Full wwPDB NMR Structure Validation Report (i)

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Title	:	D11 bound IGF-II
Authors	:	Hexnerova, R.
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This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

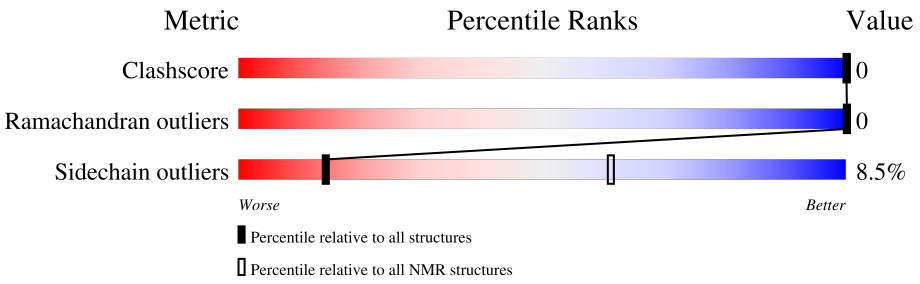
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 83%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	67	21% • 76%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:9-A:24 (16)	0.53	10

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

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

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

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1018 atoms, of which 498 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin-like growth factor II.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	67	1018	321	498	93	100	6	0

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: Insulin-like growth factor II

Chain A: 21% 76%

A1 Y2 R3 P4 S5 E6 T7 L8 C9 E12 G25 F26 Y27 F28 S29 R30 P31 A32 S33 R34 V35 S36 R37 R38 S39 R40 G41 I42 V43 E44 E45 C46 C47 F48 R49 S50 C51 D52 L53 A54 L55 L56 E57 T58 Y59 C60 A61 T62 P63 A64 K65 S66 E67

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: Insulin-like growth factor II

Chain A: 24% 76%

A1 Y2 R3 P4 S5 E6 T7 L8 G25 F26 Y27 F28 S29 R30 P31 A32 S33 R34 V35 S36 R37 R38 S39 R40 G41 I42 V43 E44 E45 C46 C47 F48 R49 S50 C51 D52 L53 A54 L55 L56 E57 T58 Y59 C60 A61 T62 P63 A64 K65 S66 E67

4.2.2 Score per residue for model 2

• Molecule 1: Insulin-like growth factor II

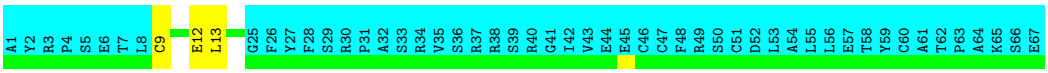
Chain A: 22% 76%

A1 Y2 R3 P4 S5 E6 T7 L8 L13 G25 F26 Y27 F28 S29 R30 P31 A32 S33 R34 V35 S36 R37 R38 S39 R40 G41 I42 V43 E44 E45 C46 C47 F48 R49 S50 C51 D52 L53 A54 L55 L56 E57 T58 Y59 C60 A61 T62 P63 A64 K65 S66 E67

4.2.3 Score per residue for model 3

- Molecule 1: Insulin-like growth factor II

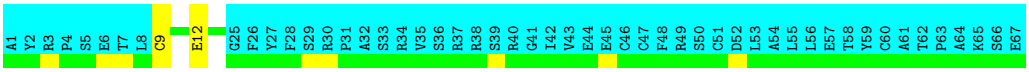
Chain A: 19% • 76%



4.2.4 Score per residue for model 4

- Molecule 1: Insulin-like growth factor II

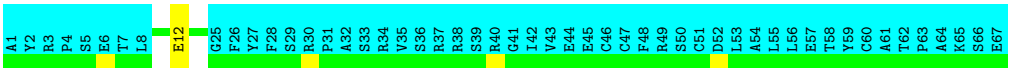
Chain A: 21% • 76%



4.2.5 Score per residue for model 5

- Molecule 1: Insulin-like growth factor II

Chain A: 22% • 76%



4.2.6 Score per residue for model 6

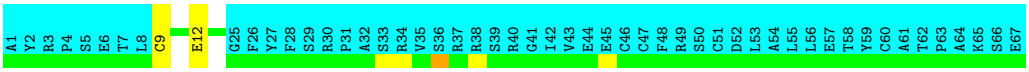
- Molecule 1: Insulin-like growth factor II

Chain A: 19% • 76%

4.2.7 Score per residue for model 7

- Molecule 1: Insulin-like growth factor II

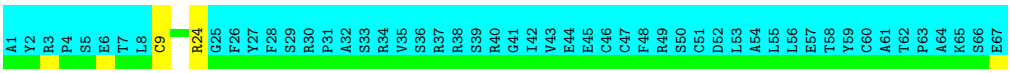
Chain A: 21% • 76%



4.2.8 Score per residue for model 8

- Molecule 1: Insulin-like growth factor II

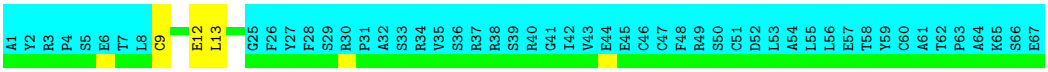
Chain A: 21% • 76%



4.2.9 Score per residue for model 9

- Molecule 1: Insulin-like growth factor II

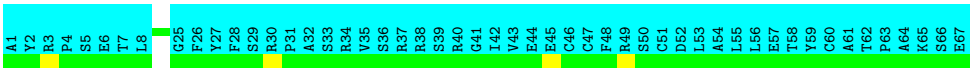
Chain A: 19% • 76%



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Insulin-like growth factor II

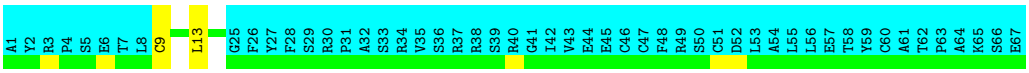
Chain A: 24% 76%



4.2.11 Score per residue for model 11

- Molecule 1: Insulin-like growth factor II

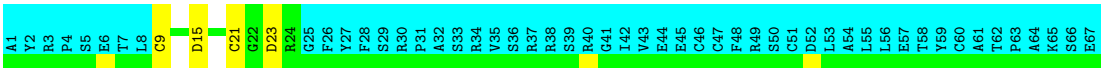
Chain A: 21% • 76%



4.2.12 Score per residue for model 12

- Molecule 1: Insulin-like growth factor II

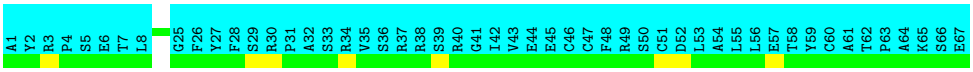
Chain A: 18% 6% 76%



4.2.13 Score per residue for model 13

- Molecule 1: Insulin-like growth factor II

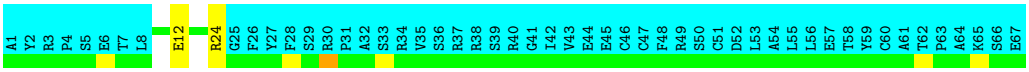
Chain A: 24% 76%



4.2.14 Score per residue for model 14

- Molecule 1: Insulin-like growth factor II

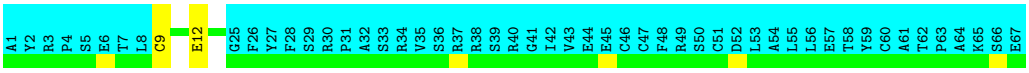
Chain A: 21% • 76%



4.2.15 Score per residue for model 15

- Molecule 1: Insulin-like growth factor II

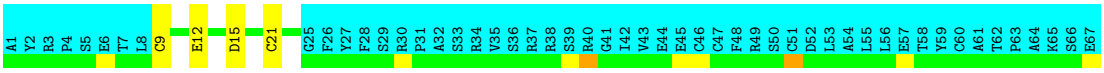
Chain A: 21% • 76%



4.2.16 Score per residue for model 16

- Molecule 1: Insulin-like growth factor II

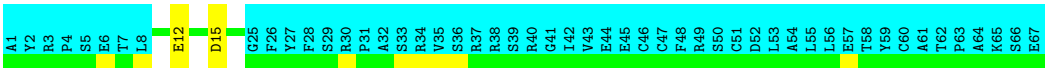
Chain A: 18% 6% 76%



4.2.17 Score per residue for model 17

- Molecule 1: Insulin-like growth factor II

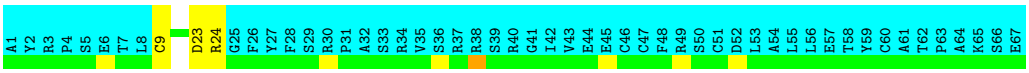
Chain A: 21% • 76%



4.2.18 Score per residue for model 18

- Molecule 1: Insulin-like growth factor II

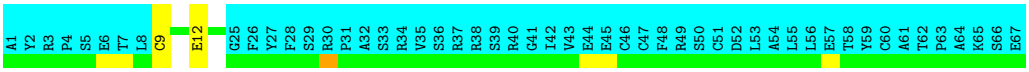
Chain A: 19% • 76%



4.2.19 Score per residue for model 19

- Molecule 1: Insulin-like growth factor II

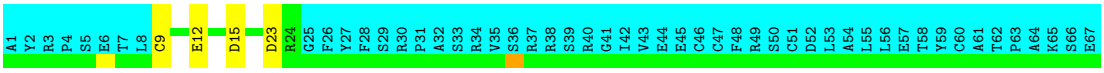
Chain A: 21% • 76%



4.2.20 Score per residue for model 20

- Molecule 1: Insulin-like growth factor II

Chain A: 18% 6% 76%



5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	Classification	Version
CYANA	structure calculation	
YASARA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	694
Number of shifts mapped to atoms	693
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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	0.84±0.05	1±0/118 (0.5± 0.4%)	0.80±0.13	1±1/159 (0.4± 0.7%)
All	All	0.84	12/2360 (0.5%)	0.81	14/3180 (0.4%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	12	GLU	CD-OE1	-5.76	1.19	1.25	5	12

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	15	ASP	CB-CG-OD1	6.36	124.03	118.30	17	4
1	A	23	ASP	CB-CG-OD1	5.88	123.59	118.30	18	2
1	A	24	ARG	NE-CZ-NH1	5.78	123.19	120.30	8	2
1	A	15	ASP	CB-CG-OD2	-5.53	113.32	118.30	12	4
1	A	23	ASP	CB-CG-OD2	-5.34	113.49	118.30	18	2

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
All	All	2340	2160	2160	-

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

There are no clashes.

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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	16/67 (24%)	15±1 (96±5%)	1±1 (4±5%)	0±0 (0±0%)	100	100
All	All	320/1340 (24%)	308 (96%)	12 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	13/57 (23%)	12±1 (92±6%)	1±1 (8±6%)	14	61
All	All	260/1140 (23%)	238 (92%)	22 (8%)	14	61

All 5 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	9	CYS	13
1	A	13	LEU	5
1	A	21	CYS	2
1	A	24	ARG	1
1	A	23	ASP	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *wt.star*

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	694
Number of shifts mapped to atoms	693
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	ALA	H	8.595	0.020	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	34	-0.53 ± 0.35	None needed (imprecise)
$^{13}C_{\beta}$	60	-0.03 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	64	0.94 ± 0.48	None needed (imprecise)

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 83%, i.e. 164 atoms were assigned a chemical shift out of a possible 197. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	63/83 (76%)	35/35 (100%)	12/32 (38%)	16/16 (100%)
Sidechain	93/104 (89%)	63/67 (94%)	28/33 (85%)	2/4 (50%)
Aromatic	8/10 (80%)	5/5 (100%)	3/5 (60%)	0/0 (—%)
Overall	164/197 (83%)	103/107 (96%)	43/70 (61%)	18/20 (90%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 693 atoms were assigned a chemical shift out of a possible 884. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	234/334 (70%)	136/136 (100%)	34/134 (25%)	64/64 (100%)
Sidechain	409/483 (85%)	279/312 (89%)	122/145 (84%)	8/26 (31%)
Aromatic	50/67 (75%)	32/32 (100%)	18/35 (51%)	0/0 (—%)
Overall	693/884 (78%)	447/480 (93%)	174/314 (55%)	72/90 (80%)

7.1.4 Statistically unusual chemical shifts (i)

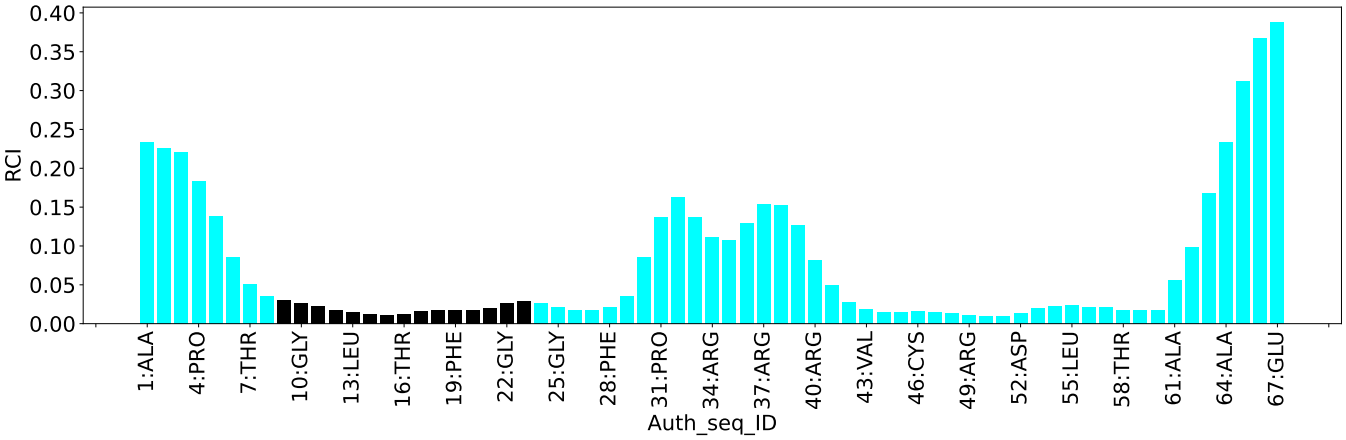
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	16	THR	HG1	5.17	0.08 – 2.19	19.1

