9.47	99.53	109.00	11	24
1	A	14	HIS	CE1-NE2-CD2	-9.26	99.74	109.00	8	24
1	A	7	LYS	N-CA-C	8.58	123.04	112.23	3	3
1	A	13	LYS	N-CA-C	8.18	128.22	110.80	11	2
1	A	9	PHE	CB-CA-C	8.09	122.26	110.04	18	5
1	A	6	ASN	CA-CB-CG	7.76	120.36	112.60	6	11
1	A	7	LYS	N-CA-CB	7.65	121.48	110.16	12	4
1	A	8	ASP	CA-C-N	7.36	134.72	123.47	6	2
1	A	8	ASP	C-N-CA	7.36	134.72	123.47	6	2
1	A	12	ASN	CB-CA-C	7.17	124.70	110.42	22	2
1	A	18	HIS	CB-CG-CD2	-7.14	121.92	131.20	11	24
1	A	8	ASP	CB-CA-C	7.09	122.15	111.80	17	6
1	A	10	ILE	CB-CA-C	7.07	122.88	111.29	14	13
1	A	20	HIS	CB-CG-CD2	-6.61	122.61	131.20	6	24
1	A	1	SER	N-CA-CB	-6.61	99.26	110.50	14	1
1	A	3	THR	N-CA-C	6.41	118.83	111.02	15	3
1	A	5	TYR	N-CA-C	-6.39	97.19	110.80	22	2
1	A	18	HIS	CG-ND1-CE1	-6.33	98.54	109.30	22	24
1	A	20	HIS	CG-ND1-CE1	-6.30	98.58	109.30	7	24
1	A	5	TYR	CB-CA-C	6.29	119.87	111.82	12	1
1	A	14	HIS	CG-ND1-CE1	-6.23	98.71	109.30	8	24
1	A	2	ASP	CA-CB-CG	6.08	118.68	112.60	3	4
1	A	9	PHE	CA-CB-CG	6.03	119.83	113.80	18	6
1	A	6	ASN	CB-CA-C	-6.03	98.42	110.42	20	1
1	A	18	HIS	CA-CB-CG	5.95	119.75	113.80	11	1
1	A	3	THR	N-CA-CB	-5.89	100.54	110.49	8	2
1	A	8	ASP	N-CA-C	-5.81	103.33	110.65	24	2
1	A	8	ASP	CA-CB-CG	5.64	118.24	112.60	17	8
1	A	9	PHE	CA-C-O	-5.57	112.54	120.51	20	1
1	A	11	ASN	CB-CA-C	5.55	120.29	111.51	10	1
1	A	4	ARG	N-CA-C	-5.48	103.75	110.65	12	1
1	A	3	THR	CB-CA-C	5.45	119.63	111.89	5	4
1	A	4	ARG	NE-CZ-NH2	5.42	124.08	119.20	21	8
1	A	14	HIS	CB-CG-CD2	-5.40	124.18	131.20	8	1
1	A	5	TYR	CA-CB-CG	5.36	123.55	113.90	22	1
1	A	1	SER	CB-CA-C	5.33	120.23	110.10	1	4
1	A	12	ASN	CA-CB-CG	5.31	117.91	112.60	18	1
1	A	18	HIS	CB-CA-C	5.24	120.84	110.42	11	1
1	A	16	ASN	CB-CA-C	5.18	119.67	112.11	13	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	HIS	ND1-CG-CD2	5.11	111.21	106.10	22	14
1	A	10	ILE	N-CA-C	-5.04	98.85	109.34	10	1
1	A	19	ALA	CB-CA-C	5.03	120.43	110.42	15	2
1	A	20	HIS	ND1-CG-CD2	5.03	111.13	106.10	20	2
1	A	7	LYS	O-C-N	-5.01	115.92	122.59	19	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	174	161	157	0±0
All	All	4176	3864	3611	3

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ILE:HG22	1:A:11:ASN:H	0.54	1.62	14	1
1:A:7:LYS:C	1:A:9:PHE:H	0.52	2.11	6	1
1:A:9:PHE:C	1:A:10:ILE:HG13	0.45	2.36	1	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	18/20 (90%)	10±2 (53±10%)	7±2 (37±9%)	2±1 (10±7%)	1	10
All	All	432/480 (90%)	229 (53%)	161 (37%)	42 (10%)	1	10

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	3	THR	10
1	A	18	HIS	7
1	A	12	ASN	5
1	A	6	ASN	4
1	A	10	ILE	3
1	A	19	ALA	3
1	A	5	TYR	2
1	A	7	LYS	2
1	A	13	LYS	2
1	A	14	HIS	2
1	A	11	ASN	1
1	A	9	PHE	1

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	19/19 (100%)	18±1 (95±5%)	1±1 (5±5%)	22	72
All	All	456/456 (100%)	432 (95%)	24 (5%)	22	72

All 8 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	3	THR	7
1	A	7	LYS	6
1	A	20	HIS	4
1	A	10	ILE	2
1	A	14	HIS	2
1	A	2	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	13	LYS	1
1	A	9	PHE	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](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 49% for the well-defined parts and 49% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: 38145.txt

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	139
Number of shifts mapped to atoms	139
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 49%, i.e. 138 atoms were assigned a chemical shift out of a possible 281. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	39/100 (39%)	39/40 (98%)	0/40 (0%)	0/20 (0%)
Sidechain	85/141 (60%)	85/88 (97%)	0/44 (0%)	0/9 (0%)
Aromatic	14/40 (35%)	14/21 (67%)	0/16 (0%)	0/3 (0%)
Overall	138/281 (49%)	138/149 (93%)	0/100 (0%)	0/32 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 49%, i.e. 138 atoms were assigned a chemical shift out of a possible 281. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	39/100 (39%)	39/40 (98%)	0/40 (0%)	0/20 (0%)
Sidechain	85/141 (60%)	85/88 (97%)	0/44 (0%)	0/9 (0%)
Aromatic	14/40 (35%)	14/21 (67%)	0/16 (0%)	0/3 (0%)
Overall	138/281 (49%)	138/149 (93%)	0/100 (0%)	0/32 (0%)

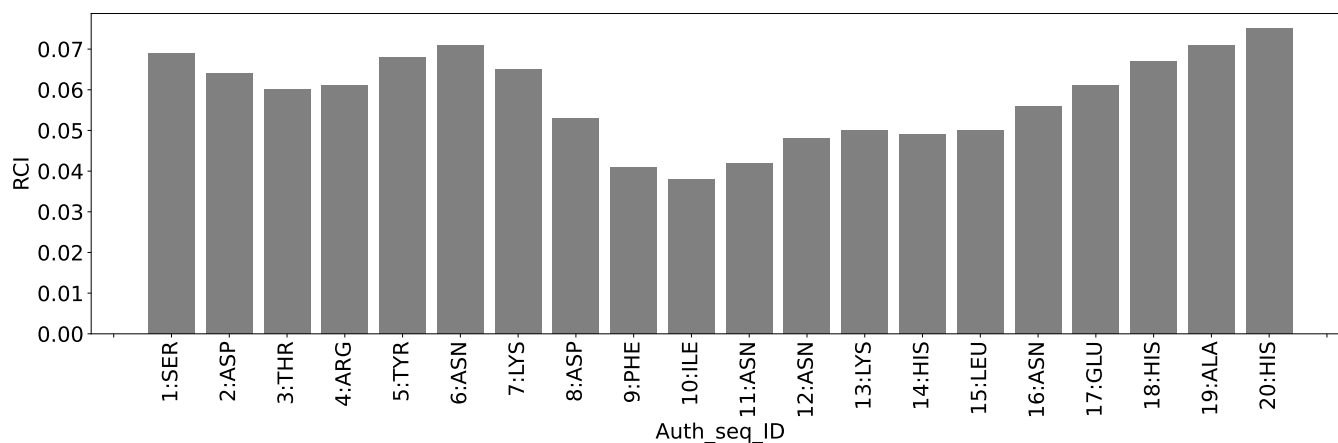
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



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	179
Intra-residue ($ i-j =0$)	109
Sequential ($ i-j =1$)	38
Medium range ($ i-j >1$ and $ i-j <5$)	28
Long range ($ i-j \geq 5$)	0
Inter-chain	0
Hydrogen bond restraints	4
Disulfide bond restraints	0
Total dihedral-angle restraints	19
Number of unmapped restraints	0
Number of restraints per residue	9.9
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	10.7	0.2
0.2-0.5 (Medium)	11.6	0.5
>0.5 (Large)	6.4	1.07

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)	4.6	3.57
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

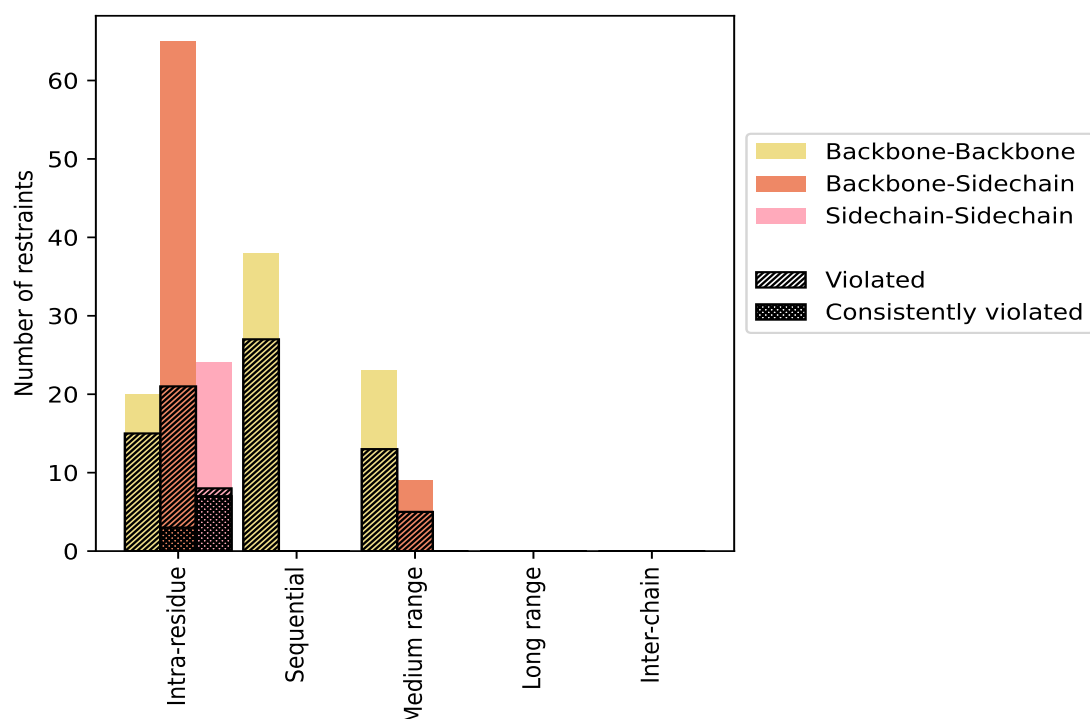
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	109	60.9	44	40.4	24.6	10	9.2	5.6
Backbone-Backbone	20	11.2	15	75.0	8.4	0	0.0	0.0
Backbone-Sidechain	65	36.3	21	32.3	11.7	3	4.6	1.7
Sidechain-Sidechain	24	13.4	8	33.3	4.5	7	29.2	3.9
Sequential (i-j =1)	38	21.2	27	71.1	15.1	0	0.0	0.0
Backbone-Backbone	38	21.2	27	71.1	15.1	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	28	15.6	15	53.6	8.4	0	0.0	0.0
Backbone-Backbone	23	12.8	13	56.5	7.3	0	0.0	0.0
Backbone-Sidechain	5	2.8	2	40.0	1.1	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	4	2.2	3	75.0	1.7	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	179	100.0	89	49.7	49.7	10	5.6	5.6
Backbone-Backbone	81	45.3	55	67.9	30.7	0	0.0	0.0
Backbone-Sidechain	74	41.3	26	35.1	14.5	3	4.1	1.7
Sidechain-Sidechain	24	13.4	8	33.3	4.5	7	29.2	3.9

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	20	6	5	0	0	31	0.3	0.83	0.23	0.23
2	19	6	3	0	0	28	0.36	0.84	0.22	0.28
3	17	4	5	0	0	26	0.34	0.83	0.2	0.32
4	18	5	5	0	0	28	0.35	0.84	0.2	0.28
5	18	2	5	0	0	25	0.38	1.07	0.27	0.29
6	23	6	4	0	0	33	0.31	0.83	0.19	0.24
7	15	3	5	0	0	23	0.34	0.83	0.23	0.31
8	21	4	4	0	0	29	0.32	0.84	0.21	0.24
9	20	5	4	0	0	29	0.3	0.83	0.2	0.22
10	21	7	5	0	0	33	0.31	0.82	0.2	0.21

