Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 05:18 pm BST

PDB ID	:	6ZUY
BMRB ID	:	34535
Title	:	Human TFIIS N-terminal domain (TND)
Authors	:	Veverka, V.
Deposited on	:	2020-07-23

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

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

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

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

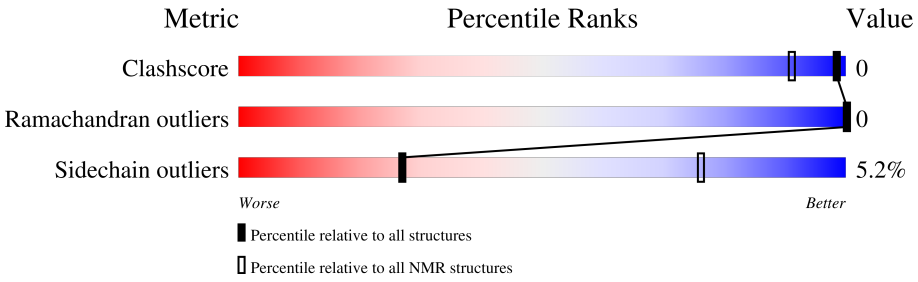
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 94%.

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	81	93% • 5%

2 Ensemble composition and analysis (i)

This entry contains 40 models. Model 17 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:1-A:77 (77)	0.28	17

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 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 15, 17, 19, 20, 21, 22, 23, 24, 25, 26, 28, 29, 30, 31, 32, 33, 36, 37, 39
2	18, 27, 40
3	14, 16
4	34, 35
Single-model clusters	1; 12; 38

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1311 atoms, of which 681 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	81	Total	C	H	N	O	S	0
			1311	395	681	109	121	5	

There are 2 discrepancies between the modelled and reference sequences:

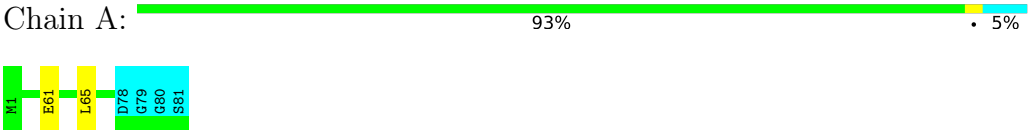
Chain	Residue	Modelled	Actual	Comment	Reference
A	80	GLY	-	expression tag	UNP P23193
A	81	SER	-	expression tag	UNP P23193

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Transcription elongation factor A protein 1

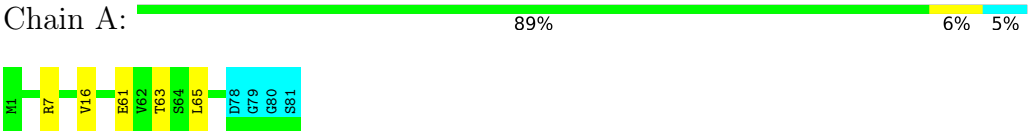


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

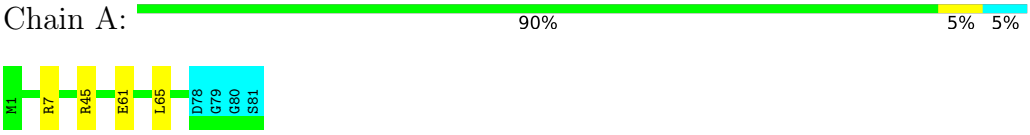
4.2.1 Score per residue for model 1

• Molecule 1: Transcription elongation factor A protein 1



4.2.2 Score per residue for model 2

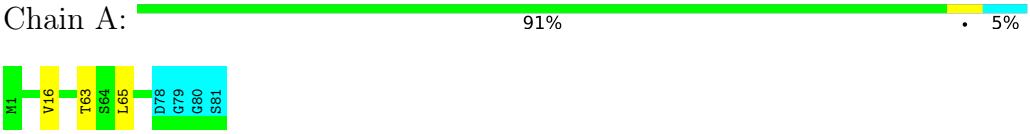
• Molecule 1: Transcription elongation factor A protein 1



4.2.3 Score per residue for model 3

• Molecule 1: Transcription elongation factor A protein 1

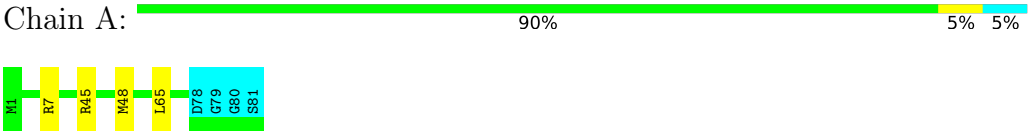
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Transcription elongation factor A protein 1

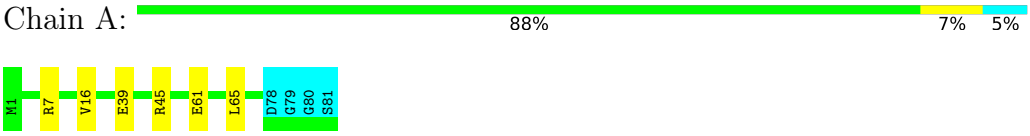
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Transcription elongation factor A protein 1