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1:ALA
4:PRO
7:THR
10:GLY
13:LEU
16:THR
19:PHE
22:GLY
25:GLY
28:PHE
31:PRO
34:ARG
37:ARG
40:ARG
43:VAL
46:CYS
49:ARG
52:ASP
55:LEU
58:THR
61:ALA
64:ALA
67:GLU
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	1046
Intra-residue (|i-j|=0)	306
Sequential (|i-j|=1)	323
Medium range (|i-j|>1 and |i-j|<5)	160
Long range (|i-j|≥5)	248
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	9
Total dihedral-angle restraints	46
Number of unmapped restraints	0
Number of restraints per residue	16.3
Number of long range restraints per residue[1]	3.8

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

8.2 Residual restraint violations (i)

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 (i)

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)	4.6	0.2
0.2-0.5 (Medium)	2.0	0.5
>0.5 (Large)	1.9	1.47

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)	1.3	5.0
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

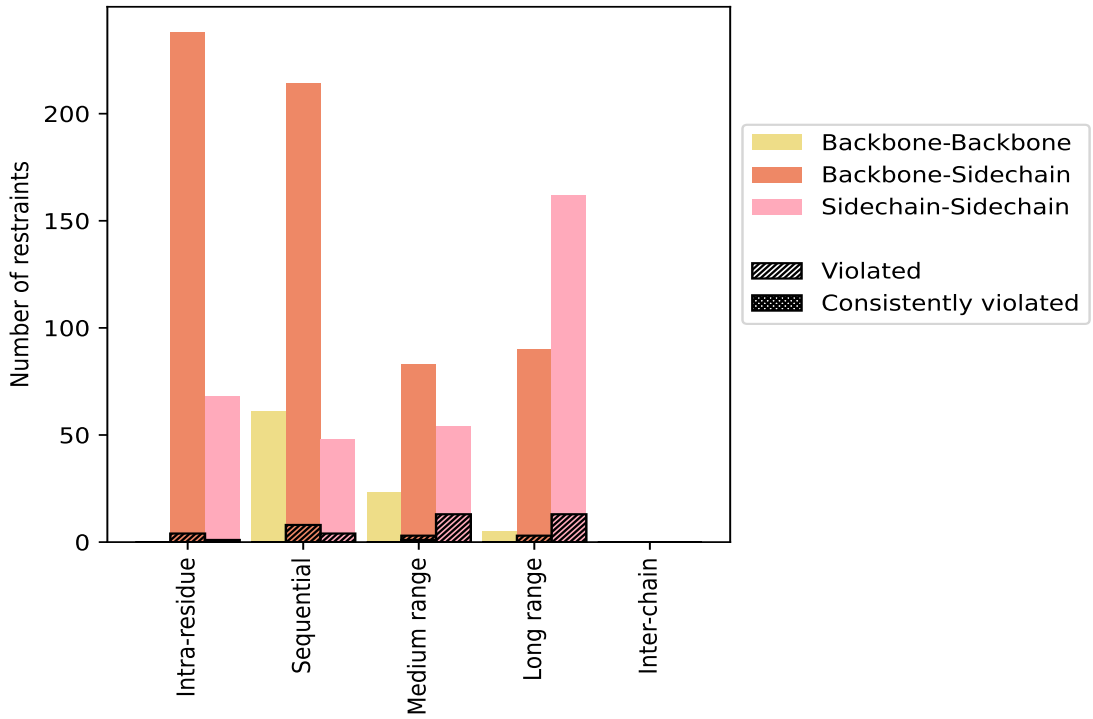
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	306	29.3	5	1.6	0.5	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	238	22.8	4	1.7	0.4	0	0.0	0.0
Sidechain-Sidechain	68	6.5	1	1.5	0.1	0	0.0	0.0
Sequential (|i-j|=1)	323	30.9	12	3.7	1.1	0	0.0	0.0
Backbone-Backbone	61	5.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	214	20.5	8	3.7	0.8	0	0.0	0.0
Sidechain-Sidechain	48	4.6	4	8.3	0.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	160	15.3	16	10.0	1.5	1	0.6	0.1
Backbone-Backbone	23	2.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	83	7.9	3	3.6	0.3	1	1.2	0.1
Sidechain-Sidechain	54	5.2	13	24.1	1.2	0	0.0	0.0
Long range (|i-j|≥5)	248	23.7	16	6.5	1.5	0	0.0	0.0
Backbone-Backbone	5	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	90	8.6	3	3.3	0.3	0	0.0	0.0
Sidechain-Sidechain	153	14.6	13	8.5	1.2	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	9	0.9	0	0.0	0.0	0	0.0	0.0
Total	1046	100.0	49	4.7	4.7	1	0.1	0.1
Backbone-Backbone	89	8.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	625	59.8	18	2.9	1.7	1	0.2	0.1
Sidechain-Sidechain	332	31.7	31	9.3	3.0	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	3	2	2	0	7	0.35	0.84	0.25	0.26
2	0	3	3	6	0	12	0.34	0.95	0.25	0.26
3	0	2	2	3	0	7	0.44	1.3	0.42	0.22
4	0	3	1	3	0	7	0.47	1.38	0.45	0.19
5	0	2	1	1	0	4	0.62	1.41	0.51	0.46
6	0	4	2	3	0	9	0.39	1.46	0.41	0.22
7	0	3	1	3	0	7	0.43	1.39	0.43	0.24
8	0	2	2	5	0	9	0.36	0.98	0.3	0.23
9	2	3	3	2	0	10	0.36	1.28	0.35	0.2
10	0	2	3	1	0	6	0.49	1.3	0.41	0.32
11	0	2	5	4	0	11	0.32	1.02	0.27	0.21

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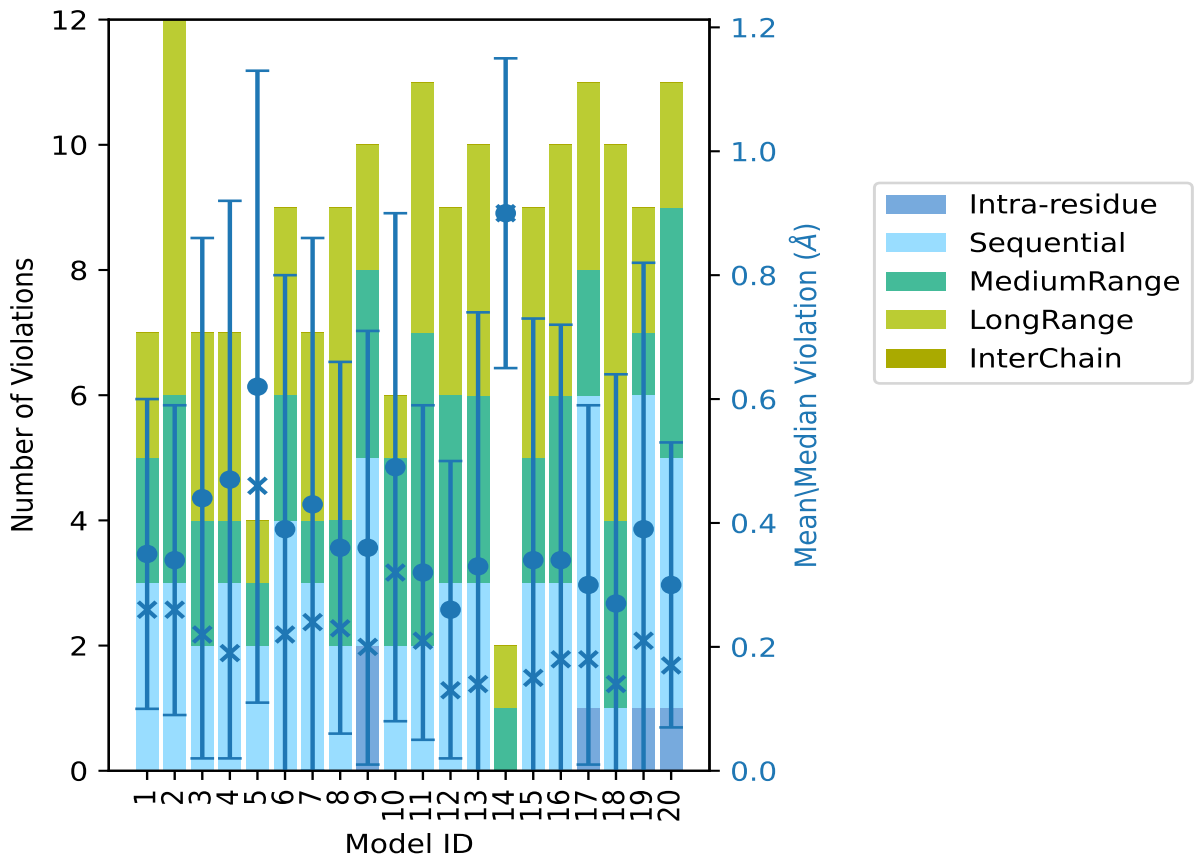
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	3	3	3	0	9	0.26	0.85	0.24	0.13
13	0	3	3	4	0	10	0.33	1.47	0.41	0.14
14	0	0	1	1	0	2	0.9	1.15	0.25	0.9
15	0	3	2	4	0	9	0.34	1.28	0.39	0.15
16	0	3	3	4	0	10	0.34	1.32	0.38	0.18
17	1	5	2	3	0	11	0.3	1.1	0.29	0.18
18	0	1	3	6	0	10	0.27	1.38	0.37	0.14
19	1	5	1	2	0	9	0.39	1.45	0.43	0.21
20	1	4	4	2	0	11	0.3	0.83	0.23	0.17

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

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



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

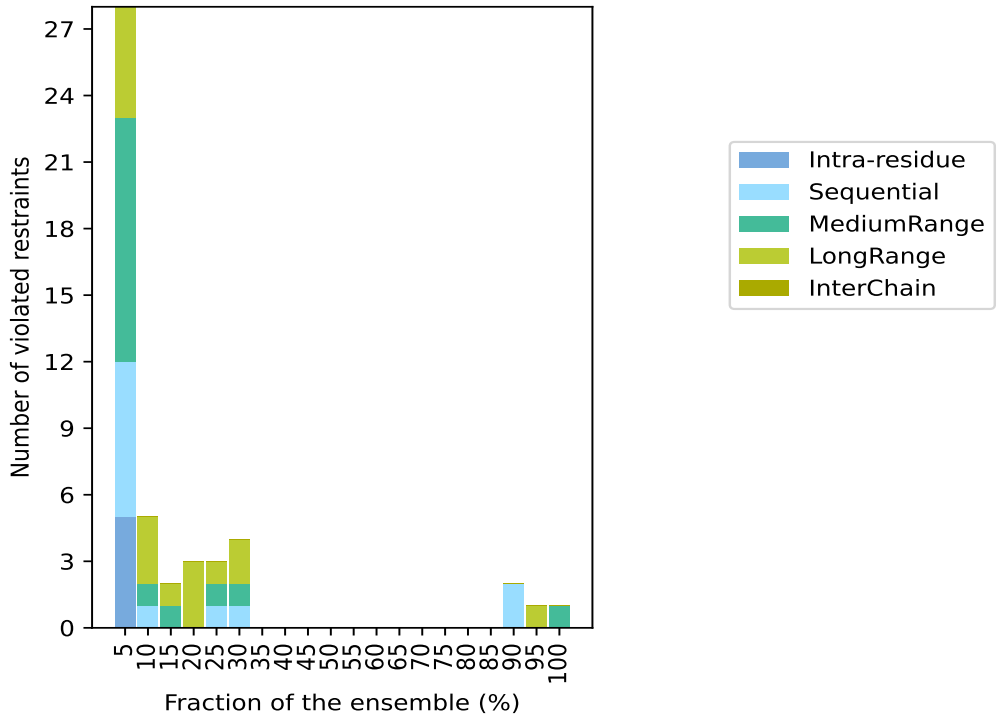
9.3 Distance violation statistics for the ensemble (i)

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, 988(IR:301, SQ:311, MR:144, LR:232, 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]	%
5	7	11	5	0	28	1	5.0
0	1	1	3	0	5	2	10.0
0	0	1	1	0	2	3	15.0
0	0	0	3	0	3	4	20.0
0	1	1	1	0	3	5	25.0
0	1	1	2	0	4	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	2	0	0	0	2	18	90.0
0	0	0	1	0	1	19	95.0
0	0	1	0	0	1	20	100.0