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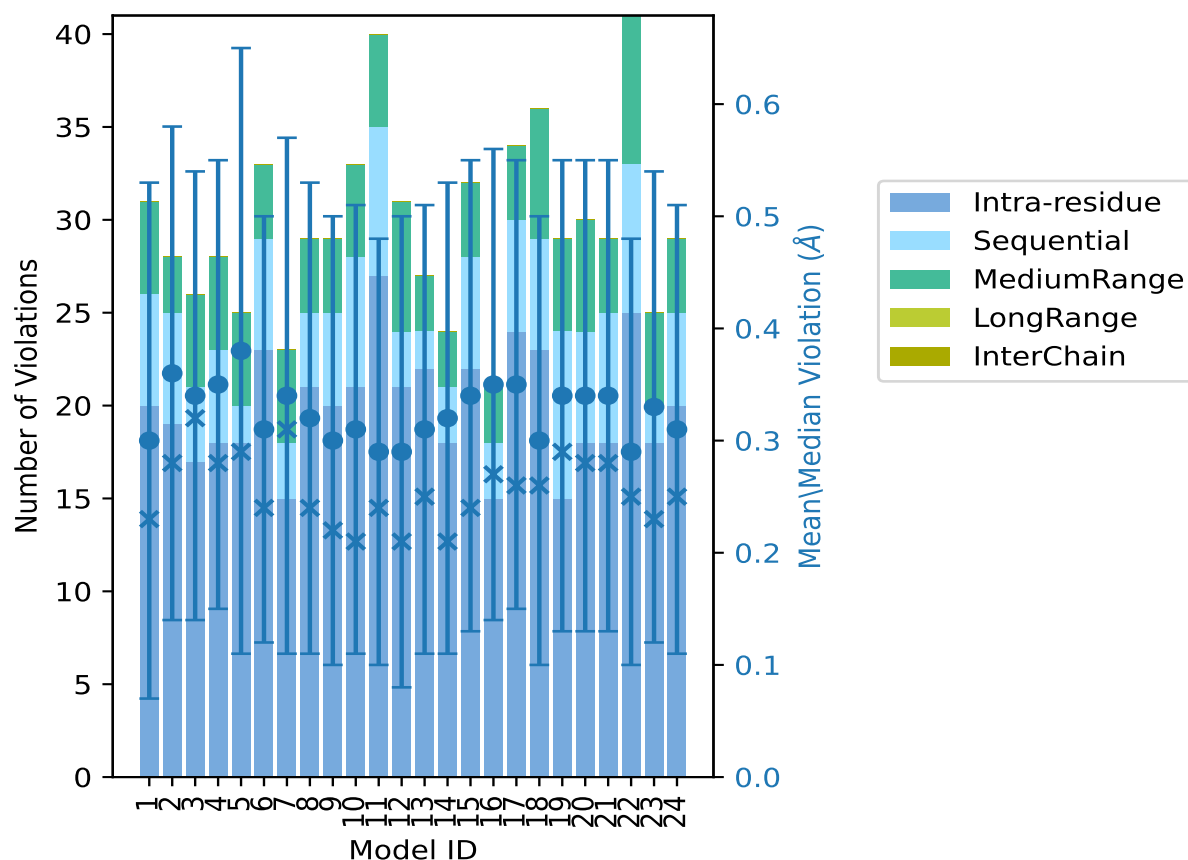
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	27	8	5	0	0	40	0.29	0.82	0.19	0.24
12	21	3	7	0	0	31	0.29	0.84	0.21	0.21
13	22	2	3	0	0	27	0.31	0.82	0.2	0.25
14	18	3	3	0	0	24	0.32	0.83	0.21	0.21
15	22	6	4	0	0	32	0.34	0.83	0.21	0.24
16	15	3	3	0	0	21	0.35	0.83	0.21	0.27
17	24	6	4	0	0	34	0.35	0.83	0.2	0.26
18	23	6	7	0	0	36	0.3	0.82	0.2	0.26
19	15	9	5	0	0	29	0.34	0.83	0.21	0.29
20	18	6	6	0	0	30	0.34	0.83	0.21	0.28
21	18	7	4	0	0	29	0.34	0.83	0.21	0.28
22	25	8	8	0	0	41	0.29	0.82	0.19	0.25
23	18	2	5	0	0	25	0.33	0.82	0.21	0.23
24	20	5	4	0	0	29	0.31	0.84	0.2	0.25

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 89(IR:65, SQ:11, MR:13, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	5	2	0	0	9	1	4.2
6	5	1	0	0	12	2	8.3
3	4	5	0	0	12	3	12.5
1	5	0	0	0	6	4	16.7
2	2	0	0	0	4	5	20.8
2	2	1	0	0	5	6	25.0

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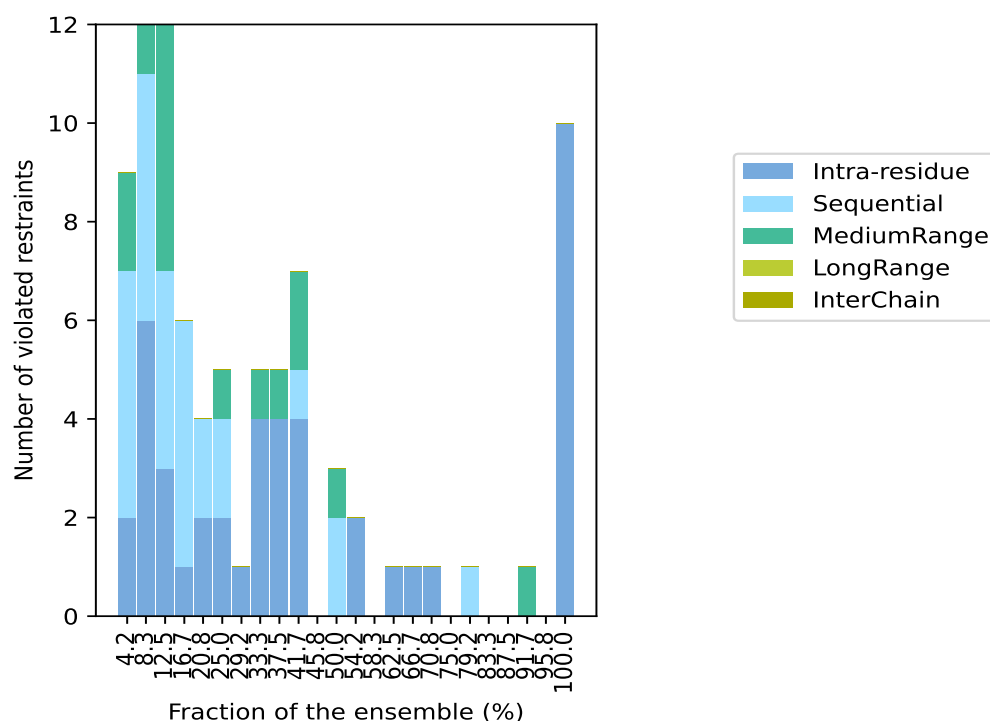
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	0	0	0	0	1	7	29.2
4	0	1	0	0	5	8	33.3
4	0	1	0	0	5	9	37.5
4	1	2	0	0	7	10	41.7
0	0	0	0	0	0	11	45.8
0	2	1	0	0	3	12	50.0
2	0	0	0	0	2	13	54.2
0	0	0	0	0	0	14	58.3
1	0	0	0	0	1	15	62.5
1	0	0	0	0	1	16	66.7
1	0	0	0	0	1	17	70.8
0	0	0	0	0	0	18	75.0
0	1	0	0	0	1	19	79.2
0	0	0	0	0	0	20	83.3
0	0	0	0	0	0	21	87.5
0	0	1	0	0	1	22	91.7
0	0	0	0	0	0	23	95.8
10	0	0	0	0	10	24	100.0

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

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

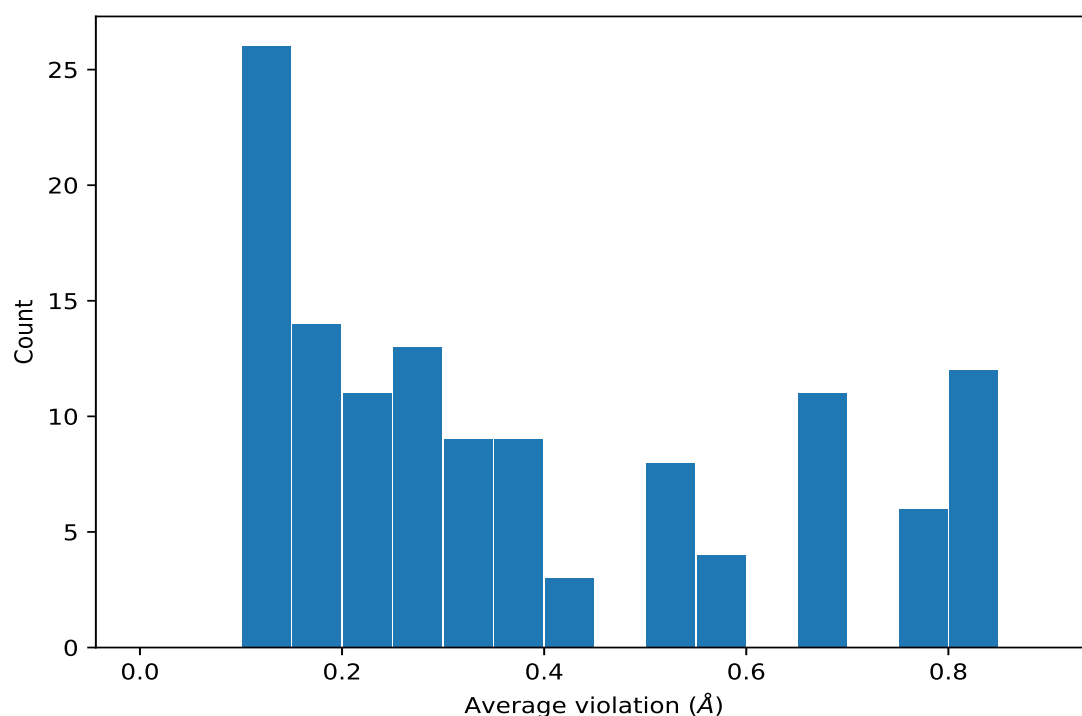
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	24	0.83	0.01	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	24	0.83	0.01	0.83
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	24	0.79	0.0	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	24	0.79	0.0	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	24	0.79	0.0	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	24	0.79	0.0	0.79