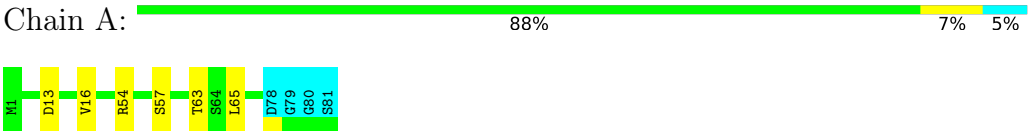
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Transcription elongation factor A protein 1

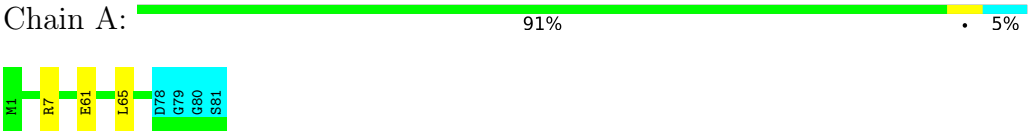
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Transcription elongation factor A protein 1

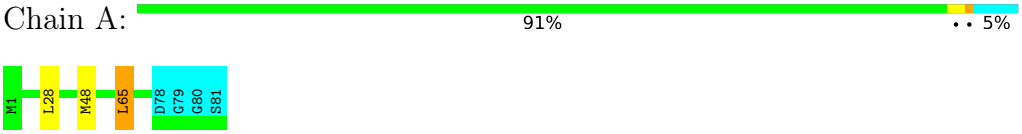
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Transcription elongation factor A protein 1

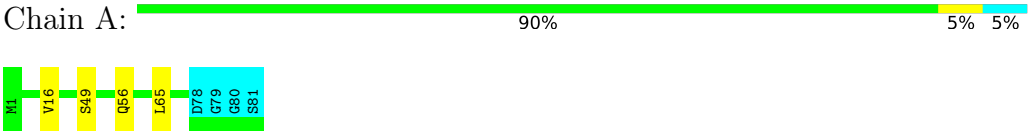
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Transcription elongation factor A protein 1

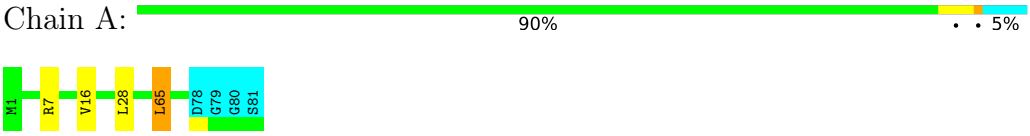
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Transcription elongation factor A protein 1

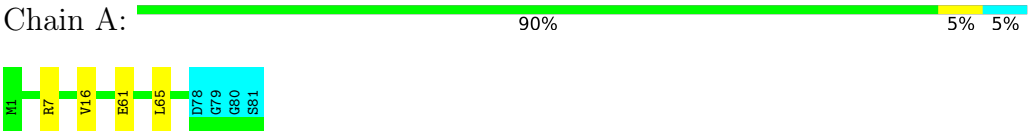
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Transcription elongation factor A protein 1

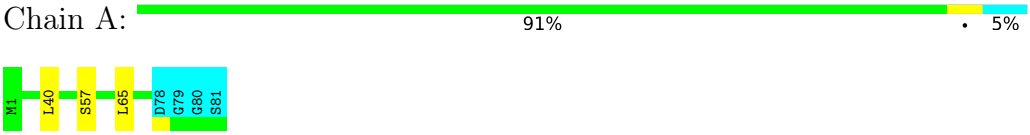
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Transcription elongation factor A protein 1

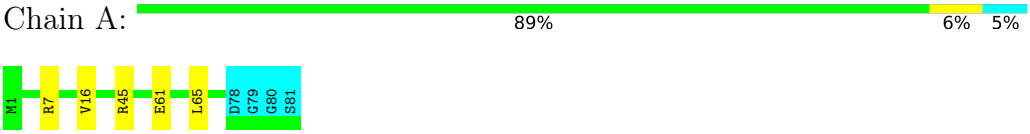
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Transcription elongation factor A protein 1

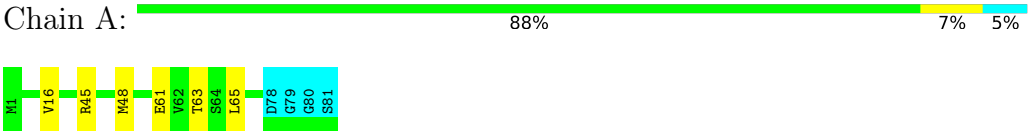
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Transcription elongation factor A protein 1

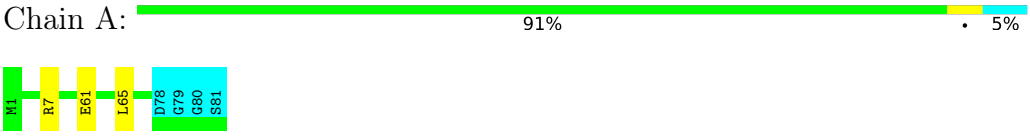
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Transcription elongation factor A protein 1

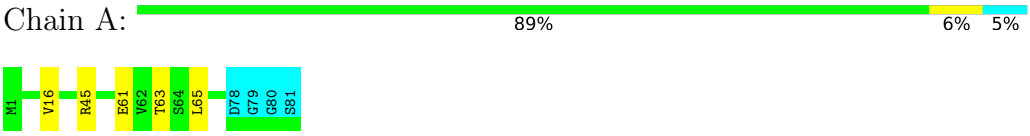
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Transcription elongation factor A protein 1