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

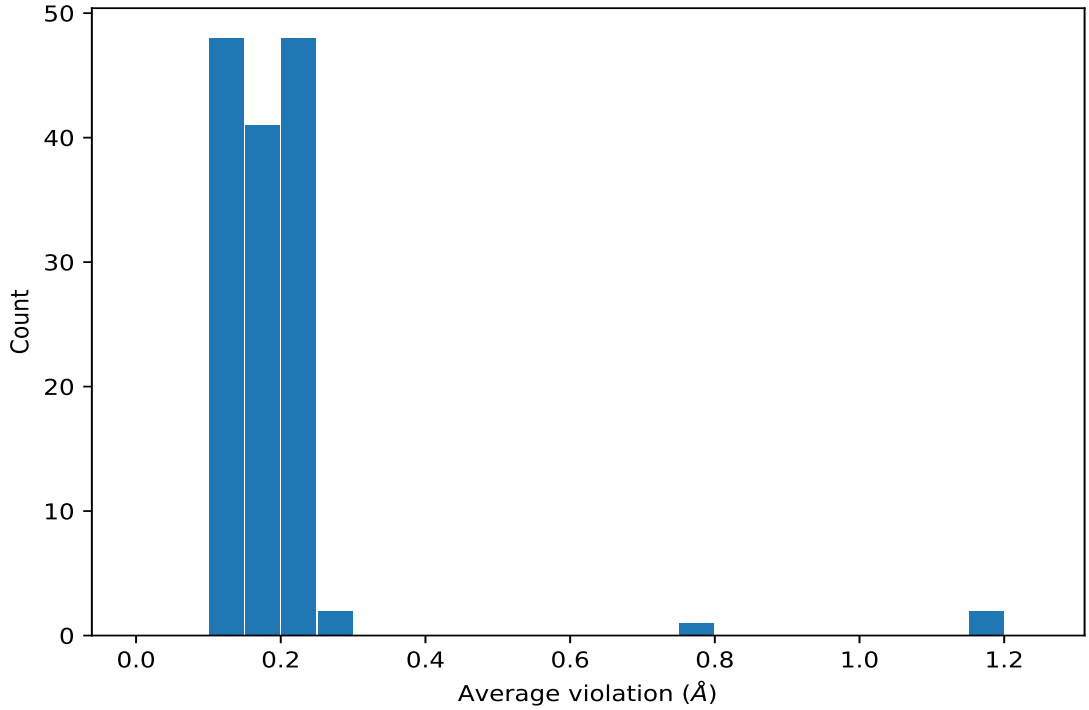
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	20	0.75	0.2	0.76
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	19	1.18	0.27	1.3
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	19	1.18	0.27	1.3
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	18	0.21	0.05	0.21
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	18	0.21	0.05	0.21
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	18	0.21	0.05	0.21
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	18	0.21	0.05	0.21
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	18	0.21	0.05	0.21
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	18	0.21	0.05	0.21
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	18	0.17	0.04	0.16
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	18	0.17	0.04	0.16
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	18	0.17	0.04	0.16
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	18	0.17	0.04	0.16
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	18	0.17	0.04	0.16
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	18	0.17	0.04	0.16
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD11	6	0.22	0.13	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD12	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD13	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD21	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD22	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD23	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD11	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD12	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD13	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD21	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD22	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD23	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD11	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD12	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD13	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD21	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD22	6	0.22	0.13	0.17
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD23	6	0.22	0.13	0.17
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD11	6	0.21	0.03	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD12	6	0.21	0.03	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD13	6	0.21	0.03	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD21	6	0.21	0.03	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD22	6	0.21	0.03	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD23	6	0.21	0.03	0.2
(1,989)	1:A:43:VAL:HG11	1:A:48:PHE:HB3	6	0.18	0.05	0.16
(1,989)	1:A:43:VAL:HG12	1:A:48:PHE:HB3	6	0.18	0.05	0.16
(1,989)	1:A:43:VAL:HG13	1:A:48:PHE:HB3	6	0.18	0.05	0.16
(1,989)	1:A:43:VAL:HG21	1:A:48:PHE:HB3	6	0.18	0.05	0.16
(1,989)	1:A:43:VAL:HG22	1:A:48:PHE:HB3	6	0.18	0.05	0.16
(1,989)	1:A:43:VAL:HG23	1:A:48:PHE:HB3	6	0.18	0.05	0.16
(1,635)	1:A:55:LEU:HD11	1:A:56:LEU:H	6	0.13	0.01	0.12
(1,635)	1:A:55:LEU:HD12	1:A:56:LEU:H	6	0.13	0.01	0.12
(1,635)	1:A:55:LEU:HD13	1:A:56:LEU:H	6	0.13	0.01	0.12
(1,635)	1:A:55:LEU:HD21	1:A:56:LEU:H	6	0.13	0.01	0.12
(1,635)	1:A:55:LEU:HD22	1:A:56:LEU:H	6	0.13	0.01	0.12
(1,635)	1:A:55:LEU:HD23	1:A:56:LEU:H	6	0.13	0.01	0.12
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD2	5	0.27	0.03	0.27
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD3	5	0.27	0.03	0.27
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD2	5	0.18	0.06	0.17
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD3	5	0.18	0.06	0.17
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD2	5	0.18	0.06	0.17
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD3	5	0.18	0.06	0.17
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD2	5	0.18	0.06	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD3	5	0.18	0.06	0.17
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD11	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD12	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD13	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD11	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD12	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD13	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD11	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD12	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD13	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD11	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD12	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD13	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD11	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD12	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD13	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD11	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD12	5	0.15	0.02	0.14
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD13	5	0.15	0.02	0.14
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD11	4	0.24	0.04	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD12	4	0.24	0.04	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD13	4	0.24	0.04	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD21	4	0.24	0.04	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD22	4	0.24	0.04	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD23	4	0.24	0.04	0.22
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG11	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG12	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG13	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG21	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG22	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG23	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG11	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG12	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG13	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG21	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG22	4	0.19	0.03	0.18
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG23	4	0.19	0.03	0.18
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD21	4	0.18	0.07	0.15
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD22	4	0.18	0.07	0.15
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD23	4	0.18	0.07	0.15
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD21	4	0.18	0.07	0.15
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD22	4	0.18	0.07	0.15