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	24	0.79	0.0	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	24	0.79	0.0	0.79
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	24	0.66	0.01	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	24	0.66	0.01	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	24	0.66	0.01	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	24	0.66	0.01	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	24	0.66	0.01	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	24	0.66	0.01	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	24	0.66	0.01	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	24	0.66	0.01	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	24	0.66	0.01	0.66
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	24	0.58	0.01	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	24	0.58	0.01	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	24	0.58	0.01	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	24	0.58	0.01	0.58
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	24	0.53	0.0	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	24	0.53	0.0	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	24	0.53	0.0	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	24	0.53	0.0	0.53
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	24	0.36	0.04	0.35
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	24	0.36	0.04	0.35
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	24	0.34	0.11	0.36
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	24	0.34	0.11	0.36
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	24	0.34	0.11	0.36
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	24	0.34	0.11	0.36
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	24	0.3	0.01	0.3
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	24	0.3	0.01	0.3
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	24	0.28	0.07	0.26
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	24	0.28	0.07	0.26
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	24	0.15	0.02	0.15
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	22	0.18	0.02	0.18
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	19	0.22	0.03	0.22
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	17	0.39	0.15	0.35
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	17	0.39	0.15	0.35
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	16	0.36	0.15	0.4
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	16	0.36	0.15	0.4
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	15	0.12	0.01	0.12
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	13	0.34	0.07	0.35
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	13	0.34	0.07	0.35
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	13	0.15	0.03	0.16
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	12	0.4	0.15	0.39
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	12	0.23	0.04	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	12	0.16	0.07	0.15
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	10	0.37	0.07	0.38
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	10	0.37	0.07	0.38
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	10	0.3	0.11	0.27
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	10	0.3	0.11	0.36
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	10	0.3	0.11	0.36
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	10	0.18	0.08	0.13
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	10	0.17	0.03	0.18
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	10	0.13	0.03	0.11
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	10	0.12	0.02	0.12
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB2	9	0.29	0.07	0.26
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB3	9	0.29	0.07	0.26
(2,166)	1:12:A:ASN:H	1:8:A:ASP:HA	9	0.23	0.08	0.2
(2,28)	1:3:A:THR:HB	1:3:A:THR:HA	9	0.18	0.01	0.18
(2,4)	1:4:A:ARG:H	1:4:A:ARG:HA	9	0.16	0.04	0.17
(2,6)	1:6:A:ASN:H	1:6:A:ASN:HA	9	0.15	0.03	0.15
(2,27)	1:3:A:THR:H	1:3:A:THR:HG21	8	0.5	0.21	0.54
(2,27)	1:3:A:THR:H	1:3:A:THR:HG22	8	0.5	0.21	0.54
(2,27)	1:3:A:THR:H	1:3:A:THR:HG23	8	0.5	0.21	0.54
(2,164)	1:11:A:ASN:H	1:7:A:LYS:HA	8	0.38	0.06	0.41
(2,62)	1:10:A:ILE:H	1:10:A:ILE:HB	8	0.21	0.01	0.22
(2,7)	1:7:A:LYS:H	1:7:A:LYS:HA	8	0.13	0.02	0.12
(2,8)	1:8:A:ASP:H	1:8:A:ASP:HA	7	0.22	0.03	0.22
(2,171)	1:7:A:LYS:HB2	1:10:A:ILE:HA	6	0.65	0.02	0.64
(2,171)	1:7:A:LYS:HB3	1:10:A:ILE:HA	6	0.65	0.02	0.64
(2,119)	1:10:A:ILE:H	1:11:A:ASN:H	6	0.16	0.05	0.15
(2,136)	1:9:A:PHE:H	1:8:A:ASP:HA	6	0.15	0.08	0.11
(2,9)	1:9:A:PHE:H	1:9:A:PHE:HA	6	0.14	0.02	0.14
(2,91)	1:15:A:LEU:HG	1:15:A:LEU:HA	6	0.11	0.01	0.11
(2,138)	1:11:A:ASN:H	1:10:A:ILE:HA	5	0.4	0.03	0.39
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB2	5	0.28	0.07	0.31
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB3	5	0.28	0.07	0.31
(2,133)	1:6:A:ASN:H	1:5:A:TYR:HA	5	0.15	0.02	0.15
(2,112)	1:3:A:THR:H	1:4:A:ARG:H	4	0.29	0.13	0.29
(2,121)	1:12:A:ASN:H	1:13:A:LYS:H	4	0.24	0.08	0.22
(2,135)	1:8:A:ASP:H	1:7:A:LYS:HA	4	0.22	0.08	0.22
(2,12)	1:12:A:ASN:H	1:12:A:ASN:HA	4	0.15	0.01	0.15
(2,113)	1:4:A:ARG:H	1:5:A:TYR:H	4	0.15	0.04	0.13
(2,111)	1:2:A:ASP:H	1:3:A:THR:H	4	0.13	0.02	0.12
(1,2)	1:10:A:ILE:O	1:14:A:HIS:H	3	0.52	0.27	0.7
(2,146)	1:19:A:ALA:H	1:18:A:HIS:HA	3	0.33	0.02	0.34
(2,167)	1:13:A:LYS:H	1:9:A:PHE:HA	3	0.29	0.06	0.29