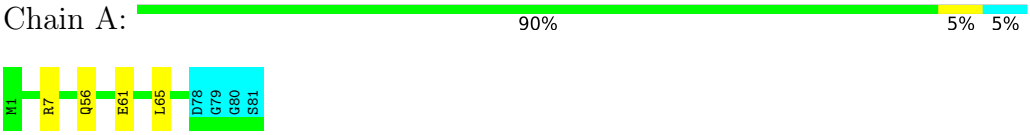
Chain A:



4.2.17 Score per residue for model 17 (medoid)

• Molecule 1: Transcription elongation factor A protein 1

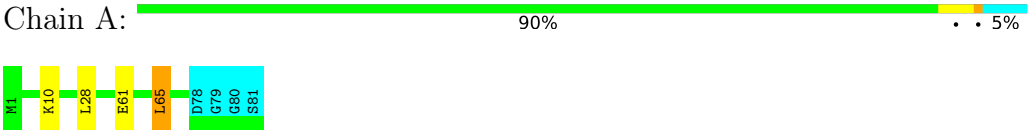
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Transcription elongation factor A protein 1

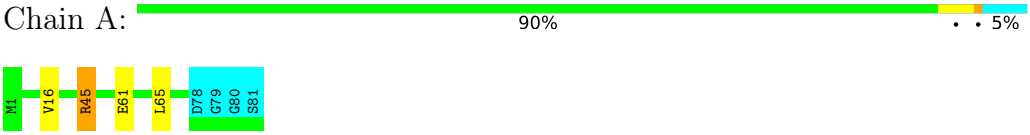
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Transcription elongation factor A protein 1

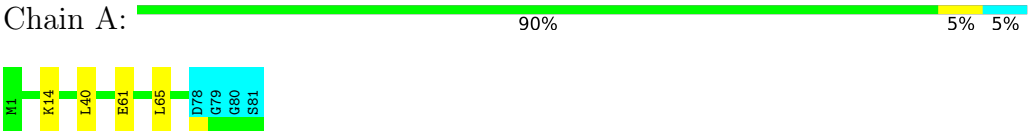
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Transcription elongation factor A protein 1

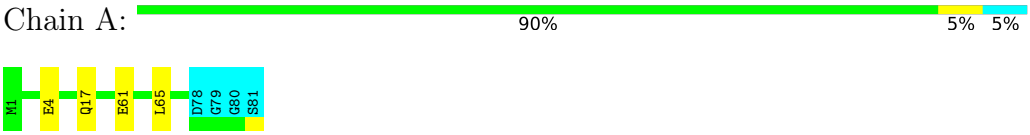
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Transcription elongation factor A protein 1

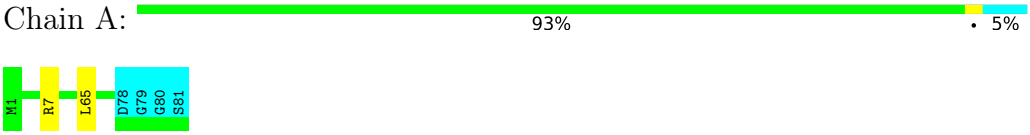
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Transcription elongation factor A protein 1

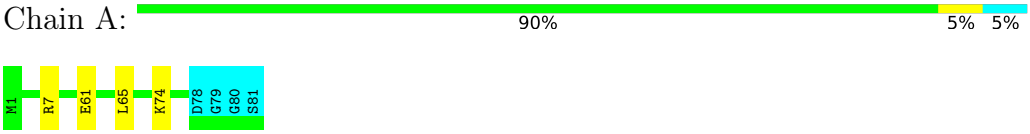
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: Transcription elongation factor A protein 1

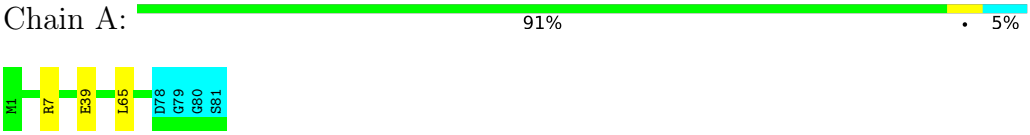
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: Transcription elongation factor A protein 1

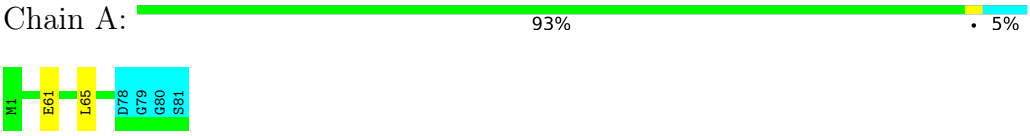
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: Transcription elongation factor A protein 1

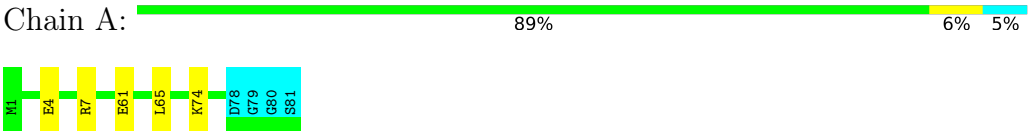
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: Transcription elongation factor A protein 1