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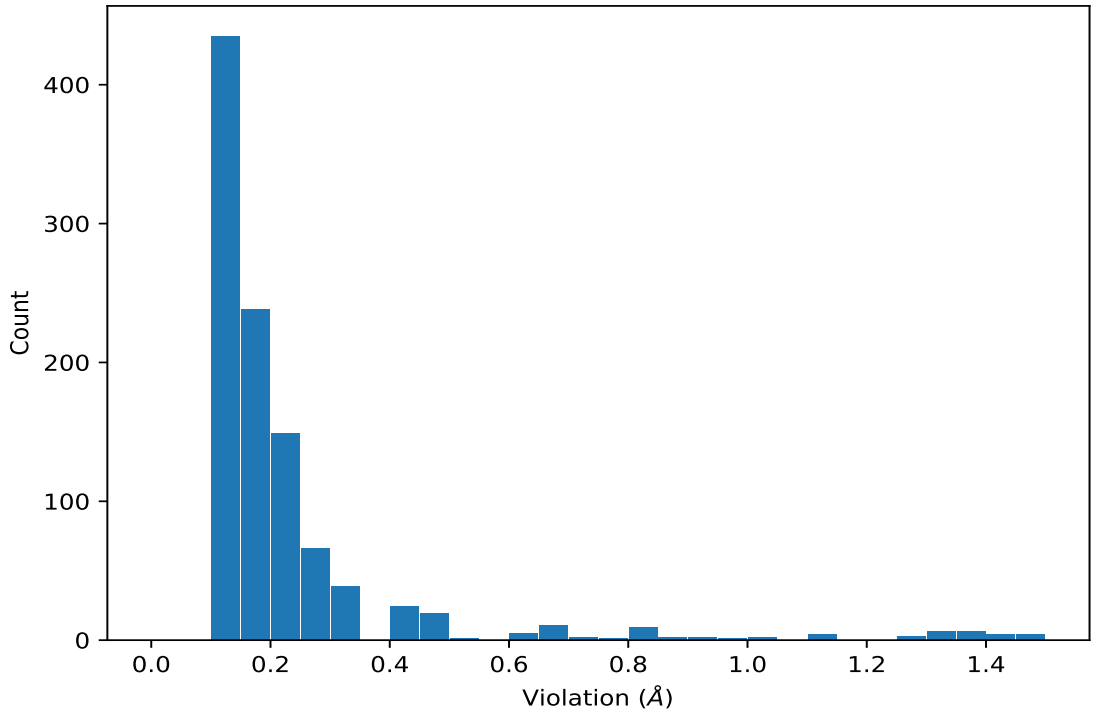
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD23	4	0.18	0.07	0.15
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD21	4	0.18	0.07	0.15
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD22	4	0.18	0.07	0.15
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD23	4	0.18	0.07	0.15
(1,485)	1:A:35:VAL:HG21	1:A:37:ARG:HD2	3	0.2	0.06	0.18
(1,485)	1:A:35:VAL:HG21	1:A:37:ARG:HD3	3	0.2	0.06	0.18
(1,485)	1:A:35:VAL:HG22	1:A:37:ARG:HD2	3	0.2	0.06	0.18
(1,485)	1:A:35:VAL:HG22	1:A:37:ARG:HD3	3	0.2	0.06	0.18
(1,485)	1:A:35:VAL:HG23	1:A:37:ARG:HD2	3	0.2	0.06	0.18
(1,485)	1:A:35:VAL:HG23	1:A:37:ARG:HD3	3	0.2	0.06	0.18
(1,901)	1:A:20:VAL:HG11	1:A:56:LEU:HA	3	0.15	0.03	0.16
(1,901)	1:A:20:VAL:HG12	1:A:56:LEU:HA	3	0.15	0.03	0.16
(1,901)	1:A:20:VAL:HG13	1:A:56:LEU:HA	3	0.15	0.03	0.16
(1,901)	1:A:20:VAL:HG21	1:A:56:LEU:HA	3	0.15	0.03	0.16
(1,901)	1:A:20:VAL:HG22	1:A:56:LEU:HA	3	0.15	0.03	0.16
(1,901)	1:A:20:VAL:HG23	1:A:56:LEU:HA	3	0.15	0.03	0.16
(1,769)	1:A:8:LEU:HD11	1:A:13:LEU:H	2	0.2	0.0	0.2
(1,769)	1:A:8:LEU:HD12	1:A:13:LEU:H	2	0.2	0.0	0.2
(1,769)	1:A:8:LEU:HD13	1:A:13:LEU:H	2	0.2	0.0	0.2
(1,769)	1:A:8:LEU:HD21	1:A:13:LEU:H	2	0.2	0.0	0.2
(1,769)	1:A:8:LEU:HD22	1:A:13:LEU:H	2	0.2	0.0	0.2
(1,769)	1:A:8:LEU:HD23	1:A:13:LEU:H	2	0.2	0.0	0.2
(1,172)	1:A:39:SER:HB2	1:A:40:ARG:H	2	0.18	0.0	0.18
(1,172)	1:A:39:SER:HB3	1:A:40:ARG:H	2	0.18	0.0	0.18
(1,561)	1:A:43:VAL:HG21	1:A:48:PHE:HD1	2	0.12	0.0	0.12
(1,561)	1:A:43:VAL:HG21	1:A:48:PHE:HD2	2	0.12	0.0	0.12
(1,561)	1:A:43:VAL:HG22	1:A:48:PHE:HD1	2	0.12	0.0	0.12
(1,561)	1:A:43:VAL:HG22	1:A:48:PHE:HD2	2	0.12	0.0	0.12
(1,561)	1:A:43:VAL:HG23	1:A:48:PHE:HD1	2	0.12	0.0	0.12
(1,561)	1:A:43:VAL:HG23	1:A:48:PHE:HD2	2	0.12	0.0	0.12
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD11	2	0.11	0.0	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD12	2	0.11	0.0	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD13	2	0.11	0.0	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD21	2	0.11	0.0	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD22	2	0.11	0.0	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD23	2	0.11	0.0	0.11
(1,687)	1:A:27:TYR:HD1	1:A:61:ALA:HB1	2	0.11	0.0	0.11
(1,687)	1:A:27:TYR:HD1	1:A:61:ALA:HB2	2	0.11	0.0	0.11
(1,687)	1:A:27:TYR:HD1	1:A:61:ALA:HB3	2	0.11	0.0	0.11
(1,687)	1:A:27:TYR:HD2	1:A:61:ALA:HB1	2	0.11	0.0	0.11
(1,687)	1:A:27:TYR:HD2	1:A:61:ALA:HB2	2	0.11	0.0	0.11
(1,687)	1:A:27:TYR:HD2	1:A:61:ALA:HB3	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	13	1.47
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	13	1.47
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	6	1.46
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	6	1.46
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	19	1.45
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	19	1.45
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	5	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	5	1.41
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	7	1.39
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	7	1.39
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	4	1.38
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	4	1.38
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	18	1.38
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	18	1.38
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	16	1.32
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	16	1.32
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	3	1.3
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	3	1.3
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	10	1.3
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	10	1.3
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	15	1.28
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	15	1.28
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	9	1.28
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	14	1.15
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	14	1.15
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	17	1.1
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	17	1.1
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	11	1.02
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	11	1.02
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	8	0.98
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	2	0.95
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	2	0.95
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	4	0.87
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	3	0.86
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	12	0.85
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	12	0.85
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	1	0.84
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	8	0.83
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	8	0.83
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	19	0.83
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	20	0.83
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	2	0.82
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	15	0.8
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	16	0.79
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	5	0.74
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	6	0.71
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	10	0.7
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	11	0.69
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	20	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	20	0.68
(1,833)	1:A:14:VAL:HG11	1:A:18:GLN:HE21	9	0.66
(1,833)	1:A:14:VAL:HG12	1:A:18:GLN:HE21	9	0.66
(1,833)	1:A:14:VAL:HG13	1:A:18:GLN:HE21	9	0.66
(1,833)	1:A:14:VAL:HG21	1:A:18:GLN:HE21	9	0.66
(1,833)	1:A:14:VAL:HG22	1:A:18:GLN:HE21	9	0.66
(1,833)	1:A:14:VAL:HG23	1:A:18:GLN:HE21	9	0.66
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	7	0.65
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	14	0.64
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	13	0.62
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE1	1	0.61
(1,451)	1:A:18:GLN:HE21	1:A:26:PHE:HE2	1	0.61
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	17	0.61
(1,280)	1:A:18:GLN:HB2	1:A:18:GLN:HE21	9	0.5
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	12	0.49
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD11	4	0.45
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD12	4	0.45
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD13	4	0.45
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD21	4	0.45
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD22	4	0.45
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD23	4	0.45
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD11	4	0.45
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD12	4	0.45
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD13	4	0.45
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD21	4	0.45
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD22	4	0.45
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD23	4	0.45
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD11	4	0.45
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD12	4	0.45
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD13	4	0.45
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD21	4	0.45
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD22	4	0.45
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD23	4	0.45
(1,486)	1:A:35:VAL:HG21	1:A:37:ARG:HG2	10	0.42
(1,486)	1:A:35:VAL:HG21	1:A:37:ARG:HG3	10	0.42
(1,486)	1:A:35:VAL:HG22	1:A:37:ARG:HG2	10	0.42
(1,486)	1:A:35:VAL:HG22	1:A:37:ARG:HG3	10	0.42
(1,486)	1:A:35:VAL:HG23	1:A:37:ARG:HG2	10	0.42
(1,486)	1:A:35:VAL:HG23	1:A:37:ARG:HG3	10	0.42
(1,905)	1:A:20:VAL:HG11	1:A:56:LEU:HD11	11	0.4
(1,905)	1:A:20:VAL:HG11	1:A:56:LEU:HD12	11	0.4
(1,905)	1:A:20:VAL:HG11	1:A:56:LEU:HD13	11	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,905)	1:A:20:VAL:HG12	1:A:56:LEU:HD11	11	0.4
(1,905)	1:A:20:VAL:HG12	1:A:56:LEU:HD12	11	0.4
(1,905)	1:A:20:VAL:HG12	1:A:56:LEU:HD13	11	0.4
(1,905)	1:A:20:VAL:HG13	1:A:56:LEU:HD11	11	0.4
(1,905)	1:A:20:VAL:HG13	1:A:56:LEU:HD12	11	0.4
(1,905)	1:A:20:VAL:HG13	1:A:56:LEU:HD13	11	0.4
(1,905)	1:A:20:VAL:HG21	1:A:56:LEU:HD11	11	0.4
(1,905)	1:A:20:VAL:HG21	1:A:56:LEU:HD12	11	0.4
(1,905)	1:A:20:VAL:HG21	1:A:56:LEU:HD13	11	0.4
(1,905)	1:A:20:VAL:HG22	1:A:56:LEU:HD11	11	0.4
(1,905)	1:A:20:VAL:HG22	1:A:56:LEU:HD12	11	0.4
(1,905)	1:A:20:VAL:HG22	1:A:56:LEU:HD13	11	0.4
(1,905)	1:A:20:VAL:HG23	1:A:56:LEU:HD11	11	0.4
(1,905)	1:A:20:VAL:HG23	1:A:56:LEU:HD12	11	0.4
(1,905)	1:A:20:VAL:HG23	1:A:56:LEU:HD13	11	0.4
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD11	7	0.33
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD12	7	0.33
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD13	7	0.33
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD21	7	0.33
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD22	7	0.33
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD23	7	0.33
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD11	7	0.33
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD12	7	0.33
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD13	7	0.33
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD21	7	0.33
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD22	7	0.33
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD23	7	0.33
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD11	7	0.33
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD12	7	0.33
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD13	7	0.33
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD21	7	0.33
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD22	7	0.33
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD23	7	0.33
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	2	0.33
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	2	0.33
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	2	0.33
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	2	0.33
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	2	0.33
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	2	0.33
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD11	2	0.32
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD12	2	0.32
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD13	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD21	2	0.32
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD22	2	0.32
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD23	2	0.32
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD21	2	0.31
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD22	2	0.31
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD23	2	0.31
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD21	2	0.31
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD22	2	0.31
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD23	2	0.31
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD21	2	0.31
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD22	2	0.31
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD23	2	0.31
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD2	17	0.3
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD3	17	0.3
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD2	19	0.29
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD3	19	0.29
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	8	0.29
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	8	0.29
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	8	0.29
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	8	0.29
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	8	0.29
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	8	0.29
(1,485)	1:A:35:VAL:HG21	1:A:37:ARG:HD2	20	0.29
(1,485)	1:A:35:VAL:HG21	1:A:37:ARG:HD3	20	0.29
(1,485)	1:A:35:VAL:HG22	1:A:37:ARG:HD2	20	0.29
(1,485)	1:A:35:VAL:HG22	1:A:37:ARG:HD3	20	0.29
(1,485)	1:A:35:VAL:HG23	1:A:37:ARG:HD2	20	0.29
(1,485)	1:A:35:VAL:HG23	1:A:37:ARG:HD3	20	0.29
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD2	20	0.29
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD3	20	0.29
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD2	20	0.29
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD3	20	0.29
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD2	20	0.29
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD3	20	0.29
(1,1030)	1:A:60:CYS:HB2	1:A:61:ALA:HB1	20	0.29
(1,1030)	1:A:60:CYS:HB2	1:A:61:ALA:HB2	20	0.29
(1,1030)	1:A:60:CYS:HB2	1:A:61:ALA:HB3	20	0.29
(1,1030)	1:A:60:CYS:HB3	1:A:61:ALA:HB1	20	0.29
(1,1030)	1:A:60:CYS:HB3	1:A:61:ALA:HB2	20	0.29
(1,1030)	1:A:60:CYS:HB3	1:A:61:ALA:HB3	20	0.29
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD2	1	0.27
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD3	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	2	0.27
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	2	0.27
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	2	0.27
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	2	0.27
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	2	0.27
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	2	0.27
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD11	2	0.26
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD12	2	0.26
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD13	2	0.26
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD21	2	0.26
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD22	2	0.26
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD23	2	0.26
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	1	0.26
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	1	0.26
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	1	0.26
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	1	0.26
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	1	0.26
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	1	0.26
(1,989)	1:A:43:VAL:HG11	1:A:48:PHE:HB3	2	0.25
(1,989)	1:A:43:VAL:HG12	1:A:48:PHE:HB3	2	0.25
(1,989)	1:A:43:VAL:HG13	1:A:48:PHE:HB3	2	0.25
(1,989)	1:A:43:VAL:HG21	1:A:48:PHE:HB3	2	0.25
(1,989)	1:A:43:VAL:HG22	1:A:48:PHE:HB3	2	0.25
(1,989)	1:A:43:VAL:HG23	1:A:48:PHE:HB3	2	0.25
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	8	0.25
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	8	0.25
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	8	0.25
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	8	0.25
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	8	0.25
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	8	0.25
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	19	0.25
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	19	0.25
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	19	0.25
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	19	0.25
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	19	0.25
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	19	0.25
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD2	7	0.24
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD3	7	0.24
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD11	11	0.24
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD12	11	0.24
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD13	11	0.24
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD21	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD22	11	0.24
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD23	11	0.24
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	17	0.24
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	17	0.24
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	17	0.24
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	17	0.24
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	17	0.24
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	17	0.24
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	3	0.24
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	3	0.24
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	3	0.24
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	3	0.24
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	3	0.24
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	3	0.24
(1,989)	1:A:43:VAL:HG11	1:A:48:PHE:HB3	8	0.23
(1,989)	1:A:43:VAL:HG12	1:A:48:PHE:HB3	8	0.23
(1,989)	1:A:43:VAL:HG13	1:A:48:PHE:HB3	8	0.23
(1,989)	1:A:43:VAL:HG21	1:A:48:PHE:HB3	8	0.23
(1,989)	1:A:43:VAL:HG22	1:A:48:PHE:HB3	8	0.23
(1,989)	1:A:43:VAL:HG23	1:A:48:PHE:HB3	8	0.23
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD2	6	0.23
(1,936)	1:A:30:ARG:HA	1:A:31:PRO:HD3	6	0.23
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG11	12	0.23
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG12	12	0.23
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG13	12	0.23
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG21	12	0.23
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG22	12	0.23
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG23	12	0.23
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG11	12	0.23
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG12	12	0.23
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG13	12	0.23
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG21	12	0.23
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG22	12	0.23
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG23	12	0.23
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD11	6	0.23
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD12	6	0.23
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD13	6	0.23
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD21	6	0.23
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD22	6	0.23
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD23	6	0.23
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	13	0.23
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	13	0.23
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	13	0.23
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	13	0.23
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	13	0.23
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	16	0.23
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	16	0.23
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	16	0.23
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	16	0.23
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	16	0.23
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	16	0.23
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD11	3	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD12	3	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD13	3	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD21	3	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD22	3	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD23	3	0.22
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	1	0.22
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	1	0.22
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	1	0.22
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	1	0.22
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	1	0.22
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	1	0.22
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	6	0.22
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	6	0.22
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	6	0.22
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	6	0.22
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	6	0.22
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	6	0.22
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD11	11	0.21
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD12	11	0.21
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD13	11	0.21
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD21	11	0.21
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD22	11	0.21
(1,759)	1:A:8:LEU:HB2	1:A:13:LEU:HD23	11	0.21
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	19	0.21
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	19	0.21
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	19	0.21
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	19	0.21
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	19	0.21
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	19	0.21