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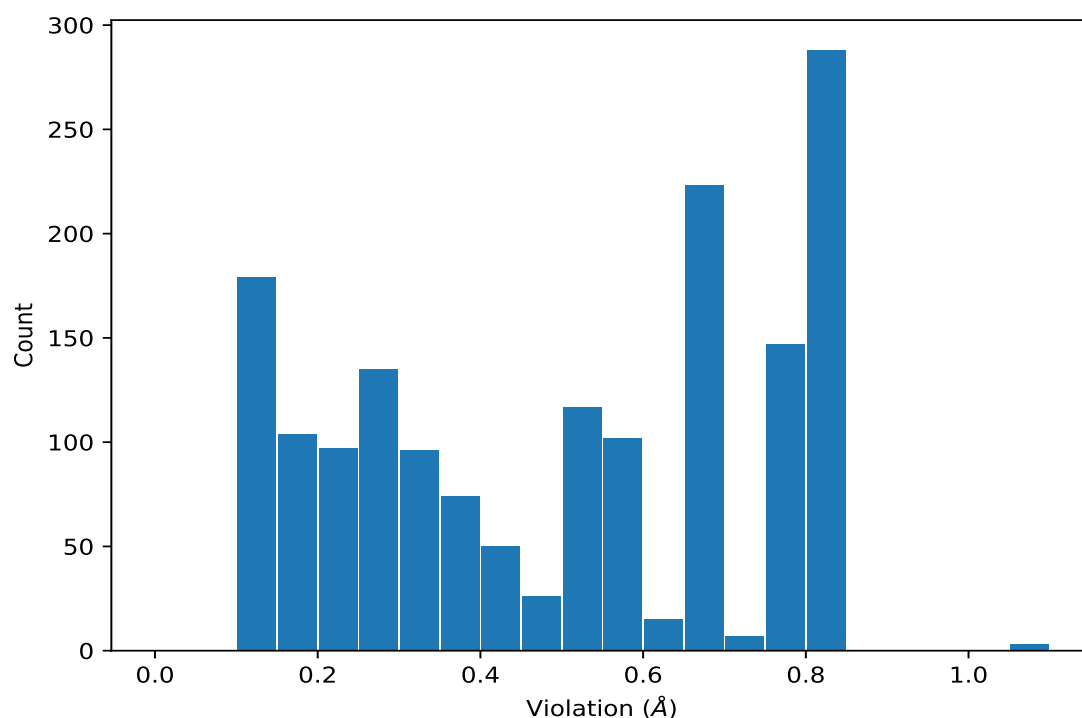
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,154)	1:13:A:LYS:H	1:11:A:ASN:HA	3	0.23	0.09	0.29
(2,147)	1:20:A:HIS:H	1:19:A:ALA:HA	3	0.22	0.01	0.23
(2,122)	1:13:A:LYS:H	1:14:A:HIS:H	3	0.2	0.06	0.24
(2,130)	1:3:A:THR:H	1:2:A:ASP:HA	3	0.19	0.06	0.21
(2,18)	1:18:A:HIS:H	1:18:A:HIS:HA	3	0.17	0.0	0.17
(2,168)	1:16:A:ASN:H	1:12:A:ASN:HA	3	0.16	0.04	0.18
(2,157)	1:13:A:LYS:H	1:10:A:ILE:HA	3	0.15	0.03	0.17
(2,161)	1:15:A:LEU:H	1:12:A:ASN:HA	3	0.14	0.03	0.14
(2,10)	1:10:A:ILE:H	1:10:A:ILE:HA	3	0.13	0.02	0.15
(2,26)	1:3:A:THR:H	1:3:A:THR:HB	3	0.11	0.0	0.11
(1,3)	1:12:A:ASN:O	1:16:A:ASN:H	2	0.42	0.01	0.42
(2,81)	1:13:A:LYS:H	1:13:A:LYS:HG2	2	0.34	0.01	0.34
(2,81)	1:13:A:LYS:H	1:13:A:LYS:HG3	2	0.34	0.01	0.34
(2,140)	1:13:A:LYS:H	1:12:A:ASN:HA	2	0.21	0.0	0.21
(2,134)	1:7:A:LYS:H	1:6:A:ASN:HA	2	0.18	0.03	0.18
(2,123)	1:14:A:HIS:H	1:15:A:LEU:H	2	0.16	0.01	0.16
(2,57)	1:9:A:PHE:H	1:9:A:PHE:HB2	2	0.16	0.05	0.16
(2,57)	1:9:A:PHE:H	1:9:A:PHE:HB3	2	0.16	0.05	0.16
(2,24)	1:2:A:ASP:H	1:2:A:ASP:HB3	2	0.15	0.02	0.15
(2,24)	1:2:A:ASP:H	1:2:A:ASP:HB2	2	0.15	0.02	0.15
(2,11)	1:11:A:ASN:H	1:11:A:ASN:HA	2	0.14	0.01	0.14
(2,141)	1:14:A:HIS:H	1:13:A:LYS:HA	2	0.13	0.0	0.13
(2,170)	1:15:A:LEU:H	1:11:A:ASN:HA	2	0.12	0.02	0.12
(2,128)	1:19:A:ALA:H	1:20:A:HIS:H	2	0.12	0.02	0.12
(2,13)	1:13:A:LYS:H	1:13:A:LYS:HA	2	0.11	0.0	0.11
(2,70)	1:10:A:ILE:HG12	1:10:A:ILE:HG13	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,175)	1:6:A:ASN:HA	1:3:A:THR:HG21	5	1.07
(2,175)	1:6:A:ASN:HA	1:3:A:THR:HG22	5	1.07
(2,175)	1:6:A:ASN:HA	1:3:A:THR:HG23	5	1.07
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	2	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	2	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	2	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	2	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	2	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	2	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	2	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	2	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	2	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	2	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	2	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	2	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	4	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	4	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	4	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	4	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	4	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	4	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	4	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	4	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	4	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	4	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	4	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	4	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	8	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	8	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	8	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	8	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	8	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	8	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	8	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	8	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	8	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	8	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	8	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	8	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	12	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	12	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	12	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	12	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	12	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	12	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	12	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	12	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	12	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	12	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	12	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	12	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	24	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	24	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	24	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	24	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	24	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	24	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	24	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	24	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	24	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	24	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	24	0.84
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	24	0.84
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	1	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	1	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	1	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	1	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	1	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	1	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	1	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	1	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	1	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	1	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	1	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	1	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	3	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	3	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	3	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	3	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	3	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	3	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	3	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	3	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	3	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	3	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	3	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	3	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	5	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	5	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	5	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	5	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	5	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	5	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	5	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	5	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	5	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	5	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	5	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	5	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	6	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	6	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	6	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	6	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	6	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	6	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	6	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	6	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	6	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	6	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	6	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	6	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	7	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	7	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	7	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	7	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	7	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	7	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	7	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	7	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	7	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	7	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	7	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	7	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	9	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	9	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	9	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	9	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	9	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	9	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	9	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	9	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	9	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	9	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	9	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	9	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	14	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	14	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	14	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	14	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	14	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	14	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	14	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	14	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	14	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	14	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	14	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	14	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	15	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	15	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	15	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	15	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	15	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	15	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	15	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	15	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	15	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	15	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	15	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	15	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	16	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	16	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	16	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	16	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	16	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	16	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	16	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	16	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	16	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	16	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	16	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	16	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	17	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	17	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	17	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	17	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	17	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	17	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	17	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	17	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	17	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	17	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	17	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	17	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	19	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	19	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	19	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	19	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	19	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	19	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	19	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	19	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	19	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	19	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	19	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	19	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	20	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	20	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	20	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	20	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	20	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	20	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	20	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	20	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	20	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	20	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	20	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	20	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	21	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	21	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	21	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	21	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	21	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	21	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	21	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	21	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	21	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	21	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	21	0.83
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	21	0.83
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	10	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	10	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	10	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	10	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	10	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	10	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	10	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	10	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	10	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	10	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	10	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	10	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	11	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	11	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	11	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	11	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	11	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	11	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	11	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	11	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	11	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	11	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	11	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	11	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	13	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	13	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	13	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	13	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	13	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	13	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	13	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	13	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	13	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	13	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	13	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	13	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	18	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	18	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	18	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	18	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	18	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	18	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	18	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	18	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	18	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	18	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	18	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	18	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	22	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	22	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	22	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	22	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	22	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	22	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	22	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	22	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	22	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	22	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	22	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	22	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD11	23	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD12	23	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD13	23	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	23	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	23	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	23	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD21	23	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD22	23	0.82
(2,94)	1:15:A:LEU:HB2	1:15:A:LEU:HD23	23	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD21	23	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD22	23	0.82
(2,94)	1:15:A:LEU:HB3	1:15:A:LEU:HD23	23	0.82
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	1	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	1	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	1	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	1	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	1	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	1	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	2	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	2	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	2	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	2	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	2	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	2	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	3	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	3	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	3	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	3	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	3	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	3	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	4	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	4	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	4	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	4	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	4	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	4	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	5	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	5	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	5	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	5	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	5	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	5	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	6	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	6	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	6	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	6	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	6	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	6	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	7	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	7	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	7	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	7	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	7	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	7	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	8	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	8	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	8	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	8	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	8	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	8	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	9	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	9	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	9	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	9	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	9	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	9	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	10	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	10	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	10	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	10	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	10	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	10	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	11	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	11	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	11	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	11	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	11	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	11	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	12	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	12	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	12	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	12	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	12	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	12	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	13	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	13	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	13	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	13	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	13	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	13	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	14	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	14	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	14	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	14	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	14	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	14	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	15	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	15	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	15	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	15	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	15	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	15	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	16	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	16	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	16	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	16	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	16	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	16	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	17	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	17	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	17	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	17	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	17	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	17	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	18	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	18	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	18	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	18	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	18	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	18	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	19	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	19	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	19	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	19	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	19	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	19	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	20	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	20	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	20	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	20	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	20	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	20	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	21	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	21	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	21	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	21	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	21	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	21	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	22	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	22	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	22	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	22	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	22	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	22	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	23	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	23	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	23	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	23	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	23	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	23	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD11	24	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD12	24	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD13	24	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD21	24	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD22	24	0.79
(2,95)	1:15:A:LEU:HG	1:15:A:LEU:HD23	24	0.79
(2,27)	1:3:A:THR:H	1:3:A:THR:HG21	8	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:3:A:THR:H	1:3:A:THR:HG22	8	0.75
(2,27)	1:3:A:THR:H	1:3:A:THR:HG23	8	0.75
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	1	0.74
(2,27)	1:3:A:THR:H	1:3:A:THR:HG21	1	0.72
(2,27)	1:3:A:THR:H	1:3:A:THR:HG22	1	0.72
(2,27)	1:3:A:THR:H	1:3:A:THR:HG23	1	0.72
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	20	0.71
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	20	0.71
(1,2)	1:10:A:ILE:O	1:14:A:HIS:H	22	0.71
(1,2)	1:10:A:ILE:O	1:14:A:HIS:H	11	0.7
(2,171)	1:7:A:LYS:HB2	1:10:A:ILE:HA	19	0.68
(2,171)	1:7:A:LYS:HB3	1:10:A:ILE:HA	19	0.68
(2,171)	1:7:A:LYS:HB2	1:10:A:ILE:HA	21	0.67
(2,171)	1:7:A:LYS:HB3	1:10:A:ILE:HA	21	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	2	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	2	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	2	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	2	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	2	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	2	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	2	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	2	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	2	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	4	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	4	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	4	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	4	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	4	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	4	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	4	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	4	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	4	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	8	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	8	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	8	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	8	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	8	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	8	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	8	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	8	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	8	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	14	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	14	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	14	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	14	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	14	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	14	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	14	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	14	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	14	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	21	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	21	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	21	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	21	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	21	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	21	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	21	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	21	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	21	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	24	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	24	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	24	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	24	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	24	0.67
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	24	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	24	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	24	0.67
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	24	0.67