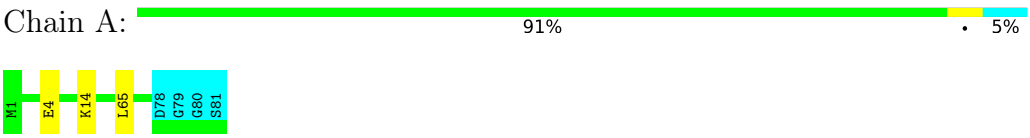
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: Transcription elongation factor A protein 1

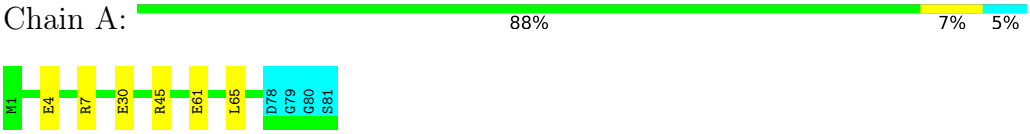
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: Transcription elongation factor A protein 1

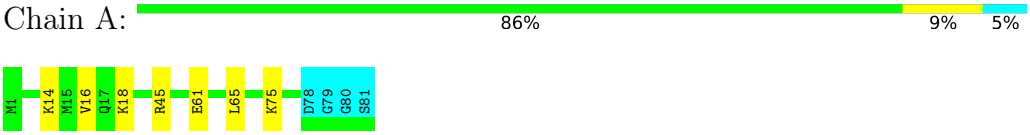
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: Transcription elongation factor A protein 1

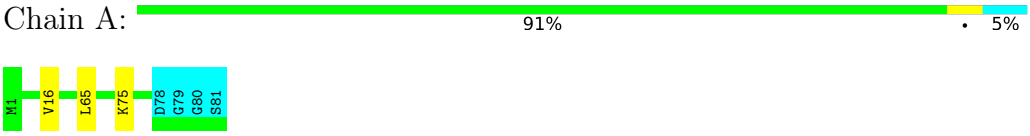
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: Transcription elongation factor A protein 1

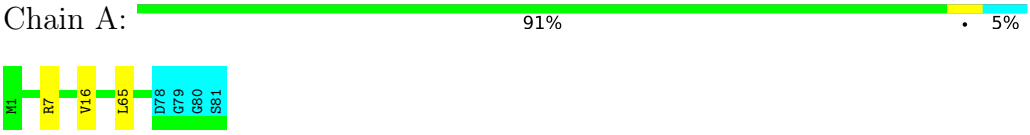
Chain A:



4.2.31 Score per residue for model 31

• Molecule 1: Transcription elongation factor A protein 1

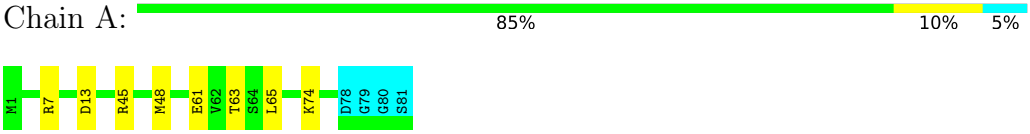
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: Transcription elongation factor A protein 1

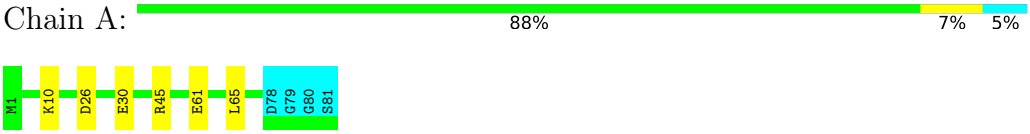
Chain A:



4.2.33 Score per residue for model 33

• Molecule 1: Transcription elongation factor A protein 1

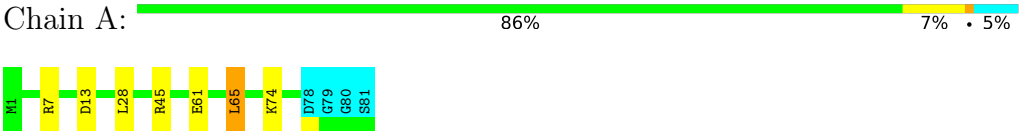
Chain A:



4.2.34 Score per residue for model 34

• Molecule 1: Transcription elongation factor A protein 1

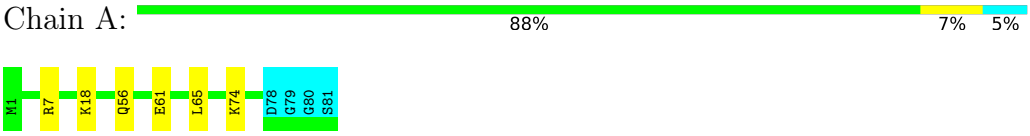
Chain A:



4.2.35 Score per residue for model 35

• Molecule 1: Transcription elongation factor A protein 1

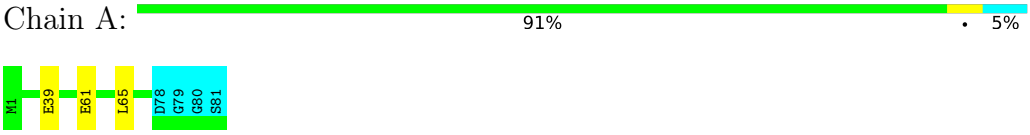
Chain A:



4.2.36 Score per residue for model 36

• Molecule 1: Transcription elongation factor A protein 1

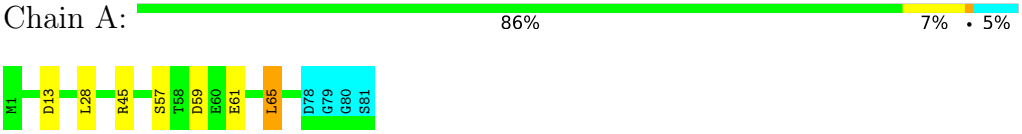
Chain A:



4.2.37 Score per residue for model 37

• Molecule 1: Transcription elongation factor A protein 1

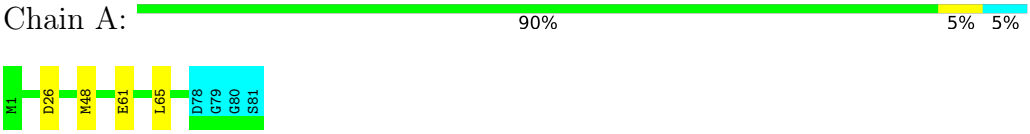
Chain A:



4.2.38 Score per residue for model 38

• Molecule 1: Transcription elongation factor A protein 1

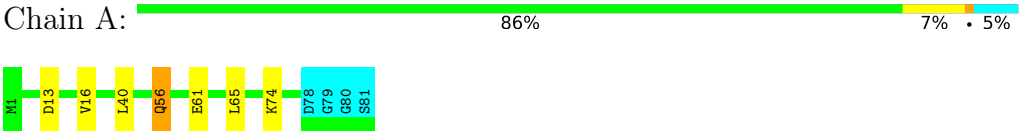
Chain A:



4.2.39 Score per residue for model 39

• Molecule 1: Transcription elongation factor A protein 1

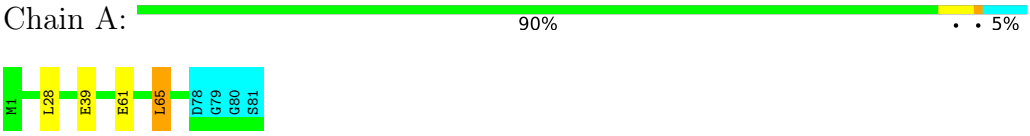
Chain A:



4.2.40 Score per residue for model 40

• Molecule 1: Transcription elongation factor A protein 1

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 40 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	
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	1049
Number of shifts mapped to atoms	1049
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality

6.1 Standard geometry

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	0.53±0.02	0±0/611 (0.0± 0.0%)	0.70±0.03	1±1/815 (0.1± 0.1%)
All	All	0.54	0/24440 (0.0%)	0.70	28/32600 (0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	7	ARG	NE-CZ-NH1	6.12	123.36	120.30	28	17
1	A	45	ARG	NE-CZ-NH1	5.84	123.22	120.30	4	10
1	A	54	ARG	NE-CZ-NH1	5.64	123.12	120.30	6	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	607	666	666	0±0
All	All	24280	26640	26640	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:VAL:HG23	1:A:56:GLN:HG3	0.44	1.88	39	1
1:A:28:LEU:HB3	1:A:65:LEU:HD12	0.43	1.89	37	6

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	76/81 (94%)	74±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	100	100
All	All	3040/3240 (94%)	2972 (98%)	68 (2%)	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	69/71 (97%)	65±1 (95±2%)	4±1 (5±2%)	27	76
All	All	2760/2840 (97%)	2616 (95%)	144 (5%)	27	76

All 23 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	65	LEU	40
1	A	61	GLU	28
1	A	16	VAL	14
1	A	63	THR	6
1	A	74	LYS	6
1	A	48	MET	5
1	A	13	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	39	GLU	4
1	A	56	GLN	4
1	A	45	ARG	4
1	A	4	GLU	4
1	A	57	SER	3
1	A	40	LEU	3
1	A	14	LYS	3
1	A	7	ARG	2
1	A	10	LYS	2
1	A	30	GLU	2
1	A	18	LYS	2
1	A	75	LYS	2
1	A	26	ASP	2
1	A	49	SER	1
1	A	17	GLN	1
1	A	59	ASP	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *tfiis_dep.star*

7.1.1 Bookkeeping

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

Total number of shifts	1049
Number of shifts mapped to atoms	1049
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	78	-0.49 ± 0.19	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	76	0.15 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	78	-0.52 ± 0.13	Should be applied
^{15}N	76	0.30 ± 0.17	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 1033 atoms were assigned a chemical shift out of a possible 1102. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	378/385 (98%)	152/155 (98%)	152/154 (99%)	74/76 (97%)
Sidechain	635/695 (91%)	437/452 (97%)	192/216 (89%)	6/27 (22%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	20/22 (91%)	11/11 (100%)	8/10 (80%)	1/1 (100%)
Overall	1033/1102 (94%)	600/618 (97%)	352/380 (93%)	81/104 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1047 atoms were assigned a chemical shift out of a possible 1131. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	389/407 (96%)	157/165 (95%)	156/162 (96%)	76/80 (95%)
Sidechain	638/702 (91%)	439/456 (96%)	193/219 (88%)	6/27 (22%)
Aromatic	20/22 (91%)	11/11 (100%)	8/10 (80%)	1/1 (100%)
Overall	1047/1131 (93%)	607/632 (96%)	357/391 (91%)	83/108 (77%)