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	10	0.21
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	10	0.21
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	10	0.21
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	10	0.21
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	10	0.21
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	11	0.21
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	11	0.21
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	11	0.21
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	11	0.21
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	11	0.21
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	11	0.21
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	17	0.21
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	17	0.21
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	17	0.21
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	17	0.21
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	17	0.21
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	17	0.21
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG11	2	0.2
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG12	2	0.2
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG13	2	0.2
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG21	2	0.2
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG22	2	0.2
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG23	2	0.2
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG11	2	0.2
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG12	2	0.2
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG13	2	0.2
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG21	2	0.2
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG22	2	0.2
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG23	2	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD11	6	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD12	6	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD13	6	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD21	6	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD22	6	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD23	6	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD11	9	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD12	9	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD13	9	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD21	9	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD22	9	0.2
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD23	9	0.2
(1,769)	1:A:8:LEU:HD11	1:A:13:LEU:H	9	0.2
(1,769)	1:A:8:LEU:HD12	1:A:13:LEU:H	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:A:8:LEU:HD13	1:A:13:LEU:H	9	0.2
(1,769)	1:A:8:LEU:HD21	1:A:13:LEU:H	9	0.2
(1,769)	1:A:8:LEU:HD22	1:A:13:LEU:H	9	0.2
(1,769)	1:A:8:LEU:HD23	1:A:13:LEU:H	9	0.2
(1,769)	1:A:8:LEU:HD11	1:A:13:LEU:H	15	0.2
(1,769)	1:A:8:LEU:HD12	1:A:13:LEU:H	15	0.2
(1,769)	1:A:8:LEU:HD13	1:A:13:LEU:H	15	0.2
(1,769)	1:A:8:LEU:HD21	1:A:13:LEU:H	15	0.2
(1,769)	1:A:8:LEU:HD22	1:A:13:LEU:H	15	0.2
(1,769)	1:A:8:LEU:HD23	1:A:13:LEU:H	15	0.2
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	9	0.2
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	9	0.2
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	9	0.2
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	9	0.2
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	9	0.2
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	9	0.2
(1,366)	1:A:14:VAL:HA	1:A:18:GLN:HE21	18	0.2
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD11	11	0.19
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD12	11	0.19
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD13	11	0.19
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD11	11	0.19
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD12	11	0.19
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD13	11	0.19
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD11	11	0.19
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD12	11	0.19
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD13	11	0.19
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD11	11	0.19
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD12	11	0.19
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD13	11	0.19
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD11	11	0.19
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD12	11	0.19
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD13	11	0.19
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD11	11	0.19
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD12	11	0.19
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD13	11	0.19
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	3	0.19
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	3	0.19
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	3	0.19
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	3	0.19
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	3	0.19
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	3	0.19
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD11	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD12	8	0.19
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD13	8	0.19
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD21	8	0.19
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD22	8	0.19
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD23	8	0.19
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD11	8	0.19
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD12	8	0.19
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD13	8	0.19
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD21	8	0.19
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD22	8	0.19
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD23	8	0.19
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD11	8	0.19
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD12	8	0.19
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD13	8	0.19
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD21	8	0.19
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD22	8	0.19
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD23	8	0.19
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	4	0.19
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	4	0.19
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	4	0.19
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	4	0.19
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	4	0.19
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	4	0.19
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	7	0.19
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	7	0.19
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	7	0.19
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	7	0.19
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	7	0.19
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	7	0.19
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD2	16	0.19
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD3	16	0.19
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD2	16	0.19
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD3	16	0.19
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD2	16	0.19
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD3	16	0.19
(1,901)	1:A:20:VAL:HG11	1:A:56:LEU:HA	16	0.18
(1,901)	1:A:20:VAL:HG12	1:A:56:LEU:HA	16	0.18
(1,901)	1:A:20:VAL:HG13	1:A:56:LEU:HA	16	0.18
(1,901)	1:A:20:VAL:HG21	1:A:56:LEU:HA	16	0.18
(1,901)	1:A:20:VAL:HG22	1:A:56:LEU:HA	16	0.18
(1,901)	1:A:20:VAL:HG23	1:A:56:LEU:HA	16	0.18
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD11	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD12	3	0.18
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD13	3	0.18
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD21	3	0.18
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD22	3	0.18
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD23	3	0.18
(1,485)	1:A:35:VAL:HG21	1:A:37:ARG:HD2	17	0.18
(1,485)	1:A:35:VAL:HG21	1:A:37:ARG:HD3	17	0.18
(1,485)	1:A:35:VAL:HG22	1:A:37:ARG:HD2	17	0.18
(1,485)	1:A:35:VAL:HG22	1:A:37:ARG:HD3	17	0.18
(1,485)	1:A:35:VAL:HG23	1:A:37:ARG:HD2	17	0.18
(1,485)	1:A:35:VAL:HG23	1:A:37:ARG:HD3	17	0.18
(1,172)	1:A:39:SER:HB2	1:A:40:ARG:H	6	0.18
(1,172)	1:A:39:SER:HB3	1:A:40:ARG:H	6	0.18
(1,998)	1:A:45:GLU:HG2	1:A:55:LEU:HD11	16	0.17
(1,998)	1:A:45:GLU:HG2	1:A:55:LEU:HD12	16	0.17
(1,998)	1:A:45:GLU:HG2	1:A:55:LEU:HD13	16	0.17
(1,998)	1:A:45:GLU:HG2	1:A:55:LEU:HD21	16	0.17
(1,998)	1:A:45:GLU:HG2	1:A:55:LEU:HD22	16	0.17
(1,998)	1:A:45:GLU:HG2	1:A:55:LEU:HD23	16	0.17
(1,998)	1:A:45:GLU:HG3	1:A:55:LEU:HD11	16	0.17
(1,998)	1:A:45:GLU:HG3	1:A:55:LEU:HD12	16	0.17
(1,998)	1:A:45:GLU:HG3	1:A:55:LEU:HD13	16	0.17
(1,998)	1:A:45:GLU:HG3	1:A:55:LEU:HD21	16	0.17
(1,998)	1:A:45:GLU:HG3	1:A:55:LEU:HD22	16	0.17
(1,998)	1:A:45:GLU:HG3	1:A:55:LEU:HD23	16	0.17
(1,989)	1:A:43:VAL:HG11	1:A:48:PHE:HB3	17	0.17
(1,989)	1:A:43:VAL:HG12	1:A:48:PHE:HB3	17	0.17
(1,989)	1:A:43:VAL:HG13	1:A:48:PHE:HB3	17	0.17
(1,989)	1:A:43:VAL:HG21	1:A:48:PHE:HB3	17	0.17
(1,989)	1:A:43:VAL:HG22	1:A:48:PHE:HB3	17	0.17
(1,989)	1:A:43:VAL:HG23	1:A:48:PHE:HB3	17	0.17
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG11	18	0.17
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG12	18	0.17
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG13	18	0.17
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG21	18	0.17
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG22	18	0.17
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG23	18	0.17
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG11	18	0.17
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG12	18	0.17
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG13	18	0.17
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG21	18	0.17
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG22	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG23	18	0.17
(1,846)	1:A:16:THR:HG21	1:A:20:VAL:HG11	11	0.17
(1,846)	1:A:16:THR:HG21	1:A:20:VAL:HG12	11	0.17
(1,846)	1:A:16:THR:HG21	1:A:20:VAL:HG13	11	0.17
(1,846)	1:A:16:THR:HG21	1:A:20:VAL:HG21	11	0.17
(1,846)	1:A:16:THR:HG21	1:A:20:VAL:HG22	11	0.17
(1,846)	1:A:16:THR:HG21	1:A:20:VAL:HG23	11	0.17
(1,846)	1:A:16:THR:HG22	1:A:20:VAL:HG11	11	0.17
(1,846)	1:A:16:THR:HG22	1:A:20:VAL:HG12	11	0.17
(1,846)	1:A:16:THR:HG22	1:A:20:VAL:HG13	11	0.17
(1,846)	1:A:16:THR:HG22	1:A:20:VAL:HG21	11	0.17
(1,846)	1:A:16:THR:HG22	1:A:20:VAL:HG22	11	0.17
(1,846)	1:A:16:THR:HG22	1:A:20:VAL:HG23	11	0.17
(1,846)	1:A:16:THR:HG23	1:A:20:VAL:HG11	11	0.17
(1,846)	1:A:16:THR:HG23	1:A:20:VAL:HG12	11	0.17
(1,846)	1:A:16:THR:HG23	1:A:20:VAL:HG13	11	0.17
(1,846)	1:A:16:THR:HG23	1:A:20:VAL:HG21	11	0.17
(1,846)	1:A:16:THR:HG23	1:A:20:VAL:HG22	11	0.17
(1,846)	1:A:16:THR:HG23	1:A:20:VAL:HG23	11	0.17
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	5	0.17
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	5	0.17
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	5	0.17
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	5	0.17
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	5	0.17
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	5	0.17
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	20	0.17
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	20	0.17
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	20	0.17
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	20	0.17
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	20	0.17
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	20	0.17
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	5	0.17
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	5	0.17
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	5	0.17
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	5	0.17
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	5	0.17
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	5	0.17
(1,172)	1:A:39:SER:HB2	1:A:40:ARG:H	11	0.17
(1,172)	1:A:39:SER:HB3	1:A:40:ARG:H	11	0.17
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD2	10	0.17
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD3	10	0.17
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD2	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD3	10	0.17
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD2	10	0.17
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD3	10	0.17
(1,989)	1:A:43:VAL:HG11	1:A:48:PHE:HB3	12	0.16
(1,989)	1:A:43:VAL:HG12	1:A:48:PHE:HB3	12	0.16
(1,989)	1:A:43:VAL:HG13	1:A:48:PHE:HB3	12	0.16
(1,989)	1:A:43:VAL:HG21	1:A:48:PHE:HB3	12	0.16
(1,989)	1:A:43:VAL:HG22	1:A:48:PHE:HB3	12	0.16
(1,989)	1:A:43:VAL:HG23	1:A:48:PHE:HB3	12	0.16
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG11	8	0.16
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG12	8	0.16
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG13	8	0.16
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG21	8	0.16
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG22	8	0.16
(1,933)	1:A:28:PHE:HD1	1:A:43:VAL:HG23	8	0.16
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG11	8	0.16
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG12	8	0.16
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG13	8	0.16
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG21	8	0.16
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG22	8	0.16
(1,933)	1:A:28:PHE:HD2	1:A:43:VAL:HG23	8	0.16
(1,901)	1:A:20:VAL:HG11	1:A:56:LEU:HA	9	0.16
(1,901)	1:A:20:VAL:HG12	1:A:56:LEU:HA	9	0.16
(1,901)	1:A:20:VAL:HG13	1:A:56:LEU:HA	9	0.16
(1,901)	1:A:20:VAL:HG21	1:A:56:LEU:HA	9	0.16
(1,901)	1:A:20:VAL:HG22	1:A:56:LEU:HA	9	0.16
(1,901)	1:A:20:VAL:HG23	1:A:56:LEU:HA	9	0.16
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD11	13	0.16
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD12	13	0.16
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD13	13	0.16
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD11	13	0.16
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD12	13	0.16
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD13	13	0.16
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD11	13	0.16
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD12	13	0.16
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD13	13	0.16
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD11	13	0.16
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD12	13	0.16
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD13	13	0.16
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD11	13	0.16
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD12	13	0.16
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD13	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD11	13	0.16
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD12	13	0.16
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD13	13	0.16
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD11	20	0.16
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD12	20	0.16
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD13	20	0.16
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD21	20	0.16
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD22	20	0.16
(1,794)	1:A:13:LEU:HG	1:A:17:LEU:HD23	20	0.16
(1,713)	1:A:20:VAL:HG21	1:A:56:LEU:HA	2	0.16
(1,713)	1:A:20:VAL:HG22	1:A:56:LEU:HA	2	0.16
(1,713)	1:A:20:VAL:HG23	1:A:56:LEU:HA	2	0.16
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	6	0.16
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	6	0.16
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	6	0.16
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	6	0.16
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	6	0.16
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	6	0.16
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	10	0.16
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	10	0.16
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	10	0.16
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	10	0.16
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	10	0.16
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	10	0.16
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	15	0.16
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	15	0.16
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	15	0.16
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	15	0.16
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	15	0.16
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	15	0.16
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD21	16	0.16
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD22	16	0.16
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD23	16	0.16
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD21	16	0.16
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD22	16	0.16
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD23	16	0.16
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD21	16	0.16
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD22	16	0.16
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD23	16	0.16
(1,635)	1:A:55:LEU:HD11	1:A:56:LEU:H	17	0.16
(1,635)	1:A:55:LEU:HD12	1:A:56:LEU:H	17	0.16
(1,635)	1:A:55:LEU:HD13	1:A:56:LEU:H	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:A:55:LEU:HD21	1:A:56:LEU:H	17	0.16
(1,635)	1:A:55:LEU:HD22	1:A:56:LEU:H	17	0.16
(1,635)	1:A:55:LEU:HD23	1:A:56:LEU:H	17	0.16
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	4	0.15
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	4	0.15
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	4	0.15
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	4	0.15
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	4	0.15
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	4	0.15
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	9	0.15
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	9	0.15
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	9	0.15
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	9	0.15
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	9	0.15
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	9	0.15
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD11	18	0.15
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD12	18	0.15
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD13	18	0.15
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD21	18	0.15
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD22	18	0.15
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD23	18	0.15
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD11	18	0.15
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD12	18	0.15
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD13	18	0.15
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD21	18	0.15
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD22	18	0.15
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD23	18	0.15
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD11	18	0.15
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD12	18	0.15
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD13	18	0.15
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD21	18	0.15
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD22	18	0.15
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD23	18	0.15
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	15	0.15
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	15	0.15
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	15	0.15
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	15	0.15
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	15	0.15
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	15	0.15
(1,989)	1:A:43:VAL:HG11	1:A:48:PHE:HB3	13	0.14
(1,989)	1:A:43:VAL:HG12	1:A:48:PHE:HB3	13	0.14
(1,989)	1:A:43:VAL:HG13	1:A:48:PHE:HB3	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:A:43:VAL:HG21	1:A:48:PHE:HB3	13	0.14
(1,989)	1:A:43:VAL:HG22	1:A:48:PHE:HB3	13	0.14
(1,989)	1:A:43:VAL:HG23	1:A:48:PHE:HB3	13	0.14
(1,952)	1:A:37:ARG:H	1:A:37:ARG:HB2	20	0.14
(1,952)	1:A:37:ARG:H	1:A:37:ARG:HB3	20	0.14
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD11	8	0.14
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD12	8	0.14
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD13	8	0.14
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD11	8	0.14
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD12	8	0.14