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	1	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	1	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	1	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	1	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	1	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	1	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	1	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	1	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	1	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	3	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	3	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	3	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	3	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	3	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	3	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	3	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	3	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	3	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	5	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	5	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	5	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	5	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	5	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	5	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	5	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	5	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	5	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	7	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	7	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	7	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	7	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	7	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	7	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	7	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	7	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	7	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	9	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	9	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	9	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	9	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	9	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	9	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	9	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	9	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	9	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	10	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	10	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	10	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	10	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	10	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	10	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	10	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	10	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	10	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	12	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	12	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	12	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	12	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	12	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	12	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	12	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	12	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	12	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	13	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	13	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	13	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	13	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	13	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	13	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	13	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	13	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	13	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	15	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	15	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	15	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	15	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	15	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	15	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	15	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	15	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	15	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	16	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	16	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	16	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	16	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	16	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	16	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	16	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	16	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	16	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	17	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	17	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	17	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	17	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	17	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	17	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	17	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	17	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	17	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	18	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	18	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	18	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	18	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	18	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	18	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	18	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	18	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	18	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	20	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	20	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	20	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	20	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	20	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	20	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	20	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	20	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	20	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	23	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	23	0.66
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	23	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	23	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	23	0.66
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	23	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	23	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	23	0.66
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	23	0.66
(2,171)	1:7:A:LYS:HB2	1:10:A:ILE:HA	15	0.65
(2,171)	1:7:A:LYS:HB3	1:10:A:ILE:HA	15	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	6	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	6	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	6	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	6	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	6	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	6	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	6	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	6	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	6	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	11	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	11	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	11	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	11	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	11	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	11	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	11	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	11	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	19	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	19	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	19	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	19	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	19	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	19	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	19	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	19	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	19	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD11	22	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD12	22	0.65
(2,96)	1:15:A:LEU:HD21	1:15:A:LEU:HD13	22	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD11	22	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD12	22	0.65
(2,96)	1:15:A:LEU:HD22	1:15:A:LEU:HD13	22	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD11	22	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD12	22	0.65
(2,96)	1:15:A:LEU:HD23	1:15:A:LEU:HD13	22	0.65
(2,171)	1:7:A:LYS:HB2	1:10:A:ILE:HA	2	0.64
(2,171)	1:7:A:LYS:HB3	1:10:A:ILE:HA	2	0.64
(2,27)	1:3:A:THR:H	1:3:A:THR:HG21	15	0.64
(2,27)	1:3:A:THR:H	1:3:A:THR:HG22	15	0.64
(2,27)	1:3:A:THR:H	1:3:A:THR:HG23	15	0.64
(2,171)	1:7:A:LYS:HB2	1:10:A:ILE:HA	4	0.62
(2,171)	1:7:A:LYS:HB3	1:10:A:ILE:HA	4	0.62
(2,171)	1:7:A:LYS:HB2	1:10:A:ILE:HA	17	0.62
(2,171)	1:7:A:LYS:HB3	1:10:A:ILE:HA	17	0.62
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	2	0.62
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	2	0.62
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	20	0.61
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	20	0.61
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	20	0.61
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	20	0.61
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	18	0.6
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	17	0.6
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	17	0.6
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	1	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	1	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	1	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	8	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	8	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	8	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	8	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	10	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	10	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	10	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	10	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	15	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	15	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	15	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	15	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	17	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	17	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	17	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	17	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	21	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	21	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	21	0.59
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	21	0.59
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	15	0.59
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	15	0.59
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	15	0.59
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	15	0.59
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	2	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	2	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	2	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	2	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	3	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	3	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	3	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	3	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	4	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	4	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	4	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	4	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	5	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	5	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	5	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	6	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	6	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	6	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	6	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	7	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	7	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	7	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	7	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	9	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	9	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	9	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	9	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	11	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	11	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	11	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	11	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	12	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	12	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	12	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	12	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	13	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	13	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	13	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	13	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	14	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	14	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	14	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	14	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	16	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	16	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	16	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	16	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	18	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	18	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	18	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	18	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	19	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	19	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	19	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	19	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	22	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	22	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	22	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	22	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	23	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	23	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	23	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	23	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG2	24	0.58
(2,37)	1:4:A:ARG:HD2	1:4:A:ARG:HG3	24	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG2	24	0.58
(2,37)	1:4:A:ARG:HD3	1:4:A:ARG:HG3	24	0.58
(2,27)	1:3:A:THR:H	1:3:A:THR:HG21	10	0.58
(2,27)	1:3:A:THR:H	1:3:A:THR:HG22	10	0.58
(2,27)	1:3:A:THR:H	1:3:A:THR:HG23	10	0.58
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	4	0.54
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	4	0.54
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	4	0.54
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	4	0.54
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	10	0.54
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	10	0.54
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	10	0.54
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	10	0.54
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	12	0.54
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	12	0.54
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	12	0.54
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	12	0.54
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	19	0.54
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	19	0.54
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	19	0.54
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	19	0.54
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	22	0.54
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	22	0.54
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	22	0.54
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	22	0.54
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	12	0.54
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	12	0.54
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	12	0.54
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	12	0.54
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	6	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	1	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	1	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	1	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	2	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	2	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	2	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	2	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	3	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	3	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	3	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	3	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	5	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	5	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	5	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	5	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	6	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	6	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	6	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	6	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	7	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	7	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	7	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	7	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	8	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	8	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	8	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	8	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	9	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	9	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	9	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	9	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	11	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	11	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	11	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	11	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	13	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	13	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	13	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	13	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	14	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	14	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	14	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	14	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	15	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	15	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	15	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	15	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	16	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	16	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	16	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	16	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	17	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	17	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	17	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	17	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	18	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	18	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	18	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	18	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	20	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	20	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	20	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	20	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	21	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	21	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	21	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	21	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	23	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	23	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	23	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	23	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE1	24	0.53
(2,61)	1:9:A:PHE:HD1	1:9:A:PHE:HE2	24	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE1	24	0.53
(2,61)	1:9:A:PHE:HD2	1:9:A:PHE:HE2	24	0.53
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	4	0.53
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	4	0.53
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	2	0.52
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	2	0.52
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	12	0.52
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	12	0.52
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	17	0.52
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	17	0.52
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	3	0.51
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	15	0.51
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	15	0.51
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	5	0.5
(2,27)	1:3:A:THR:H	1:3:A:THR:HG21	21	0.5
(2,27)	1:3:A:THR:H	1:3:A:THR:HG22	21	0.5
(2,27)	1:3:A:THR:H	1:3:A:THR:HG23	21	0.5
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	21	0.49
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	21	0.49
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	3	0.49
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	3	0.49
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	20	0.49
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	20	0.49
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	24	0.48
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	22	0.48
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	22	0.48
(2,112)	1:3:A:THR:H	1:4:A:ARG:H	17	0.47
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	6	0.47
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	6	0.47
(2,164)	1:11:A:ASN:H	1:7:A:LYS:HA	7	0.45
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	14	0.45
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	14	0.45
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	10	0.45
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	10	0.45
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	23	0.45
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	23	0.45
(2,27)	1:3:A:THR:H	1:3:A:THR:HG21	18	0.45
(2,27)	1:3:A:THR:H	1:3:A:THR:HG22	18	0.45
(2,27)	1:3:A:THR:H	1:3:A:THR:HG23	18	0.45
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	10	0.45
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	10	0.45
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	20	0.45
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	20	0.45
(2,164)	1:11:A:ASN:H	1:7:A:LYS:HA	13	0.44
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	2	0.44
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	2	0.44
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	2	0.44
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	2	0.44
(2,138)	1:11:A:ASN:H	1:10:A:ILE:HA	18	0.43
(2,138)	1:11:A:ASN:H	1:10:A:ILE:HA	20	0.43
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	22	0.43
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	22	0.43
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	14	0.43
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	14	0.43
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	14	0.43
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	19	0.43
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	19	0.43
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	24	0.43
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	24	0.43
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	23	0.43
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	23	0.43
(2,164)	1:11:A:ASN:H	1:7:A:LYS:HA	9	0.42
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	4	0.42
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	4	0.42
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	3	0.42
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	3	0.42
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	3	0.42
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	3	0.42
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	20	0.42
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	20	0.42
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	20	0.42
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	20	0.42
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	21	0.42
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	21	0.42
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB2	4	0.42
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB3	4	0.42
(1,3)	1:12:A:ASN:O	1:16:A:ASN:H	11	0.42
(2,164)	1:11:A:ASN:H	1:7:A:LYS:HA	5	0.41
(2,164)	1:11:A:ASN:H	1:7:A:LYS:HA	23	0.41
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	15	0.41
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	24	0.41
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	24	0.41
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	16	0.41
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	16	0.41
(1,3)	1:12:A:ASN:O	1:16:A:ASN:H	22	0.41
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	4	0.4
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	10	0.4
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	10	0.4
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	10	0.4
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	10	0.4
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	14	0.4
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	14	0.4
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	2	0.39
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	17	0.39
(2,138)	1:11:A:ASN:H	1:10:A:ILE:HA	12	0.39
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	8	0.39
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	8	0.39
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	8	0.39
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	1	0.39
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	1	0.39
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	12	0.39
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	12	0.39
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	18	0.39
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	18	0.39
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	5	0.39
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	5	0.39
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB2	10	0.39
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB3	10	0.39
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	18	0.38
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	18	0.38
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	24	0.38
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	24	0.38
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	17	0.38
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	17	0.38
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	17	0.38
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	17	0.38
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	9	0.38
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	9	0.38
(2,166)	1:12:A:ASN:H	1:8:A:ASP:HA	18	0.37
(2,138)	1:11:A:ASN:H	1:10:A:ILE:HA	11	0.37
(2,138)	1:11:A:ASN:H	1:10:A:ILE:HA	22	0.37
(2,121)	1:12:A:ASN:H	1:13:A:LYS:H	18	0.37
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	3	0.37
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	3	0.37
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	8	0.37
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	8	0.37
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	13	0.37
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	13	0.37
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	17	0.37
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	17	0.37
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	13	0.37
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	13	0.37
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	13	0.37
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	13	0.37
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	5	0.37
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	5	0.37
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	6	0.37
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	16	0.37
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	16	0.37
(2,167)	1:13:A:LYS:H	1:9:A:PHE:HA	1	0.36
(2,164)	1:11:A:ASN:H	1:7:A:LYS:HA	10	0.36
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	9	0.36
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	6	0.36
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	6	0.36
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	11	0.36
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	11	0.36
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	11	0.36
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	11	0.36
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	11	0.36
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	11	0.36
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	22	0.36
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	22	0.36
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	22	0.36
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	22	0.36
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	3	0.36
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	3	0.36
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	17	0.36
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	17	0.36
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	22	0.36
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	22	0.36
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	19	0.36
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	19	0.36
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	24	0.36
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	24	0.36
(2,146)	1:19:A:ALA:H	1:18:A:HIS:HA	6	0.35
(2,81)	1:13:A:LYS:H	1:13:A:LYS:HG2	22	0.35
(2,81)	1:13:A:LYS:H	1:13:A:LYS:HG3	22	0.35
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB2	20	0.35
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB3	20	0.35
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	15	0.35
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	15	0.35
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	9	0.35
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	9	0.35
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	23	0.35
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	23	0.35
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	23	0.35
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	23	0.35
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	8	0.35
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	2	0.35
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	2	0.35
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	14	0.35
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	14	0.35
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	15	0.35
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	15	0.35
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB2	22	0.35
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB3	22	0.35
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	21	0.34
(2,146)	1:19:A:ALA:H	1:18:A:HIS:HA	19	0.34
(2,136)	1:9:A:PHE:H	1:8:A:ASP:HA	18	0.34
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	3	0.34
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	3	0.34