7.1.4 Statistically unusual chemical shifts (i)

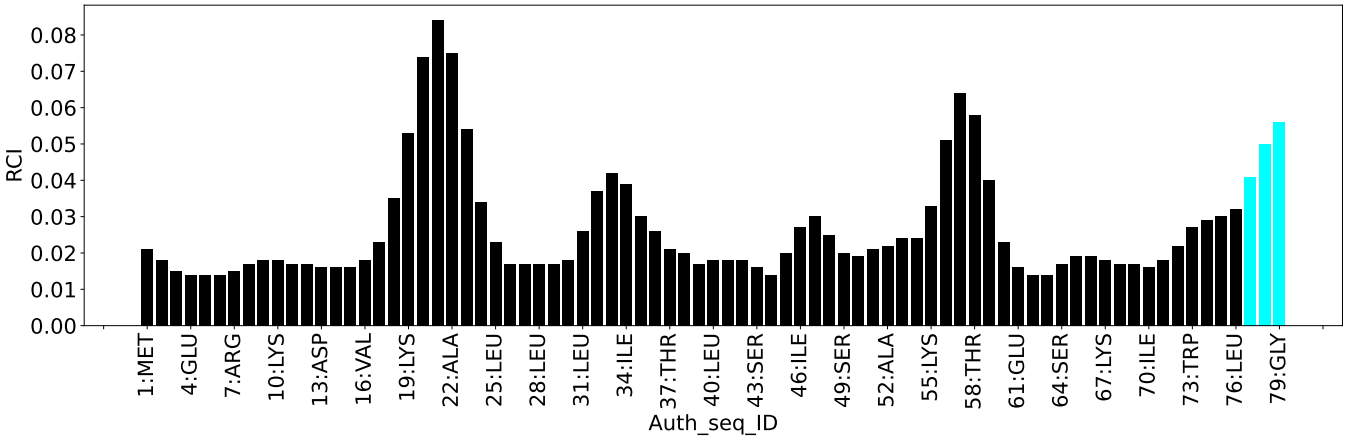
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	37	THR	HG1	5.67	0.08 – 2.19	21.5

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
1:MET
4:GLU
7:ARG
10:LYS
13:ASP
16:VAL
19:LYS
22:ALA
25:LEU
28:LEU
31:LEU
34:ILE
37:THR
40:LEU
43:SER
46:ILE
49:SER
52:ALA
55:LYS
58:THR
61:GLU
64:SER
67:LYS
70:ILE
73:TRP
76:LEU
79:GLY
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2045
Intra-residue (|i-j|=0)	486
Sequential (|i-j|=1)	407
Medium range (|i-j|>1 and |i-j|<5)	501
Long range (|i-j|≥5)	651
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	138
Number of unmapped restraints	0
Number of restraints per residue	27.0
Number of long range restraints per residue[1]	8.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.4	0.2
0.2-0.5 (Medium)	1.0	0.45
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.2	5.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

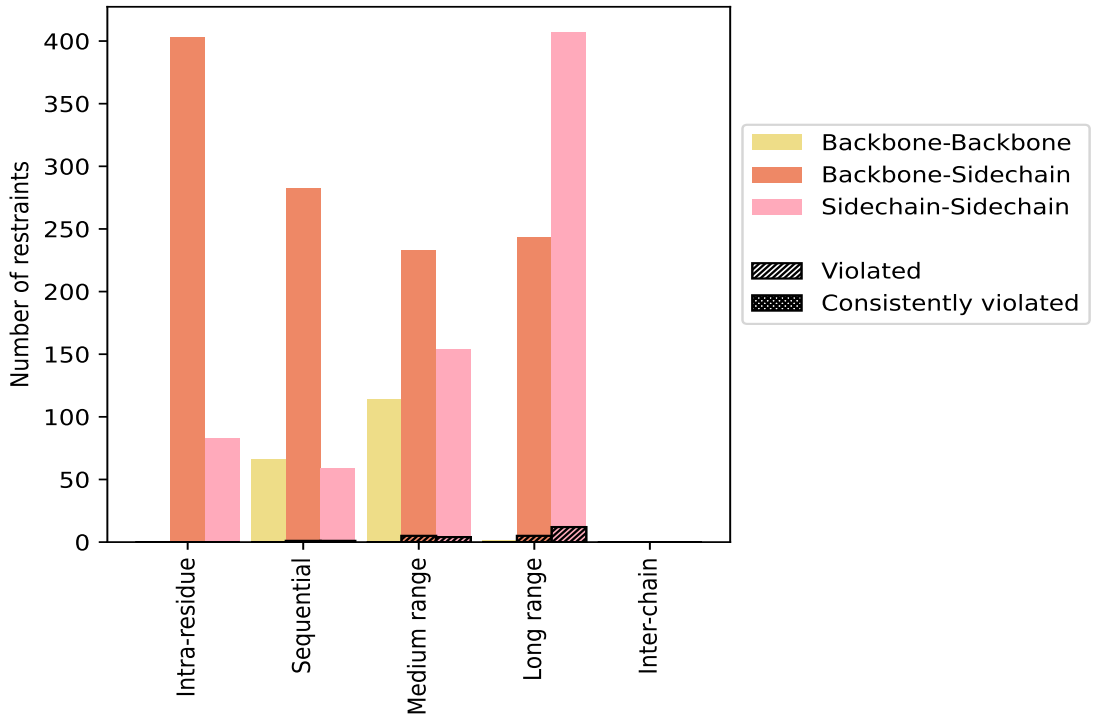
9.1 Summary of distance violations (i)