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD13	8	0.14
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD11	8	0.14
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD12	8	0.14
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD13	8	0.14
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD11	8	0.14
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD12	8	0.14
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD13	8	0.14
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD11	8	0.14
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD12	8	0.14
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD13	8	0.14
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD11	8	0.14
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD12	8	0.14
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD13	8	0.14
(1,771)	1:A:8:LEU:HD11	1:A:13:LEU:HD11	18	0.14
(1,771)	1:A:8:LEU:HD11	1:A:13:LEU:HD12	18	0.14
(1,771)	1:A:8:LEU:HD11	1:A:13:LEU:HD13	18	0.14
(1,771)	1:A:8:LEU:HD11	1:A:13:LEU:HD21	18	0.14
(1,771)	1:A:8:LEU:HD11	1:A:13:LEU:HD22	18	0.14
(1,771)	1:A:8:LEU:HD11	1:A:13:LEU:HD23	18	0.14
(1,771)	1:A:8:LEU:HD12	1:A:13:LEU:HD11	18	0.14
(1,771)	1:A:8:LEU:HD12	1:A:13:LEU:HD12	18	0.14
(1,771)	1:A:8:LEU:HD12	1:A:13:LEU:HD13	18	0.14
(1,771)	1:A:8:LEU:HD12	1:A:13:LEU:HD21	18	0.14
(1,771)	1:A:8:LEU:HD12	1:A:13:LEU:HD22	18	0.14
(1,771)	1:A:8:LEU:HD12	1:A:13:LEU:HD23	18	0.14
(1,771)	1:A:8:LEU:HD13	1:A:13:LEU:HD11	18	0.14
(1,771)	1:A:8:LEU:HD13	1:A:13:LEU:HD12	18	0.14
(1,771)	1:A:8:LEU:HD13	1:A:13:LEU:HD13	18	0.14
(1,771)	1:A:8:LEU:HD13	1:A:13:LEU:HD21	18	0.14
(1,771)	1:A:8:LEU:HD13	1:A:13:LEU:HD22	18	0.14
(1,771)	1:A:8:LEU:HD13	1:A:13:LEU:HD23	18	0.14
(1,771)	1:A:8:LEU:HD21	1:A:13:LEU:HD11	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,771)	1:A:8:LEU:HD21	1:A:13:LEU:HD12	18	0.14
(1,771)	1:A:8:LEU:HD21	1:A:13:LEU:HD13	18	0.14
(1,771)	1:A:8:LEU:HD21	1:A:13:LEU:HD21	18	0.14
(1,771)	1:A:8:LEU:HD21	1:A:13:LEU:HD22	18	0.14
(1,771)	1:A:8:LEU:HD21	1:A:13:LEU:HD23	18	0.14
(1,771)	1:A:8:LEU:HD22	1:A:13:LEU:HD11	18	0.14
(1,771)	1:A:8:LEU:HD22	1:A:13:LEU:HD12	18	0.14
(1,771)	1:A:8:LEU:HD22	1:A:13:LEU:HD13	18	0.14
(1,771)	1:A:8:LEU:HD22	1:A:13:LEU:HD21	18	0.14
(1,771)	1:A:8:LEU:HD22	1:A:13:LEU:HD22	18	0.14
(1,771)	1:A:8:LEU:HD22	1:A:13:LEU:HD23	18	0.14
(1,771)	1:A:8:LEU:HD23	1:A:13:LEU:HD11	18	0.14
(1,771)	1:A:8:LEU:HD23	1:A:13:LEU:HD12	18	0.14
(1,771)	1:A:8:LEU:HD23	1:A:13:LEU:HD13	18	0.14
(1,771)	1:A:8:LEU:HD23	1:A:13:LEU:HD21	18	0.14
(1,771)	1:A:8:LEU:HD23	1:A:13:LEU:HD22	18	0.14
(1,771)	1:A:8:LEU:HD23	1:A:13:LEU:HD23	18	0.14
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	13	0.14
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	13	0.14
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	13	0.14
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	13	0.14
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	13	0.14
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	13	0.14
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	16	0.14
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	16	0.14
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	16	0.14
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	16	0.14
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	16	0.14
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	16	0.14
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD21	20	0.14
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD22	20	0.14
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD23	20	0.14
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD21	20	0.14
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD22	20	0.14
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD23	20	0.14
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD21	20	0.14
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD22	20	0.14
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD23	20	0.14
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	20	0.14
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	20	0.14
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	20	0.14
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	20	0.14
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	20	0.14
(1,485)	1:A:35:VAL:HG21	1:A:37:ARG:HD2	18	0.14
(1,485)	1:A:35:VAL:HG21	1:A:37:ARG:HD3	18	0.14
(1,485)	1:A:35:VAL:HG22	1:A:37:ARG:HD2	18	0.14
(1,485)	1:A:35:VAL:HG22	1:A:37:ARG:HD3	18	0.14
(1,485)	1:A:35:VAL:HG23	1:A:37:ARG:HD2	18	0.14
(1,485)	1:A:35:VAL:HG23	1:A:37:ARG:HD3	18	0.14
(1,1008)	1:A:51:CYS:HB2	1:A:55:LEU:HD11	13	0.14
(1,1008)	1:A:51:CYS:HB2	1:A:55:LEU:HD12	13	0.14
(1,1008)	1:A:51:CYS:HB2	1:A:55:LEU:HD13	13	0.14
(1,1008)	1:A:51:CYS:HB2	1:A:55:LEU:HD21	13	0.14
(1,1008)	1:A:51:CYS:HB2	1:A:55:LEU:HD22	13	0.14
(1,1008)	1:A:51:CYS:HB2	1:A:55:LEU:HD23	13	0.14
(1,1008)	1:A:51:CYS:HB3	1:A:55:LEU:HD11	13	0.14
(1,1008)	1:A:51:CYS:HB3	1:A:55:LEU:HD12	13	0.14
(1,1008)	1:A:51:CYS:HB3	1:A:55:LEU:HD13	13	0.14
(1,1008)	1:A:51:CYS:HB3	1:A:55:LEU:HD21	13	0.14
(1,1008)	1:A:51:CYS:HB3	1:A:55:LEU:HD22	13	0.14
(1,1008)	1:A:51:CYS:HB3	1:A:55:LEU:HD23	13	0.14
(1,943)	1:A:33:SER:HB2	1:A:35:VAL:HG11	8	0.13
(1,943)	1:A:33:SER:HB2	1:A:35:VAL:HG12	8	0.13
(1,943)	1:A:33:SER:HB2	1:A:35:VAL:HG13	8	0.13
(1,943)	1:A:33:SER:HB3	1:A:35:VAL:HG11	8	0.13
(1,943)	1:A:33:SER:HB3	1:A:35:VAL:HG12	8	0.13
(1,943)	1:A:33:SER:HB3	1:A:35:VAL:HG13	8	0.13
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD11	4	0.13
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD12	4	0.13
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD13	4	0.13
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD11	4	0.13
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD12	4	0.13
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD13	4	0.13
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD11	4	0.13
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD12	4	0.13
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD13	4	0.13
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD11	4	0.13
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD12	4	0.13
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD13	4	0.13
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD11	4	0.13
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD12	4	0.13
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD13	4	0.13
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD11	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD12	4	0.13
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD13	4	0.13
(1,859)	1:A:17:LEU:HD11	1:A:20:VAL:HG11	18	0.13
(1,859)	1:A:17:LEU:HD11	1:A:20:VAL:HG12	18	0.13
(1,859)	1:A:17:LEU:HD11	1:A:20:VAL:HG13	18	0.13
(1,859)	1:A:17:LEU:HD11	1:A:20:VAL:HG21	18	0.13
(1,859)	1:A:17:LEU:HD11	1:A:20:VAL:HG22	18	0.13
(1,859)	1:A:17:LEU:HD11	1:A:20:VAL:HG23	18	0.13
(1,859)	1:A:17:LEU:HD12	1:A:20:VAL:HG11	18	0.13
(1,859)	1:A:17:LEU:HD12	1:A:20:VAL:HG12	18	0.13
(1,859)	1:A:17:LEU:HD12	1:A:20:VAL:HG13	18	0.13
(1,859)	1:A:17:LEU:HD12	1:A:20:VAL:HG21	18	0.13
(1,859)	1:A:17:LEU:HD12	1:A:20:VAL:HG22	18	0.13
(1,859)	1:A:17:LEU:HD12	1:A:20:VAL:HG23	18	0.13
(1,859)	1:A:17:LEU:HD13	1:A:20:VAL:HG11	18	0.13
(1,859)	1:A:17:LEU:HD13	1:A:20:VAL:HG12	18	0.13
(1,859)	1:A:17:LEU:HD13	1:A:20:VAL:HG13	18	0.13
(1,859)	1:A:17:LEU:HD13	1:A:20:VAL:HG21	18	0.13
(1,859)	1:A:17:LEU:HD13	1:A:20:VAL:HG22	18	0.13
(1,859)	1:A:17:LEU:HD13	1:A:20:VAL:HG23	18	0.13
(1,859)	1:A:17:LEU:HD21	1:A:20:VAL:HG11	18	0.13
(1,859)	1:A:17:LEU:HD21	1:A:20:VAL:HG12	18	0.13
(1,859)	1:A:17:LEU:HD21	1:A:20:VAL:HG13	18	0.13
(1,859)	1:A:17:LEU:HD21	1:A:20:VAL:HG21	18	0.13
(1,859)	1:A:17:LEU:HD21	1:A:20:VAL:HG22	18	0.13
(1,859)	1:A:17:LEU:HD21	1:A:20:VAL:HG23	18	0.13
(1,859)	1:A:17:LEU:HD22	1:A:20:VAL:HG11	18	0.13
(1,859)	1:A:17:LEU:HD22	1:A:20:VAL:HG12	18	0.13
(1,859)	1:A:17:LEU:HD22	1:A:20:VAL:HG13	18	0.13
(1,859)	1:A:17:LEU:HD22	1:A:20:VAL:HG21	18	0.13
(1,859)	1:A:17:LEU:HD22	1:A:20:VAL:HG22	18	0.13
(1,859)	1:A:17:LEU:HD22	1:A:20:VAL:HG23	18	0.13
(1,859)	1:A:17:LEU:HD23	1:A:20:VAL:HG11	18	0.13
(1,859)	1:A:17:LEU:HD23	1:A:20:VAL:HG12	18	0.13
(1,859)	1:A:17:LEU:HD23	1:A:20:VAL:HG13	18	0.13
(1,859)	1:A:17:LEU:HD23	1:A:20:VAL:HG21	18	0.13
(1,859)	1:A:17:LEU:HD23	1:A:20:VAL:HG22	18	0.13
(1,859)	1:A:17:LEU:HD23	1:A:20:VAL:HG23	18	0.13
(1,753)	1:A:3:ARG:HG2	1:A:4:PRO:HD2	4	0.13
(1,753)	1:A:3:ARG:HG2	1:A:4:PRO:HD3	4	0.13
(1,753)	1:A:3:ARG:HG3	1:A:4:PRO:HD2	4	0.13
(1,753)	1:A:3:ARG:HG3	1:A:4:PRO:HD3	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:A:17:LEU:HA	1:A:20:VAL:HG21	11	0.13
(1,712)	1:A:17:LEU:HA	1:A:20:VAL:HG22	11	0.13
(1,712)	1:A:17:LEU:HA	1:A:20:VAL:HG23	11	0.13
(1,686)	1:A:27:TYR:HE1	1:A:61:ALA:HB1	15	0.13
(1,686)	1:A:27:TYR:HE1	1:A:61:ALA:HB2	15	0.13
(1,686)	1:A:27:TYR:HE1	1:A:61:ALA:HB3	15	0.13
(1,686)	1:A:27:TYR:HE2	1:A:61:ALA:HB1	15	0.13
(1,686)	1:A:27:TYR:HE2	1:A:61:ALA:HB2	15	0.13
(1,686)	1:A:27:TYR:HE2	1:A:61:ALA:HB3	15	0.13
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	7	0.13
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	7	0.13
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	7	0.13
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	7	0.13
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	7	0.13
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	7	0.13
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD21	19	0.13
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD22	19	0.13
(1,656)	1:A:42:ILE:HD11	1:A:56:LEU:HD23	19	0.13
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD21	19	0.13
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD22	19	0.13
(1,656)	1:A:42:ILE:HD12	1:A:56:LEU:HD23	19	0.13
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD21	19	0.13
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD22	19	0.13
(1,656)	1:A:42:ILE:HD13	1:A:56:LEU:HD23	19	0.13
(1,635)	1:A:55:LEU:HD11	1:A:56:LEU:H	9	0.13
(1,635)	1:A:55:LEU:HD12	1:A:56:LEU:H	9	0.13
(1,635)	1:A:55:LEU:HD13	1:A:56:LEU:H	9	0.13
(1,635)	1:A:55:LEU:HD21	1:A:56:LEU:H	9	0.13
(1,635)	1:A:55:LEU:HD22	1:A:56:LEU:H	9	0.13
(1,635)	1:A:55:LEU:HD23	1:A:56:LEU:H	9	0.13
(1,635)	1:A:55:LEU:HD11	1:A:56:LEU:H	19	0.13
(1,635)	1:A:55:LEU:HD12	1:A:56:LEU:H	19	0.13
(1,635)	1:A:55:LEU:HD13	1:A:56:LEU:H	19	0.13
(1,635)	1:A:55:LEU:HD21	1:A:56:LEU:H	19	0.13
(1,635)	1:A:55:LEU:HD22	1:A:56:LEU:H	19	0.13
(1,635)	1:A:55:LEU:HD23	1:A:56:LEU:H	19	0.13
(1,624)	1:A:55:LEU:HD11	1:A:56:LEU:HA	12	0.13
(1,624)	1:A:55:LEU:HD12	1:A:56:LEU:HA	12	0.13
(1,624)	1:A:55:LEU:HD13	1:A:56:LEU:HA	12	0.13
(1,624)	1:A:55:LEU:HD21	1:A:56:LEU:HA	12	0.13
(1,624)	1:A:55:LEU:HD22	1:A:56:LEU:HA	12	0.13
(1,624)	1:A:55:LEU:HD23	1:A:56:LEU:HA	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:A:38:ARG:HD2	1:A:39:SER:H	13	0.13
(1,500)	1:A:38:ARG:HD3	1:A:39:SER:H	13	0.13
(1,989)	1:A:43:VAL:HG11	1:A:48:PHE:HB3	18	0.12
(1,989)	1:A:43:VAL:HG12	1:A:48:PHE:HB3	18	0.12
(1,989)	1:A:43:VAL:HG13	1:A:48:PHE:HB3	18	0.12
(1,989)	1:A:43:VAL:HG21	1:A:48:PHE:HB3	18	0.12
(1,989)	1:A:43:VAL:HG22	1:A:48:PHE:HB3	18	0.12
(1,989)	1:A:43:VAL:HG23	1:A:48:PHE:HB3	18	0.12
(1,944)	1:A:33:SER:HB2	1:A:35:VAL:HG21	12	0.12
(1,944)	1:A:33:SER:HB2	1:A:35:VAL:HG22	12	0.12
(1,944)	1:A:33:SER:HB2	1:A:35:VAL:HG23	12	0.12
(1,944)	1:A:33:SER:HB3	1:A:35:VAL:HG21	12	0.12
(1,944)	1:A:33:SER:HB3	1:A:35:VAL:HG22	12	0.12
(1,944)	1:A:33:SER:HB3	1:A:35:VAL:HG23	12	0.12
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD11	18	0.12
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD12	18	0.12
(1,878)	1:A:17:LEU:HD11	1:A:56:LEU:HD13	18	0.12
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD11	18	0.12
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD12	18	0.12
(1,878)	1:A:17:LEU:HD12	1:A:56:LEU:HD13	18	0.12
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD11	18	0.12
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD12	18	0.12
(1,878)	1:A:17:LEU:HD13	1:A:56:LEU:HD13	18	0.12
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD11	18	0.12
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD12	18	0.12
(1,878)	1:A:17:LEU:HD21	1:A:56:LEU:HD13	18	0.12
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD11	18	0.12
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD12	18	0.12
(1,878)	1:A:17:LEU:HD22	1:A:56:LEU:HD13	18	0.12
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD11	18	0.12
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD12	18	0.12
(1,878)	1:A:17:LEU:HD23	1:A:56:LEU:HD13	18	0.12
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	18	0.12
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	18	0.12
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	18	0.12
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	18	0.12
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	18	0.12
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	18	0.12
(1,635)	1:A:55:LEU:HD11	1:A:56:LEU:H	2	0.12
(1,635)	1:A:55:LEU:HD12	1:A:56:LEU:H	2	0.12
(1,635)	1:A:55:LEU:HD13	1:A:56:LEU:H	2	0.12
(1,635)	1:A:55:LEU:HD21	1:A:56:LEU:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:A:55:LEU:HD22	1:A:56:LEU:H	2	0.12
(1,635)	1:A:55:LEU:HD23	1:A:56:LEU:H	2	0.12
(1,635)	1:A:55:LEU:HD11	1:A:56:LEU:H	15	0.12
(1,635)	1:A:55:LEU:HD12	1:A:56:LEU:H	15	0.12
(1,635)	1:A:55:LEU:HD13	1:A:56:LEU:H	15	0.12
(1,635)	1:A:55:LEU:HD21	1:A:56:LEU:H	15	0.12
(1,635)	1:A:55:LEU:HD22	1:A:56:LEU:H	15	0.12
(1,635)	1:A:55:LEU:HD23	1:A:56:LEU:H	15	0.12
(1,635)	1:A:55:LEU:HD11	1:A:56:LEU:H	20	0.12
(1,635)	1:A:55:LEU:HD12	1:A:56:LEU:H	20	0.12
(1,635)	1:A:55:LEU:HD13	1:A:56:LEU:H	20	0.12
(1,635)	1:A:55:LEU:HD21	1:A:56:LEU:H	20	0.12
(1,635)	1:A:55:LEU:HD22	1:A:56:LEU:H	20	0.12
(1,635)	1:A:55:LEU:HD23	1:A:56:LEU:H	20	0.12
(1,578)	1:A:44:GLU:HG2	1:A:48:PHE:HE1	2	0.12
(1,578)	1:A:44:GLU:HG2	1:A:48:PHE:HE2	2	0.12
(1,561)	1:A:43:VAL:HG21	1:A:48:PHE:HD1	13	0.12
(1,561)	1:A:43:VAL:HG21	1:A:48:PHE:HD2	13	0.12
(1,561)	1:A:43:VAL:HG22	1:A:48:PHE:HD1	13	0.12
(1,561)	1:A:43:VAL:HG22	1:A:48:PHE:HD2	13	0.12
(1,561)	1:A:43:VAL:HG23	1:A:48:PHE:HD1	13	0.12
(1,561)	1:A:43:VAL:HG23	1:A:48:PHE:HD2	13	0.12
(1,561)	1:A:43:VAL:HG21	1:A:48:PHE:HD1	17	0.12
(1,561)	1:A:43:VAL:HG21	1:A:48:PHE:HD2	17	0.12
(1,561)	1:A:43:VAL:HG22	1:A:48:PHE:HD1	17	0.12
(1,561)	1:A:43:VAL:HG22	1:A:48:PHE:HD2	17	0.12
(1,561)	1:A:43:VAL:HG23	1:A:48:PHE:HD1	17	0.12
(1,561)	1:A:43:VAL:HG23	1:A:48:PHE:HD2	17	0.12
(1,499)	1:A:37:ARG:H	1:A:37:ARG:HD2	19	0.12
(1,499)	1:A:37:ARG:H	1:A:37:ARG:HD3	19	0.12
(1,325)	1:A:8:LEU:HD11	1:A:9:CYS:H	16	0.12
(1,325)	1:A:8:LEU:HD12	1:A:9:CYS:H	16	0.12
(1,325)	1:A:8:LEU:HD13	1:A:9:CYS:H	16	0.12
(1,307)	1:A:7:THR:HG21	1:A:8:LEU:H	19	0.12
(1,307)	1:A:7:THR:HG22	1:A:8:LEU:H	19	0.12
(1,307)	1:A:7:THR:HG23	1:A:8:LEU:H	19	0.12
(1,144)	1:A:34:ARG:H	1:A:34:ARG:HG2	17	0.12
(1,144)	1:A:34:ARG:H	1:A:34:ARG:HG3	17	0.12
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD2	15	0.12
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD3	15	0.12
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD2	15	0.12
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD3	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD2	15	0.12
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD3	15	0.12
(1,959)	1:A:40:ARG:HB2	1:A:41:GLY:H	12	0.11
(1,959)	1:A:40:ARG:HB3	1:A:41:GLY:H	12	0.11
(1,901)	1:A:20:VAL:HG11	1:A:56:LEU:HA	7	0.11
(1,901)	1:A:20:VAL:HG12	1:A:56:LEU:HA	7	0.11
(1,901)	1:A:20:VAL:HG13	1:A:56:LEU:HA	7	0.11
(1,901)	1:A:20:VAL:HG21	1:A:56:LEU:HA	7	0.11
(1,901)	1:A:20:VAL:HG22	1:A:56:LEU:HA	7	0.11
(1,901)	1:A:20:VAL:HG23	1:A:56:LEU:HA	7	0.11
(1,782)	1:A:10:GLY:H	1:A:13:LEU:HD11	16	0.11
(1,782)	1:A:10:GLY:H	1:A:13:LEU:HD12	16	0.11
(1,782)	1:A:10:GLY:H	1:A:13:LEU:HD13	16	0.11
(1,782)	1:A:10:GLY:H	1:A:13:LEU:HD21	16	0.11
(1,782)	1:A:10:GLY:H	1:A:13:LEU:HD22	16	0.11
(1,782)	1:A:10:GLY:H	1:A:13:LEU:HD23	16	0.11
(1,687)	1:A:27:TYR:HD1	1:A:61:ALA:HB1	1	0.11
(1,687)	1:A:27:TYR:HD1	1:A:61:ALA:HB2	1	0.11
(1,687)	1:A:27:TYR:HD1	1:A:61:ALA:HB3	1	0.11
(1,687)	1:A:27:TYR:HD2	1:A:61:ALA:HB1	1	0.11
(1,687)	1:A:27:TYR:HD2	1:A:61:ALA:HB2	1	0.11
(1,687)	1:A:27:TYR:HD2	1:A:61:ALA:HB3	1	0.11
(1,687)	1:A:27:TYR:HD1	1:A:61:ALA:HB1	3	0.11
(1,687)	1:A:27:TYR:HD1	1:A:61:ALA:HB2	3	0.11
(1,687)	1:A:27:TYR:HD1	1:A:61:ALA:HB3	3	0.11
(1,687)	1:A:27:TYR:HD2	1:A:61:ALA:HB1	3	0.11
(1,687)	1:A:27:TYR:HD2	1:A:61:ALA:HB2	3	0.11
(1,687)	1:A:27:TYR:HD2	1:A:61:ALA:HB3	3	0.11
(1,670)	1:A:55:LEU:HD11	1:A:56:LEU:HG	12	0.11
(1,670)	1:A:55:LEU:HD12	1:A:56:LEU:HG	12	0.11
(1,670)	1:A:55:LEU:HD13	1:A:56:LEU:HG	12	0.11
(1,670)	1:A:55:LEU:HD21	1:A:56:LEU:HG	12	0.11
(1,670)	1:A:55:LEU:HD22	1:A:56:LEU:HG	12	0.11
(1,670)	1:A:55:LEU:HD23	1:A:56:LEU:HG	12	0.11
(1,666)	1:A:56:LEU:HD11	1:A:59:TYR:HD1	1	0.11
(1,666)	1:A:56:LEU:HD11	1:A:59:TYR:HD2	1	0.11
(1,666)	1:A:56:LEU:HD12	1:A:59:TYR:HD1	1	0.11
(1,666)	1:A:56:LEU:HD12	1:A:59:TYR:HD2	1	0.11
(1,666)	1:A:56:LEU:HD13	1:A:59:TYR:HD1	1	0.11
(1,666)	1:A:56:LEU:HD13	1:A:59:TYR:HD2	1	0.11
(1,638)	1:A:55:LEU:HD11	1:A:56:LEU:HB2	17	0.11
(1,638)	1:A:55:LEU:HD12	1:A:56:LEU:HB2	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:A:55:LEU:HD13	1:A:56:LEU:HB2	17	0.11
(1,638)	1:A:55:LEU:HD21	1:A:56:LEU:HB2	17	0.11
(1,638)	1:A:55:LEU:HD22	1:A:56:LEU:HB2	17	0.11
(1,638)	1:A:55:LEU:HD23	1:A:56:LEU:HB2	17	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD11	6	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD12	6	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD13	6	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD21	6	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD22	6	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD23	6	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD11	6	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD12	6	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD13	6	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD21	6	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD22	6	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD23	6	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD11	6	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD12	6	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD13	6	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD21	6	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD22	6	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD23	6	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD11	15	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD12	15	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD13	15	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD21	15	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD22	15	0.11
(1,630)	1:A:42:ILE:HD11	1:A:55:LEU:HD23	15	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD11	15	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD12	15	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD13	15	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD21	15	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD22	15	0.11
(1,630)	1:A:42:ILE:HD12	1:A:55:LEU:HD23	15	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD11	15	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD12	15	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD13	15	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD21	15	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD22	15	0.11
(1,630)	1:A:42:ILE:HD13	1:A:55:LEU:HD23	15	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD11	11	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD12	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD13	11	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD21	11	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD22	11	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD23	11	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD11	13	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD12	13	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD13	13	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD21	13	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD22	13	0.11
(1,625)	1:A:51:CYS:HB2	1:A:55:LEU:HD23	13	0.11
(1,161)	1:A:38:ARG:H	1:A:38:ARG:HG2	9	0.11
(1,161)	1:A:38:ARG:H	1:A:38:ARG:HG3	9	0.11
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD2	12	0.11
(1,1031)	1:A:61:ALA:HB1	1:A:63:PRO:HD3	12	0.11
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD2	12	0.11
(1,1031)	1:A:61:ALA:HB2	1:A:63:PRO:HD3	12	0.11
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD2	12	0.11
(1,1031)	1:A:61:ALA:HB3	1:A:63:PRO:HD3	12	0.11