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	7	0.34
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	7	0.34
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	9	0.34
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	9	0.34
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	7	0.34
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	7	0.34
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	3	0.34
(2,164)	1:11:A:ASN:H	1:7:A:LYS:HA	8	0.33
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	18	0.33
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	18	0.33
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	8	0.33
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	8	0.33
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	10	0.33
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	10	0.33
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	23	0.33
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	23	0.33
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	3	0.32
(2,112)	1:3:A:THR:H	1:4:A:ARG:H	8	0.32
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	23	0.32
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	23	0.32
(2,81)	1:13:A:LYS:H	1:13:A:LYS:HG2	11	0.32
(2,81)	1:13:A:LYS:H	1:13:A:LYS:HG3	11	0.32
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	7	0.32
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	7	0.32
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	7	0.32
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	7	0.32
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	4	0.32
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	17	0.32
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	17	0.32
(2,166)	1:12:A:ASN:H	1:8:A:ASP:HA	6	0.31
(2,166)	1:12:A:ASN:H	1:8:A:ASP:HA	10	0.31
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	20	0.31
(2,146)	1:19:A:ALA:H	1:18:A:HIS:HA	11	0.31
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	3	0.31
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	3	0.31
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	7	0.31
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	7	0.31
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	9	0.31
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	9	0.31
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	10	0.31
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	10	0.31
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	13	0.31
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	13	0.31
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	14	0.31
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	14	0.31
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	16	0.31
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	16	0.31
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	22	0.31
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	22	0.31
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB2	11	0.31
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB3	11	0.31
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB2	22	0.31
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB3	22	0.31
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	13	0.31
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	13	0.31
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	15	0.31
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	15	0.31
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	11	0.31
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	11	0.31
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	13	0.31
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	13	0.31
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	22	0.31
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	22	0.31
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	7	0.31
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	7	0.31
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	19	0.31
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	19	0.31
(2,154)	1:13:A:LYS:H	1:11:A:ASN:HA	22	0.3
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,135)	1:8:A:ASP:H	1:7:A:LYS:HA	6	0.3
(2,135)	1:8:A:ASP:H	1:7:A:LYS:HA	19	0.3
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	18	0.3
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	5	0.3
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	5	0.3
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	8	0.3
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	8	0.3
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	18	0.3
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	18	0.3
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	19	0.3
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	19	0.3
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	24	0.3
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	24	0.3
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB2	12	0.3
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB3	12	0.3
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	4	0.3
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	4	0.3
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	4	0.3
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	4	0.3
(2,34)	1:4:A:ARG:HB2	1:4:A:ARG:HA	4	0.3
(2,34)	1:4:A:ARG:HB3	1:4:A:ARG:HA	4	0.3
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB2	8	0.3
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB3	8	0.3
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	12	0.3
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	12	0.3
(2,167)	1:13:A:LYS:H	1:9:A:PHE:HA	6	0.29
(2,154)	1:13:A:LYS:H	1:11:A:ASN:HA	11	0.29
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	19	0.29
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	2	0.29
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	2	0.29
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	4	0.29
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	4	0.29
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	6	0.29
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	6	0.29
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	1	0.29
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	1	0.29
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	11	0.29
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	11	0.29
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	5	0.29
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	5	0.29
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	5	0.29
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	19	0.29
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	19	0.29
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	19	0.29
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	19	0.29
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	18	0.29
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	18	0.29
(2,8)	1:8:A:ASP:H	1:8:A:ASP:HA	18	0.29
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	21	0.28
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	20	0.28
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	1	0.28
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	1	0.28
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	11	0.28
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	11	0.28
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	20	0.28
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	20	0.28
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	21	0.28
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	21	0.28
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	21	0.28
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	21	0.28
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	2	0.28
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	2	0.28
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	1	0.28
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	1	0.28
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	21	0.28
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	21	0.28
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	20	0.27
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	2	0.27
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	4	0.27
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	17	0.27
(2,119)	1:10:A:ILE:H	1:11:A:ASN:H	14	0.27
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	12	0.27
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	12	0.27
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	15	0.27
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	15	0.27
(2,93)	1:15:A:LEU:HB2	1:15:A:LEU:HG	17	0.27
(2,93)	1:15:A:LEU:HB3	1:15:A:LEU:HG	17	0.27
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	12	0.27
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	12	0.27
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	16	0.27
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	16	0.27
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	3	0.27
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	24	0.26
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	15	0.26
(2,121)	1:12:A:ASN:H	1:13:A:LYS:H	20	0.26
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	24	0.26
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	10	0.26
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	10	0.26
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	9	0.26
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	9	0.26
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	9	0.26
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	9	0.26
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB2	11	0.26
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB3	11	0.26
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	4	0.26
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	4	0.26
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	6	0.26
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	6	0.26
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	9	0.26
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	9	0.26
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	13	0.26
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	13	0.26
(2,164)	1:11:A:ASN:H	1:7:A:LYS:HA	16	0.25
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	19	0.25
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	19	0.25
(2,122)	1:13:A:LYS:H	1:14:A:HIS:H	22	0.25
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	3	0.25
(2,112)	1:3:A:THR:H	1:4:A:ARG:H	20	0.25
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	24	0.25
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	24	0.25
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	24	0.25
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	24	0.25
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB2	13	0.25
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB3	13	0.25
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB2	17	0.25
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB3	17	0.25
(2,27)	1:3:A:THR:H	1:3:A:THR:HG21	17	0.25
(2,27)	1:3:A:THR:H	1:3:A:THR:HG22	17	0.25
(2,27)	1:3:A:THR:H	1:3:A:THR:HG23	17	0.25
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	2	0.25
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	2	0.25
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	5	0.25
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	5	0.25
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	11	0.25
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	16	0.25
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	16	0.25
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	22	0.25
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	22	0.25
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	24	0.25
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	24	0.25
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	1	0.24
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	1	0.24
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	3	0.24
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	8	0.24
(2,130)	1:3:A:THR:H	1:2:A:ASP:HA	8	0.24
(2,122)	1:13:A:LYS:H	1:14:A:HIS:H	11	0.24
(2,116)	1:7:A:LYS:H	1:8:A:ASP:H	19	0.24
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	6	0.24
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	6	0.24
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	6	0.24
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	6	0.24
(2,33)	1:4:A:ARG:HD2	1:4:A:ARG:HA	21	0.24
(2,33)	1:4:A:ARG:HD3	1:4:A:ARG:HA	21	0.24
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB2	15	0.24
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB3	15	0.24
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	18	0.24
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	18	0.24
(2,147)	1:20:A:HIS:H	1:19:A:ALA:HA	15	0.23
(2,147)	1:20:A:HIS:H	1:19:A:ALA:HA	17	0.23
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	2	0.23
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	4	0.23
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	23	0.23
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	6	0.23
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	1	0.23
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	4	0.23
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	12	0.23
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	12	0.23
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	1	0.23
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	1	0.23
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	15	0.23
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	15	0.23
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	7	0.23
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	23	0.23
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	20	0.22
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	15	0.22
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	17	0.22
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	21	0.22
(2,129)	1:2:A:ASP:H	1:1:A:SER:HA	14	0.22
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	19	0.22
(2,62)	1:10:A:ILE:H	1:10:A:ILE:HB	2	0.22
(2,62)	1:10:A:ILE:H	1:10:A:ILE:HB	3	0.22
(2,62)	1:10:A:ILE:H	1:10:A:ILE:HB	4	0.22
(2,62)	1:10:A:ILE:H	1:10:A:ILE:HB	15	0.22
(2,62)	1:10:A:ILE:H	1:10:A:ILE:HB	17	0.22
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	1	0.22
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	1	0.22
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	1	0.22
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	1	0.22
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	16	0.22
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	16	0.22
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	16	0.22
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	16	0.22
(2,35)	1:4:A:ARG:HG2	1:4:A:ARG:HA	11	0.22
(2,35)	1:4:A:ARG:HG3	1:4:A:ARG:HA	11	0.22
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	8	0.22
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	8	0.22
(2,8)	1:8:A:ASP:H	1:8:A:ASP:HA	4	0.22
(2,8)	1:8:A:ASP:H	1:8:A:ASP:HA	15	0.22
(2,8)	1:8:A:ASP:H	1:8:A:ASP:HA	17	0.22
(2,8)	1:8:A:ASP:H	1:8:A:ASP:HA	21	0.22
(2,167)	1:13:A:LYS:H	1:9:A:PHE:HA	12	0.21
(2,166)	1:12:A:ASN:H	1:8:A:ASP:HA	13	0.21
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	10	0.21
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	10	0.21
(2,140)	1:13:A:LYS:H	1:12:A:ASN:HA	11	0.21
(2,140)	1:13:A:LYS:H	1:12:A:ASN:HA	22	0.21
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	6	0.21
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	13	0.21
(2,130)	1:3:A:THR:H	1:2:A:ASP:HA	23	0.21
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	2	0.21
(2,113)	1:4:A:ARG:H	1:5:A:TYR:H	10	0.21
(2,62)	1:10:A:ILE:H	1:10:A:ILE:HB	21	0.21
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	11	0.21
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	11	0.21
(2,57)	1:9:A:PHE:H	1:9:A:PHE:HB2	18	0.21
(2,57)	1:9:A:PHE:H	1:9:A:PHE:HB3	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	18	0.21
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	18	0.21
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	18	0.21
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	18	0.21
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	17	0.21
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	17	0.21
(2,8)	1:8:A:ASP:H	1:8:A:ASP:HA	2	0.21
(2,4)	1:4:A:ARG:H	1:4:A:ARG:HA	12	0.21
(2,4)	1:4:A:ARG:H	1:4:A:ARG:HA	15	0.21
(2,4)	1:4:A:ARG:H	1:4:A:ARG:HA	21	0.21
(2,166)	1:12:A:ASN:H	1:8:A:ASP:HA	5	0.2
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	14	0.2
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	19	0.2
(2,147)	1:20:A:HIS:H	1:19:A:ALA:HA	9	0.2
(2,134)	1:7:A:LYS:H	1:6:A:ASN:HA	4	0.2
(2,62)	1:10:A:ILE:H	1:10:A:ILE:HB	19	0.2
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	6	0.2
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	6	0.2
(2,52)	1:7:A:LYS:HD2	1:7:A:LYS:HA	13	0.2
(2,52)	1:7:A:LYS:HD3	1:7:A:LYS:HA	13	0.2
(2,168)	1:16:A:ASN:H	1:12:A:ASN:HA	22	0.19
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	5	0.19
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	6	0.19
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	13	0.19
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	14	0.19
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	15	0.19
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	17	0.19
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	21	0.19
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	23	0.19
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	7	0.19
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	6	0.19
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	21	0.19
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	10	0.19
(2,62)	1:10:A:ILE:H	1:10:A:ILE:HB	24	0.19
(2,28)	1:3:A:THR:HB	1:3:A:THR:HA	12	0.19
(2,28)	1:3:A:THR:HB	1:3:A:THR:HA	22	0.19
(2,8)	1:8:A:ASP:H	1:8:A:ASP:HA	1	0.19
(2,6)	1:6:A:ASN:H	1:6:A:ASN:HA	17	0.19
(2,4)	1:4:A:ARG:H	1:4:A:ARG:HA	8	0.19
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	14	0.19
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	22	0.19
(2,168)	1:16:A:ASN:H	1:12:A:ASN:HA	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:12:A:ASN:H	1:8:A:ASP:HA	7	0.18
(2,166)	1:12:A:ASN:H	1:8:A:ASP:HA	9	0.18
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	3	0.18
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	23	0.18
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	3	0.18
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	7	0.18
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	8	0.18
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	9	0.18
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	16	0.18
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	24	0.18
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	10	0.18
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	15	0.18
(2,117)	1:8:A:ASP:H	1:9:A:PHE:H	17	0.18
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	9	0.18
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	13	0.18
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB2	2	0.18
(2,30)	1:4:A:ARG:H	1:4:A:ARG:HB3	2	0.18
(2,28)	1:3:A:THR:HB	1:3:A:THR:HA	2	0.18
(2,28)	1:3:A:THR:HB	1:3:A:THR:HA	13	0.18
(2,28)	1:3:A:THR:HB	1:3:A:THR:HA	24	0.18
(2,25)	1:2:A:ASP:HB3	1:2:A:ASP:HA	14	0.18
(2,25)	1:2:A:ASP:HB2	1:2:A:ASP:HA	14	0.18
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	15	0.18
(2,6)	1:6:A:ASN:H	1:6:A:ASN:HA	24	0.18
(2,161)	1:15:A:LEU:H	1:12:A:ASN:HA	11	0.17
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	2	0.17
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	4	0.17
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	10	0.17
(2,157)	1:13:A:LYS:H	1:10:A:ILE:HA	16	0.17
(2,157)	1:13:A:LYS:H	1:10:A:ILE:HA	18	0.17
(2,156)	1:10:A:ILE:H	1:7:A:LYS:HA	24	0.17
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	5	0.17
(2,133)	1:6:A:ASN:H	1:5:A:TYR:HA	21	0.17
(2,131)	1:4:A:ARG:H	1:3:A:THR:HA	19	0.17
(2,123)	1:14:A:HIS:H	1:15:A:LEU:H	22	0.17
(2,121)	1:12:A:ASN:H	1:13:A:LYS:H	11	0.17
(2,119)	1:10:A:ILE:H	1:11:A:ASN:H	16	0.17
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	5	0.17
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	7	0.17
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	14	0.17
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	23	0.17
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	5	0.17
(2,28)	1:3:A:THR:HB	1:3:A:THR:HA	6	0.17
(2,28)	1:3:A:THR:HB	1:3:A:THR:HA	11	0.17
(2,28)	1:3:A:THR:HB	1:3:A:THR:HA	16	0.17
(2,24)	1:2:A:ASP:H	1:2:A:ASP:HB3	8	0.17
(2,24)	1:2:A:ASP:H	1:2:A:ASP:HB2	8	0.17
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	17	0.17
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	20	0.17
(2,18)	1:18:A:HIS:H	1:18:A:HIS:HA	6	0.17
(2,18)	1:18:A:HIS:H	1:18:A:HIS:HA	11	0.17
(2,18)	1:18:A:HIS:H	1:18:A:HIS:HA	19	0.17
(2,12)	1:12:A:ASN:H	1:12:A:ASN:HA	12	0.17
(2,6)	1:6:A:ASN:H	1:6:A:ASN:HA	3	0.17
(2,4)	1:4:A:ARG:H	1:4:A:ARG:HA	17	0.17
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	10	0.17
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	17	0.17
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	18	0.17
(2,166)	1:12:A:ASN:H	1:8:A:ASP:HA	20	0.16
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	4	0.16
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	22	0.16
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	12	0.16
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	18	0.16
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	19	0.16
(2,123)	1:14:A:HIS:H	1:15:A:LEU:H	11	0.16
(2,121)	1:12:A:ASN:H	1:13:A:LYS:H	22	0.16
(2,119)	1:10:A:ILE:H	1:11:A:ASN:H	8	0.16
(2,111)	1:2:A:ASP:H	1:3:A:THR:H	10	0.16
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	16	0.16
(2,28)	1:3:A:THR:HB	1:3:A:THR:HA	4	0.16
(2,12)	1:12:A:ASN:H	1:12:A:ASN:HA	20	0.16
(2,9)	1:9:A:PHE:H	1:9:A:PHE:HA	5	0.16
(2,9)	1:9:A:PHE:H	1:9:A:PHE:HA	10	0.16
(2,7)	1:7:A:LYS:H	1:7:A:LYS:HA	5	0.16
(2,7)	1:7:A:LYS:H	1:7:A:LYS:HA	7	0.16
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	14	0.16
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	1	0.16
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	15	0.16
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	20	0.16
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	4	0.16
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	12	0.16
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	12	0.15
(2,158)	1:16:A:ASN:H	1:13:A:LYS:HA	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,139)	1:12:A:ASN:H	1:11:A:ASN:HA	14	0.15
(2,136)	1:9:A:PHE:H	1:8:A:ASP:HA	6	0.15
(2,135)	1:8:A:ASP:H	1:7:A:LYS:HA	20	0.15
(2,134)	1:7:A:LYS:H	1:6:A:ASN:HA	1	0.15
(2,133)	1:6:A:ASN:H	1:5:A:TYR:HA	10	0.15
(2,133)	1:6:A:ASN:H	1:5:A:TYR:HA	15	0.15
(2,133)	1:6:A:ASN:H	1:5:A:TYR:HA	18	0.15
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB2	18	0.15
(2,76)	1:12:A:ASN:H	1:12:A:ASN:HB3	18	0.15
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	3	0.15
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	6	0.15
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	8	0.15
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	20	0.15
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	9	0.15
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	9	0.15
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	23	0.15
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	23	0.15
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	9	0.15
(2,11)	1:11:A:ASN:H	1:11:A:ASN:HA	12	0.15
(2,10)	1:10:A:ILE:H	1:10:A:ILE:HA	1	0.15
(2,10)	1:10:A:ILE:H	1:10:A:ILE:HA	6	0.15
(2,9)	1:9:A:PHE:H	1:9:A:PHE:HA	20	0.15
(2,6)	1:6:A:ASN:H	1:6:A:ASN:HA	8	0.15
(2,6)	1:6:A:ASN:H	1:6:A:ASN:HA	14	0.15
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	6	0.15
(2,4)	1:4:A:ARG:H	1:4:A:ARG:HA	10	0.15
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	8	0.15
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	22	0.15
(2,170)	1:15:A:LEU:H	1:11:A:ASN:HA	20	0.14
(2,166)	1:12:A:ASN:H	1:8:A:ASP:HA	23	0.14
(2,161)	1:15:A:LEU:H	1:12:A:ASN:HA	22	0.14
(2,135)	1:8:A:ASP:H	1:7:A:LYS:HA	10	0.14
(2,91)	1:15:A:LEU:HG	1:15:A:LEU:HA	11	0.14
(2,78)	1:12:A:ASN:HD22	1:12:A:ASN:HA	1	0.14
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	1	0.14
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	11	0.14
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	12	0.14
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	24	0.14
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	2	0.14
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	2	0.14
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	9	0.14
(2,12)	1:12:A:ASN:H	1:12:A:ASN:HA	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:12:A:ASN:H	1:12:A:ASN:HA	22	0.14
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	9	0.14
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	23	0.14
(1,2)	1:10:A:ILE:O	1:14:A:HIS:H	14	0.14
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	18	0.14
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	1	0.13
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	12	0.13
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	19	0.13
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	22	0.13
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	24	0.13
(2,141)	1:14:A:HIS:H	1:13:A:LYS:HA	11	0.13
(2,141)	1:14:A:HIS:H	1:13:A:LYS:HA	22	0.13
(2,128)	1:19:A:ALA:H	1:20:A:HIS:H	9	0.13
(2,119)	1:10:A:ILE:H	1:11:A:ASN:H	10	0.13
(2,113)	1:4:A:ARG:H	1:5:A:TYR:H	15	0.13
(2,113)	1:4:A:ARG:H	1:5:A:TYR:H	21	0.13
(2,111)	1:2:A:ASP:H	1:3:A:THR:H	7	0.13
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	2	0.13
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	4	0.13
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	15	0.13
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	17	0.13
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	18	0.13
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	19	0.13
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	21	0.13
(2,65)	1:10:A:ILE:HB	1:10:A:ILE:HA	22	0.13
(2,60)	1:9:A:PHE:HD1	1:9:A:PHE:HA	6	0.13
(2,60)	1:9:A:PHE:HD2	1:9:A:PHE:HA	6	0.13
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	16	0.13
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	16	0.13
(2,24)	1:2:A:ASP:H	1:2:A:ASP:HB3	17	0.13
(2,24)	1:2:A:ASP:H	1:2:A:ASP:HB2	17	0.13
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	5	0.13
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	22	0.13
(2,11)	1:11:A:ASN:H	1:11:A:ASN:HA	20	0.13
(2,9)	1:9:A:PHE:H	1:9:A:PHE:HA	9	0.13
(2,7)	1:7:A:LYS:H	1:7:A:LYS:HA	12	0.13
(2,7)	1:7:A:LYS:H	1:7:A:LYS:HA	22	0.13
(2,6)	1:6:A:ASN:H	1:6:A:ASN:HA	2	0.13
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	23	0.13
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	24	0.13
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	5	0.12
(2,162)	1:7:A:LYS:H	1:3:A:THR:HA	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:10:A:ILE:H	1:11:A:ASN:H	9	0.12
(2,91)	1:15:A:LEU:HG	1:15:A:LEU:HA	18	0.12
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB2	14	0.12
(2,41)	1:5:A:TYR:H	1:5:A:TYR:HB3	14	0.12
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB2	21	0.12
(2,36)	1:4:A:ARG:HD2	1:4:A:ARG:HB3	21	0.12
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB2	21	0.12
(2,36)	1:4:A:ARG:HD3	1:4:A:ARG:HB3	21	0.12
(2,27)	1:3:A:THR:H	1:3:A:THR:HG21	9	0.12
(2,27)	1:3:A:THR:H	1:3:A:THR:HG22	9	0.12
(2,27)	1:3:A:THR:H	1:3:A:THR:HG23	9	0.12
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	7	0.12
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	8	0.12
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	10	0.12
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	13	0.12
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	23	0.12
(2,9)	1:9:A:PHE:H	1:9:A:PHE:HA	12	0.12
(2,7)	1:7:A:LYS:H	1:7:A:LYS:HA	13	0.12
(2,7)	1:7:A:LYS:H	1:7:A:LYS:HA	23	0.12
(2,7)	1:7:A:LYS:H	1:7:A:LYS:HA	24	0.12
(2,6)	1:6:A:ASN:H	1:6:A:ASN:HA	6	0.12
(2,4)	1:4:A:ARG:H	1:4:A:ARG:HA	18	0.12
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	1	0.12
(2,168)	1:16:A:ASN:H	1:12:A:ASN:HA	18	0.11
(2,157)	1:13:A:LYS:H	1:10:A:ILE:HA	8	0.11
(2,154)	1:13:A:LYS:H	1:11:A:ASN:HA	18	0.11
(2,151)	1:9:A:PHE:H	1:7:A:LYS:HA	3	0.11
(2,137)	1:10:A:ILE:H	1:9:A:PHE:HA	10	0.11
(2,136)	1:9:A:PHE:H	1:8:A:ASP:HA	1	0.11
(2,136)	1:9:A:PHE:H	1:8:A:ASP:HA	21	0.11
(2,136)	1:9:A:PHE:H	1:8:A:ASP:HA	24	0.11
(2,133)	1:6:A:ASN:H	1:5:A:TYR:HA	22	0.11
(2,130)	1:3:A:THR:H	1:2:A:ASP:HA	3	0.11
(2,122)	1:13:A:LYS:H	1:14:A:HIS:H	1	0.11
(2,119)	1:10:A:ILE:H	1:11:A:ASN:H	13	0.11
(2,118)	1:9:A:PHE:H	1:10:A:ILE:H	20	0.11
(2,113)	1:4:A:ARG:H	1:5:A:TYR:H	12	0.11
(2,112)	1:3:A:THR:H	1:4:A:ARG:H	22	0.11
(2,111)	1:2:A:ASP:H	1:3:A:THR:H	2	0.11
(2,111)	1:2:A:ASP:H	1:3:A:THR:H	19	0.11
(2,91)	1:15:A:LEU:HG	1:15:A:LEU:HA	6	0.11
(2,91)	1:15:A:LEU:HG	1:15:A:LEU:HA	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,72)	1:11:A:ASN:H	1:11:A:ASN:HB2	10	0.11
(2,72)	1:11:A:ASN:H	1:11:A:ASN:HB3	10	0.11
(2,70)	1:10:A:ILE:HG12	1:10:A:ILE:HG13	1	0.11
(2,57)	1:9:A:PHE:H	1:9:A:PHE:HB2	19	0.11
(2,57)	1:9:A:PHE:H	1:9:A:PHE:HB3	19	0.11
(2,26)	1:3:A:THR:H	1:3:A:THR:HB	11	0.11
(2,26)	1:3:A:THR:H	1:3:A:THR:HB	16	0.11
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	1	0.11
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	14	0.11
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	21	0.11
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	24	0.11
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	5	0.11
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	7	0.11
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	23	0.11
(2,13)	1:13:A:LYS:H	1:13:A:LYS:HA	11	0.11
(2,9)	1:9:A:PHE:H	1:9:A:PHE:HA	13	0.11
(2,6)	1:6:A:ASN:H	1:6:A:ASN:HA	7	0.11
(2,6)	1:6:A:ASN:H	1:6:A:ASN:HA	13	0.11
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	11	0.11
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	13	0.11
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	17	0.11
(2,4)	1:4:A:ARG:H	1:4:A:ARG:HA	1	0.11
(2,4)	1:4:A:ARG:H	1:4:A:ARG:HA	22	0.11
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	9	0.11
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	11	0.11
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	21	0.11
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	24	0.11
(2,170)	1:15:A:LEU:H	1:11:A:ASN:HA	12	0.1
(2,163)	1:8:A:ASP:H	1:4:A:ARG:HA	7	0.1
(2,161)	1:15:A:LEU:H	1:12:A:ASN:HA	12	0.1
(2,136)	1:9:A:PHE:H	1:8:A:ASP:HA	2	0.1
(2,128)	1:19:A:ALA:H	1:20:A:HIS:H	18	0.1
(2,115)	1:6:A:ASN:H	1:7:A:LYS:H	1	0.1
(2,91)	1:15:A:LEU:HG	1:15:A:LEU:HA	9	0.1
(2,91)	1:15:A:LEU:HG	1:15:A:LEU:HA	12	0.1
(2,70)	1:10:A:ILE:HG12	1:10:A:ILE:HG13	6	0.1
(2,26)	1:3:A:THR:H	1:3:A:THR:HB	6	0.1
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	3	0.1
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	11	0.1
(2,20)	1:20:A:HIS:H	1:20:A:HIS:HA	15	0.1
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	10	0.1
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:19:A:ALA:H	1:19:A:ALA:HA	22	0.1
(2,13)	1:13:A:LYS:H	1:13:A:LYS:HA	22	0.1
(2,10)	1:10:A:ILE:H	1:10:A:ILE:HA	18	0.1
(2,7)	1:7:A:LYS:H	1:7:A:LYS:HA	3	0.1
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	8	0.1
(2,5)	1:5:A:TYR:H	1:5:A:TYR:HA	18	0.1
(2,2)	1:2:A:ASP:H	1:2:A:ASP:HA	5	0.1
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	8	0.1
(1,1)	1:2:A:ASP:O	1:6:A:ASN:H	15	0.1