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)	486	23.8	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	403	19.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	83	4.1	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	407	19.9	2	0.5	0.1	0	0.0	0.0
Backbone-Backbone	66	3.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	282	13.8	1	0.4	0.0	0	0.0	0.0
Sidechain-Sidechain	59	2.9	1	1.7	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	501	24.5	9	1.8	0.4	0	0.0	0.0
Backbone-Backbone	114	5.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	233	11.4	5	2.1	0.2	0	0.0	0.0
Sidechain-Sidechain	154	7.5	4	2.6	0.2	0	0.0	0.0
Long range (|i-j|≥5)	651	31.8	17	2.6	0.8	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	243	11.9	5	2.1	0.2	0	0.0	0.0
Sidechain-Sidechain	407	19.9	12	2.9	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2045	100.0	28	1.4	1.4	0	0.0	0.0
Backbone-Backbone	181	8.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1161	56.8	11	0.9	0.5	0	0.0	0.0
Sidechain-Sidechain	703	34.4	17	2.4	0.8	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



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	2	3	0	5	0.16	0.21	0.03	0.17
2	0	0	5	6	0	11	0.15	0.24	0.04	0.13
3	0	0	3	6	0	9	0.18	0.34	0.07	0.18
4	0	0	2	6	0	8	0.17	0.24	0.04	0.16
5	0	0	2	6	0	8	0.15	0.21	0.03	0.16
6	0	1	3	7	0	11	0.16	0.23	0.04	0.16
7	0	0	3	3	0	6	0.15	0.21	0.03	0.14
8	0	1	3	5	0	9	0.15	0.22	0.04	0.15
9	0	0	4	5	0	9	0.18	0.28	0.06	0.18
10	0	0	2	4	0	6	0.15	0.17	0.02	0.16
11	0	0	5	7	0	12	0.15	0.25	0.04	0.14

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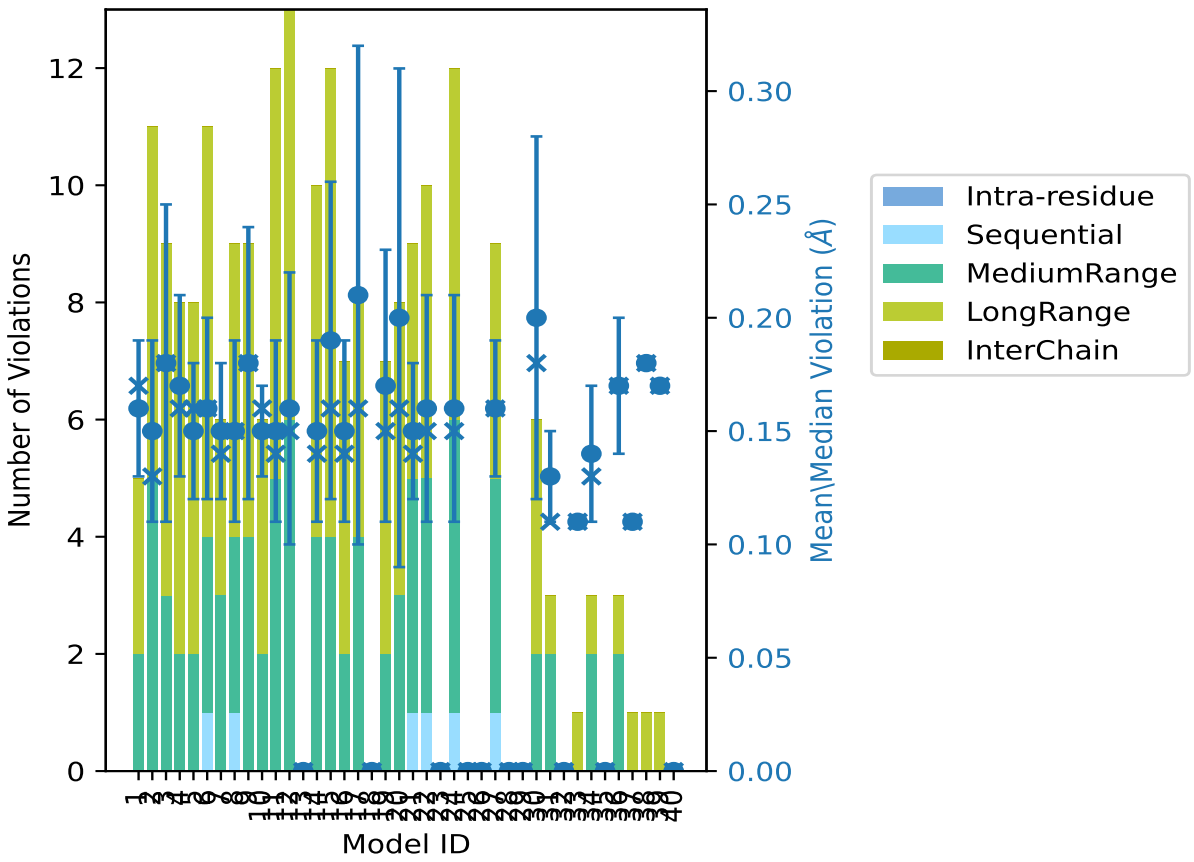
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	6	7	0	13	0.16	0.35	0.06	0.15
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	4	6	0	10	0.15	0.22	0.04	0.14
15	0	0	4	8	0	12	0.19	0.35	0.07	0.16
16	0	0	2	5	0	7	0.15	0.23	0.04	0.14
17	0	0	4	4	0	8	0.21	0.43	0.11	0.16
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	2	5	0	7	0.17	0.28	0.06	0.15
20	0	0	3	5	0	8	0.2	0.45	0.11	0.16
21	0	1	4	4	0	9	0.15	0.22	0.03	0.14
22	0	1	4	5	0	10	0.16	0.24	0.05	0.15
23	0	0	0	0	0	0	0.0	0.0	0.0	0.0
24	0	1	5	6	0	12	0.16	0.3	0.05	0.15
25	0	0	0	0	0	0	0.0	0.0	0.0	0.0
26	0	0	0	0	0	0	0.0	0.0	0.0	0.0
27	0	1	4	4	0	9	0.16	0.21	0.03	0.16
28	0	0	0	0	0	0	0.0	0.0	0.0	0.0
29	0	0	0	0	0	0	0.0	0.0	0.0	0.0
30	0	0	2	4	0	6	0.2	0.35	0.08	0.18
31	0	0	2	1	0	3	0.13	0.16	0.02	0.11
32	0	0	0	0	0	0	0.0	0.0	0.0	0.0
33	0	0	0	1	0	1	0.11	0.11	0.0	0.11
34	0	0	2	1	0	3	0.14	0.19	0.03	0.13
35	0	0	0	0	0	0	0.0	0.0	0.0	0.0
36	0	0	2	1	0	3	0.17	0.2	0.03	0.17
37	0	0	0	1	0	1	0.11	0.11	0.0	0.11
38	0	0	0	1	0	1	0.18	0.18	0.0	0.18
39	0	0	0	1	0	1	0.17	0.17	0.0	0.17
40	0	0	0	0	0	0	0.0	0.0	0.0	0.0