10 Dihedral-angle violation analysis (i)

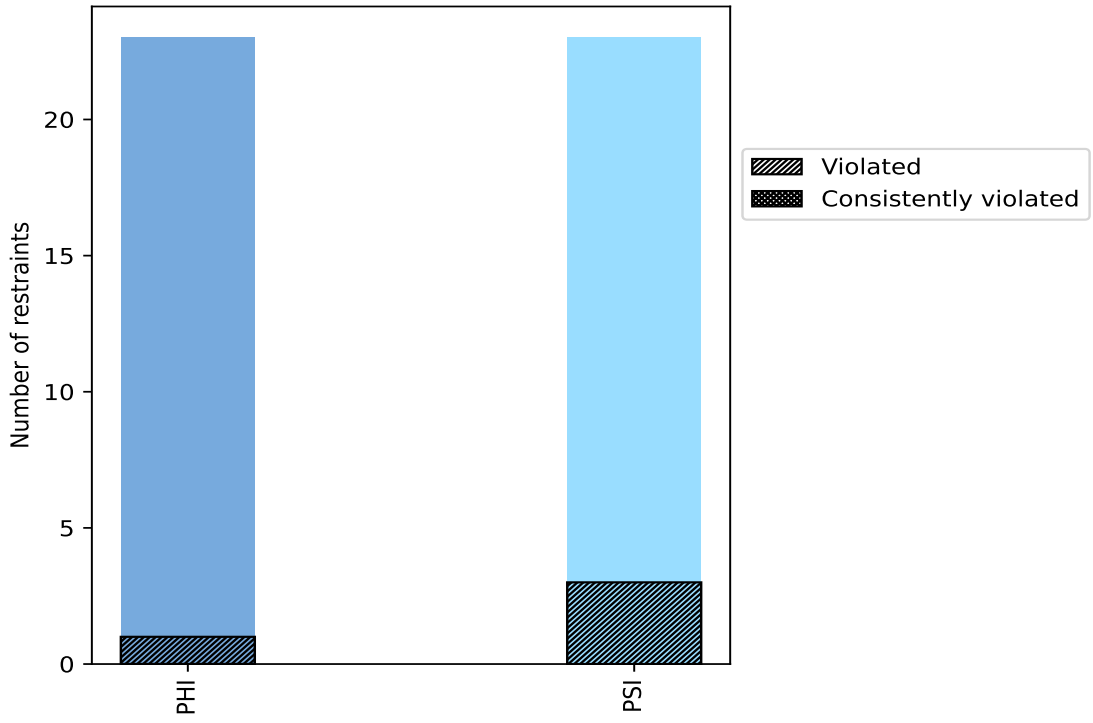
10.1 Summary of dihedral-angle violations (i)