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

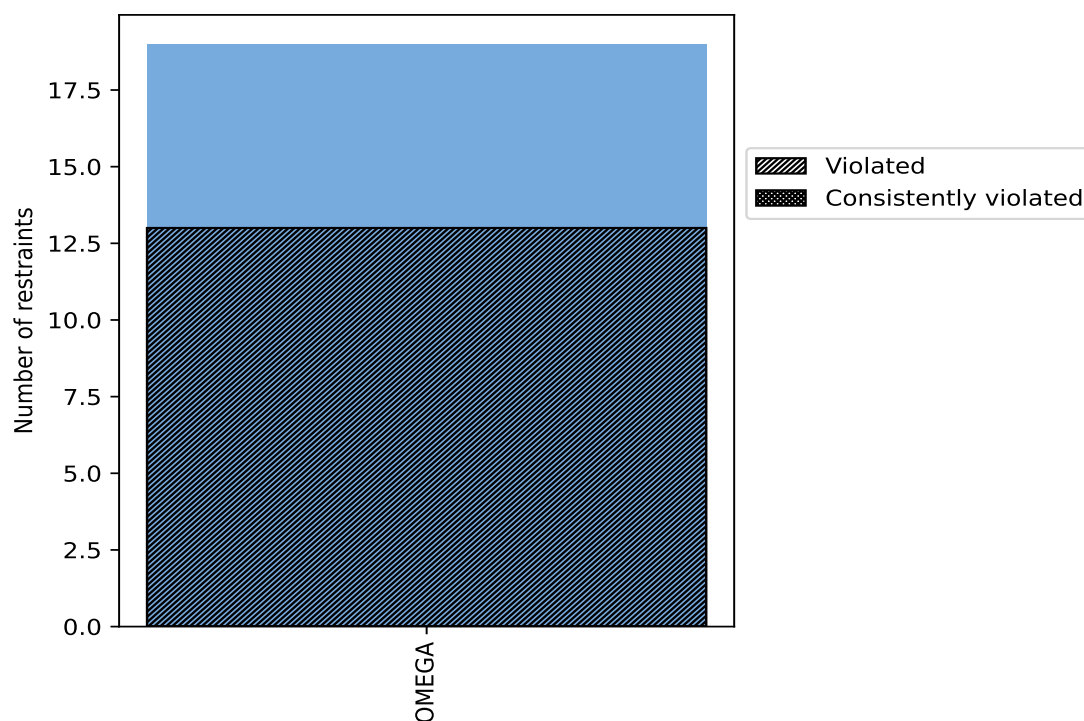
10.1 Summary of dihedral-angle violations [i](#)

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
OMEGA	19	100.0	13	68.4	68.4	0	0.0	0.0
Total	19	100.0	13	68.4	68.4	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](#)



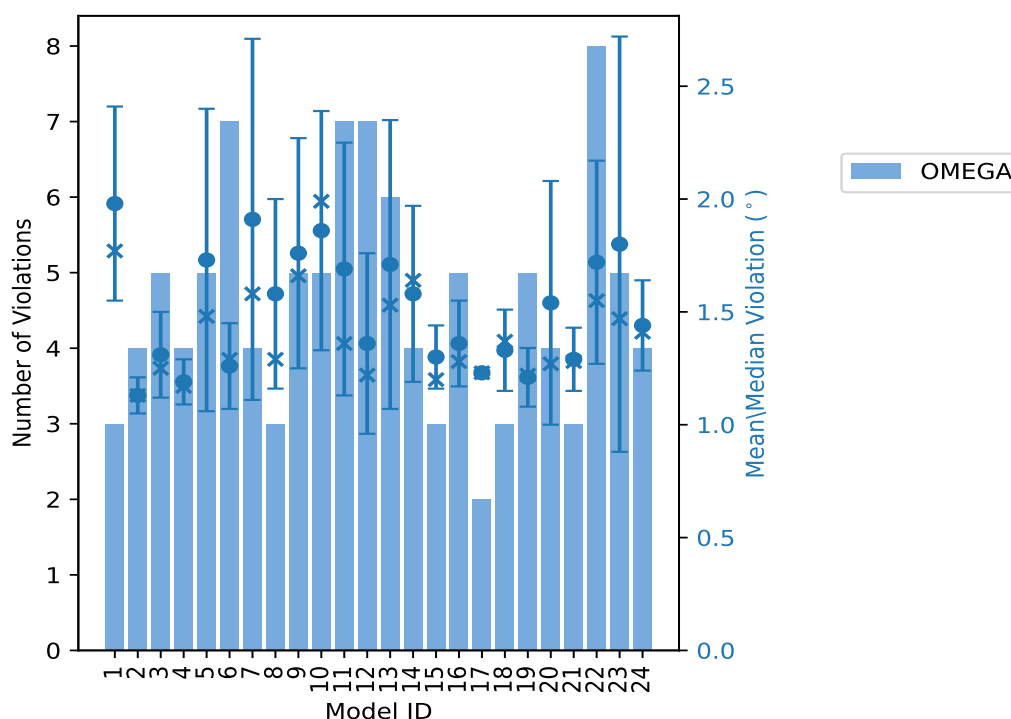
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations		Mean (°)	Max (°)	SD (°)	Median (°)
	OMEGA	Total				
1	3	3	1.98	2.58	0.43	1.77
2	4	4	1.13	1.24	0.08	1.13
3	5	5	1.31	1.65	0.19	1.25
4	4	4	1.19	1.34	0.1	1.17
5	5	5	1.73	3.01	0.67	1.48
6	7	7	1.26	1.51	0.19	1.29
7	4	4	1.91	3.27	0.8	1.58
8	3	3	1.58	2.17	0.42	1.29
9	5	5	1.76	2.7	0.51	1.66
10	5	5	1.86	2.69	0.53	1.99
11	7	7	1.69	2.67	0.56	1.36
12	7	7	1.36	2.3	0.4	1.22
13	6	6	1.71	3.07	0.64	1.53
14	4	4	1.58	2.03	0.39	1.64
15	3	3	1.3	1.5	0.14	1.2
16	5	5	1.36	1.72	0.19	1.28
17	2	2	1.23	1.24	0.01	1.23
18	3	3	1.33	1.53	0.18	1.37
19	5	5	1.21	1.43	0.13	1.22
20	4	4	1.54	2.47	0.54	1.27
21	3	3	1.29	1.47	0.14	1.28
22	8	8	1.72	2.72	0.45	1.55
23	5	5	1.8	3.57	0.92	1.47
24	4	4	1.44	1.75	0.2	1.41

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



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

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

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

Number of violated restraints		Fraction of the ensemble	
OMEGA	Total	Count ¹	%
2	2	1	4.2
1	1	2	8.3
2	2	3	12.5
1	1	4	16.7
1	1	5	20.8
1	1	6	25.0
0	0	7	29.2
0	0	8	33.3
0	0	9	37.5
2	2	10	41.7
0	0	11	45.8

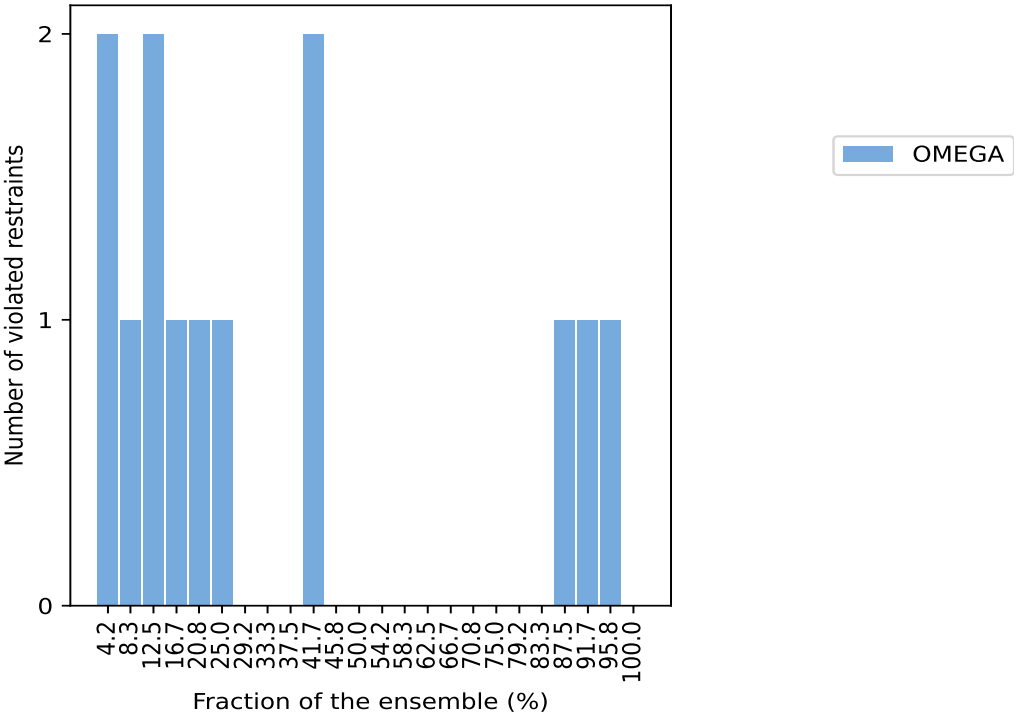
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Number of violated restraints		Fraction of the ensemble	
OMEGA	Total	Count ¹	%
0	0	12	50.0
0	0	13	54.2
0	0	14	58.3
0	0	15	62.5
0	0	16	66.7
0	0	17	70.8
0	0	18	75.0
0	0	19	79.2
0	0	20	83.3
1	1	21	87.5
1	1	22	91.7
1	1	23	95.8
0	0	24	100.0