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]
PHI	23	50.0	1	4.3	2.2	0	0.0	0.0
PSI	23	50.0	3	13.0	6.5	0	0.0	0.0
Total	46	100.0	4	8.7	8.7	0	0.0	0.0

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

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



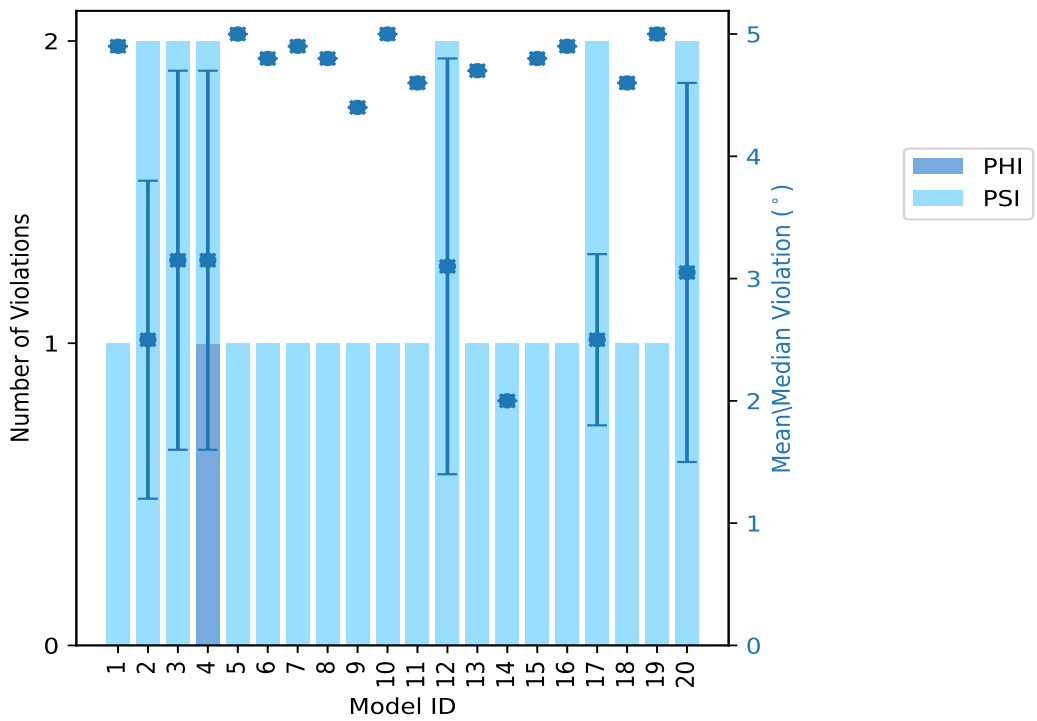
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	1	1	4.9	4.9	0.0	4.9
2	0	2	2	2.5	3.8	1.3	2.5
3	0	2	2	3.15	4.7	1.55	3.15
4	1	1	2	3.15	4.7	1.55	3.15
5	0	1	1	5.0	5.0	0.0	5.0
6	0	1	1	4.8	4.8	0.0	4.8
7	0	1	1	4.9	4.9	0.0	4.9
8	0	1	1	4.8	4.8	0.0	4.8
9	0	1	1	4.4	4.4	0.0	4.4
10	0	1	1	5.0	5.0	0.0	5.0
11	0	1	1	4.6	4.6	0.0	4.6
12	0	2	2	3.1	4.8	1.7	3.1
13	0	1	1	4.7	4.7	0.0	4.7
14	0	1	1	2.0	2.0	0.0	2.0
15	0	1	1	4.8	4.8	0.0	4.8
16	0	1	1	4.9	4.9	0.0	4.9
17	0	2	2	2.5	3.2	0.7	2.5
18	0	1	1	4.6	4.6	0.0	4.6
19	0	1	1	5.0	5.0	0.0	5.0
20	0	2	2	3.05	4.6	1.55	3.05

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	
PHI	PSI	Total	Count[1]	%
1	1	2	1	5.0
0	0	0	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	1	1	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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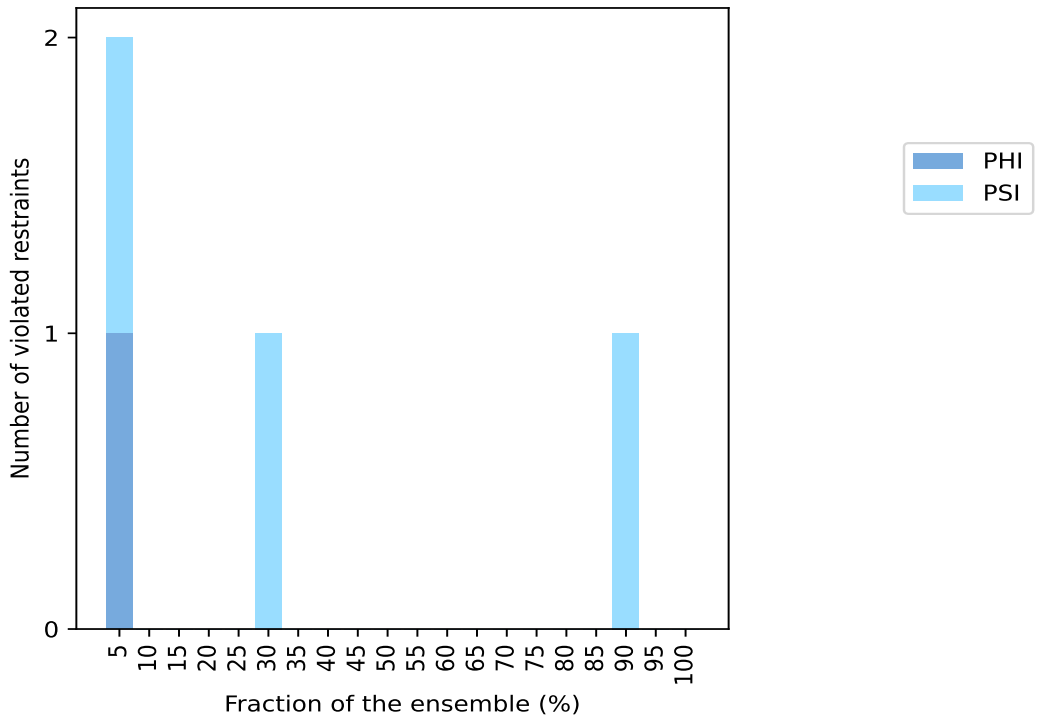
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

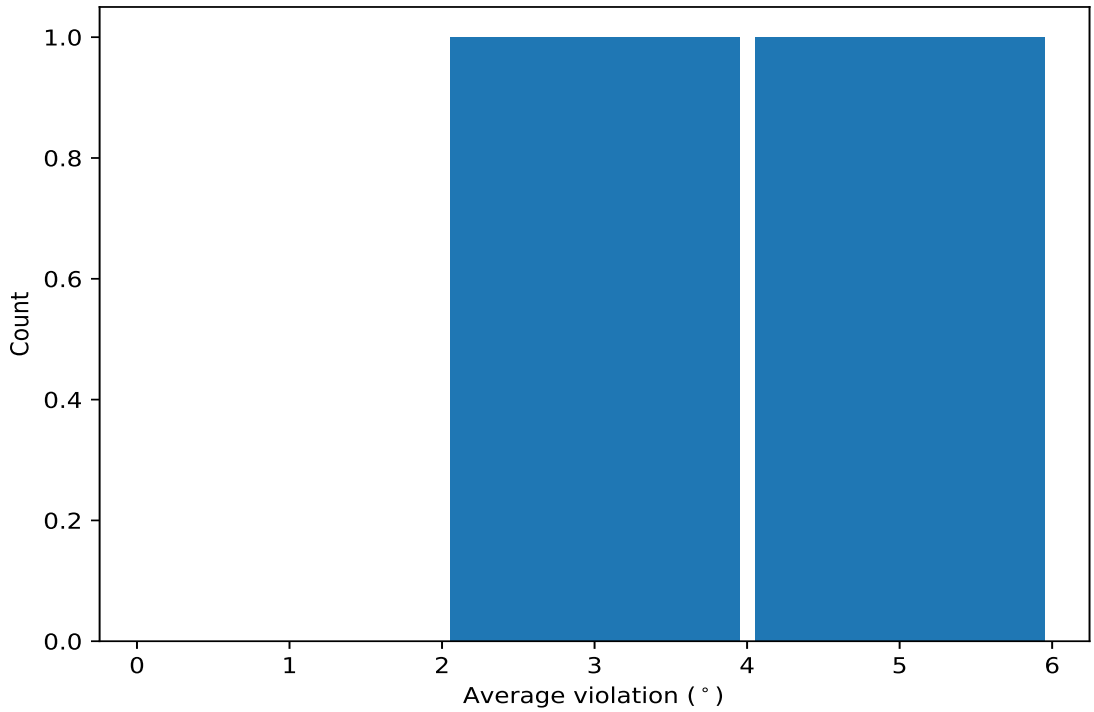


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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.

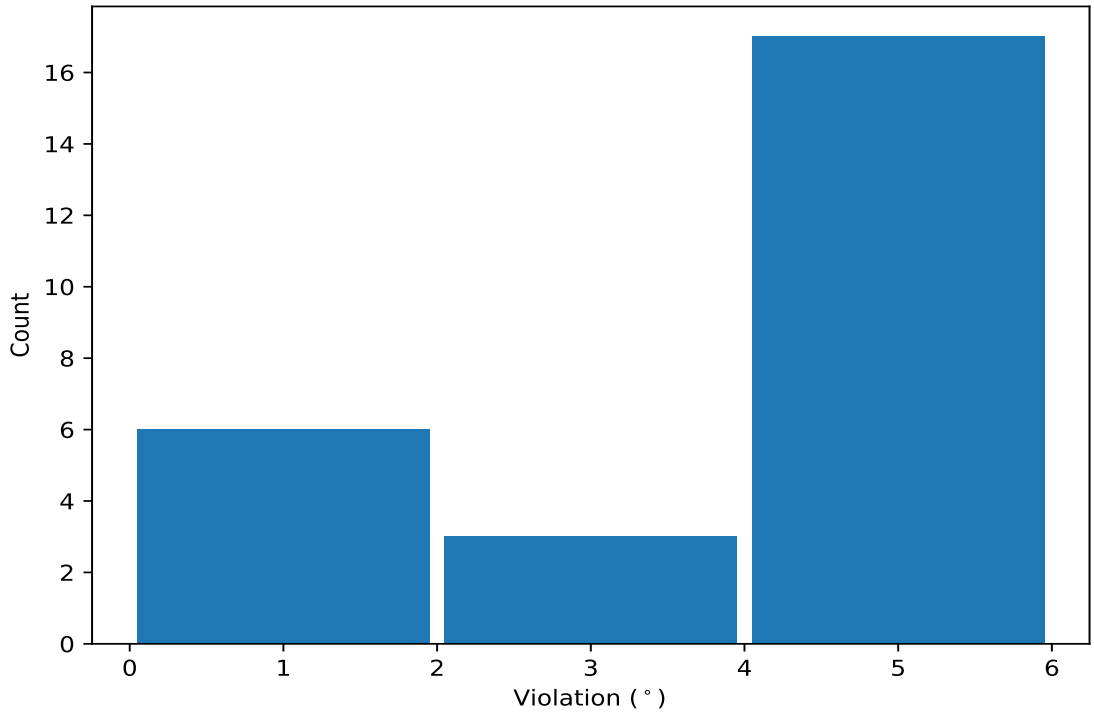
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	18	4.64	0.44	4.8
(1,18)	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	1:A:24:ARG:N	6	2.02	1.17	1.55

[1] Number of violated models, [2]Standard 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 (°)
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	5	5.0
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	10	5.0
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	19	5.0
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	1	4.9
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	7	4.9
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	16	4.9
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	6	4.8
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	8	4.8
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	12	4.8
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	15	4.8
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	3	4.7
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	4	4.7
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	13	4.7
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	11	4.6
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	20	4.6
(1,18)	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	1:A:24:ARG:N	18	4.6
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	9	4.4
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	2	3.8
(1,46)	1:A:58:THR:N	1:A:58:THR:CA	1:A:58:THR:C	1:A:59:TYR:N	17	3.2
(1,20)	1:A:24:ARG:N	1:A:24:ARG:CA	1:A:24:ARG:C	1:A:25:GLY:N	14	2.0
(1,18)	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	1:A:24:ARG:N	17	1.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,29)	1:A:42:ILE:C	1:A:43:VAL:N	1:A:43:VAL:CA	1:A:43:VAL:C	4	1.6
(1,18)	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	1:A:24:ARG:N	3	1.6
(1,18)	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	1:A:24:ARG:N	20	1.5
(1,18)	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	1:A:24:ARG:N	12	1.4
(1,18)	1:A:23:ASP:N	1:A:23:ASP:CA	1:A:23:ASP:C	1:A:24:ARG:N	2	1.2