¹ Number of models with violations

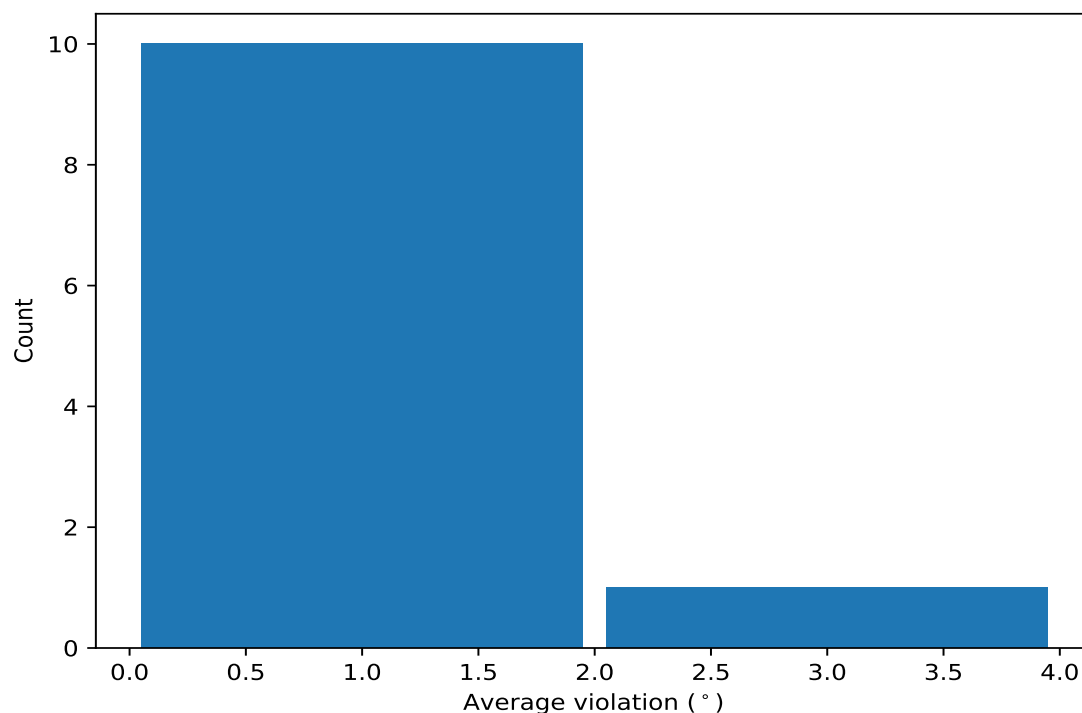
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

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

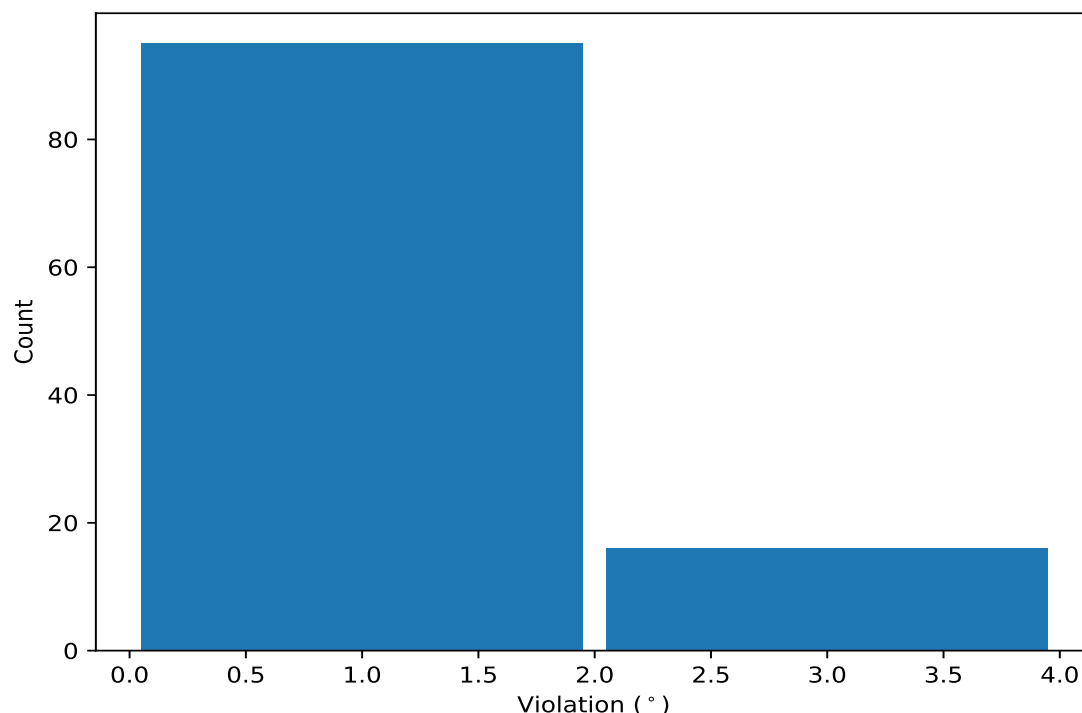
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	23	1.36	0.42	1.24
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	22	1.42	0.23	1.4
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	21	1.96	0.79	1.51
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	10	1.52	0.27	1.54
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	10	1.45	0.39	1.34
(1,10)	1:10:A:ILE:CA	1:10:A:ILE:C	1:11:A:ASN:N	1:11:A:ASN:CA	6	1.29	0.32	1.15
(1,6)	1:6:A:ASN:CA	1:6:A:ASN:C	1:7:A:LYS:N	1:7:A:LYS:CA	5	1.52	0.5	1.35
(1,15)	1:15:A:LEU:CA	1:15:A:LEU:C	1:16:A:ASN:N	1:16:A:ASN:CA	4	1.45	0.29	1.44
(1,11)	1:11:A:ASN:CA	1:11:A:ASN:C	1:12:A:ASN:N	1:12:A:ASN:CA	3	2.01	0.35	2.18
(1,3)	1:3:A:THR:CA	1:3:A:THR:C	1:4:A:ARG:N	1:4:A:ARG:CA	3	1.19	0.12	1.2
(1,12)	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:LYS:N	1:13:A:LYS:CA	2	1.33	0.04	1.33

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

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

10.5.1 Histogram : Distribution of violations [i](#)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	23	3.57
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	7	3.27
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	13	3.07
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	5	3.01
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	22	2.72
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	9	2.7
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	10	2.69
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	11	2.67
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	1	2.58
(1,6)	1:6:A:ASN:CA	1:6:A:ASN:C	1:7:A:LYS:N	1:7:A:LYS:CA	20	2.47
(1,11)	1:11:A:ASN:CA	1:11:A:ASN:C	1:12:A:ASN:N	1:12:A:ASN:CA	11	2.33
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	12	2.3
(1,11)	1:11:A:ASN:CA	1:11:A:ASN:C	1:12:A:ASN:N	1:12:A:ASN:CA	22	2.18
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	8	2.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	14	2.03
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	10	2.0
(1,10)	1:10:A:ILE:CA	1:10:A:ILE:C	1:11:A:ASN:N	1:11:A:ASN:CA	10	1.99
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	14	1.86
(1,15)	1:15:A:LEU:CA	1:15:A:LEU:C	1:16:A:ASN:N	1:16:A:ASN:CA	11	1.85
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	9	1.82
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	1	1.77
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	13	1.76
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	23	1.75
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	24	1.75
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	5	1.74
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	16	1.72
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	7	1.66
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	9	1.66
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	3	1.65
(1,5)	1:5:A:TYR:CA	1:5:A:TYR:C	1:6:A:ASN:N	1:6:A:ASN:CA	22	1.6
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	1	1.59
(1,15)	1:15:A:LEU:CA	1:15:A:LEU:C	1:16:A:ASN:N	1:16:A:ASN:CA	22	1.58
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	13	1.56
(1,11)	1:11:A:ASN:CA	1:11:A:ASN:C	1:12:A:ASN:N	1:12:A:ASN:CA	18	1.53
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	22	1.52
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	6	1.51
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	10	1.5
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	15	1.5
(1,6)	1:6:A:ASN:CA	1:6:A:ASN:C	1:7:A:LYS:N	1:7:A:LYS:CA	6	1.5
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	13	1.5
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	7	1.49
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	5	1.48
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	24	1.48
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	23	1.47
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	21	1.47
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	22	1.46
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	9	1.45
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	19	1.43
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	14	1.42
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	22	1.42
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	12	1.41
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	16	1.4
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	18	1.37
(1,12)	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:LYS:N	1:13:A:LYS:CA	11	1.36
(1,6)	1:6:A:ASN:CA	1:6:A:ASN:C	1:7:A:LYS:N	1:7:A:LYS:CA	3	1.35
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	4	1.34
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	24	1.34
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	6	1.33
(1,3)	1:3:A:THR:CA	1:3:A:THR:C	1:4:A:ARG:N	1:4:A:ARG:CA	20	1.33
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	12	1.32
(1,15)	1:15:A:LEU:CA	1:15:A:LEU:C	1:16:A:ASN:N	1:16:A:ASN:CA	6	1.29
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	8	1.29
(1,12)	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:LYS:N	1:13:A:LYS:CA	22	1.29
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	21	1.28
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	8	1.28

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,6)	1:6:A:ASN:CA	1:6:A:ASN:C	1:7:A:LYS:N	1:7:A:LYS:CA	16	1.28
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	19	1.26
(1,10)	1:10:A:ILE:CA	1:10:A:ILE:C	1:11:A:ASN:N	1:11:A:ASN:CA	13	1.26
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	11	1.26
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	5	1.25
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	3	1.25
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	2	1.24
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	17	1.24
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	11	1.23
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	7	1.22
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	20	1.22
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	12	1.22
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	4	1.22
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	17	1.22
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	19	1.22
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	16	1.22
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	3	1.2
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	15	1.2
(1,3)	1:3:A:THR:CA	1:3:A:THR:C	1:4:A:ARG:N	1:4:A:ARG:CA	24	1.2
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	9	1.19
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	16	1.19
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	15	1.19
(1,10)	1:10:A:ILE:CA	1:10:A:ILE:C	1:11:A:ASN:N	1:11:A:ASN:CA	5	1.18
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	6	1.17
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	2	1.16
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	13	1.13
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	21	1.13
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	4	1.13
(1,10)	1:10:A:ILE:CA	1:10:A:ILE:C	1:11:A:ASN:N	1:11:A:ASN:CA	12	1.12
(1,10)	1:10:A:ILE:CA	1:10:A:ILE:C	1:11:A:ASN:N	1:11:A:ASN:CA	23	1.12
(1,8)	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:PHE:N	1:9:A:PHE:CA	20	1.12
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	11	1.12
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	10	1.11
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	3	1.1
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	2	1.1
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	12	1.09
(1,10)	1:10:A:ILE:CA	1:10:A:ILE:C	1:11:A:ASN:N	1:11:A:ASN:CA	18	1.09
(1,15)	1:15:A:LEU:CA	1:15:A:LEU:C	1:16:A:ASN:N	1:16:A:ASN:CA	19	1.08
(1,14)	1:14:A:HIS:CA	1:14:A:HIS:C	1:15:A:LEU:N	1:15:A:LEU:CA	23	1.08
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	4	1.08
(1,9)	1:9:A:PHE:CA	1:9:A:PHE:C	1:10:A:ILE:N	1:10:A:ILE:CA	19	1.06
(1,3)	1:3:A:THR:CA	1:3:A:THR:C	1:4:A:ARG:N	1:4:A:ARG:CA	12	1.04
(1,7)	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:ASP:N	1:8:A:ASP:CA	2	1.03
(1,6)	1:6:A:ASN:CA	1:6:A:ASN:C	1:7:A:LYS:N	1:7:A:LYS:CA	14	1.02
(1,4)	1:4:A:ARG:CA	1:4:A:ARG:C	1:5:A:TYR:N	1:5:A:TYR:CA	6	1.02
(1,16)	1:16:A:ASN:CA	1:16:A:ASN:C	1:17:A:GLU:N	1:17:A:GLU:CA	6	1.0