[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, 2017(IR:486, SQ:405, MR:492, LR:634, 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]	%
0	1	2	6	0	9	1	2.5
0	0	1	3	0	4	2	5.0
0	0	0	1	0	1	3	7.5
0	0	1	0	0	1	4	10.0
0	1	0	0	0	1	5	12.5
0	0	0	1	0	1	6	15.0

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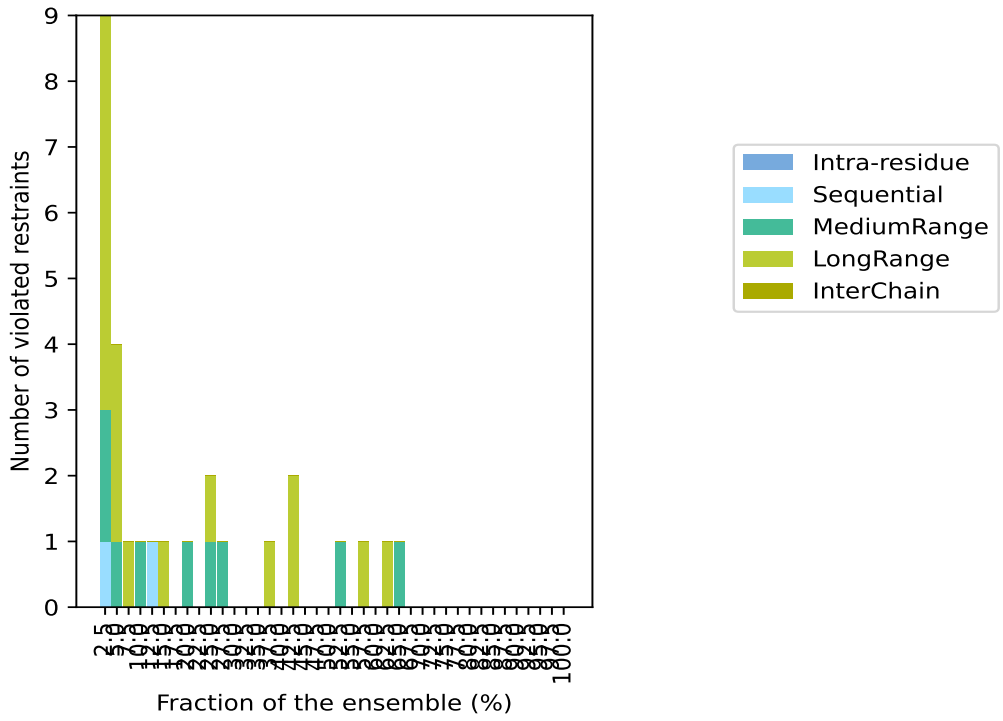
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	7	17.5
0	0	1	0	0	1	8	20.0
0	0	0	0	0	0	9	22.5
0	0	1	1	0	2	10	25.0
0	0	1	0	0	1	11	27.5
0	0	0	0	0	0	12	30.0
0	0	0	0	0	0	13	32.5
0	0	0	0	0	0	14	35.0
0	0	0	1	0	1	15	37.5
0	0	0	0	0	0	16	40.0
0	0	0	2	0	2	17	42.5
0	0	0	0	0	0	18	45.0
0	0	0	0	0	0	19	47.5
0	0	0	0	0	0	20	50.0
0	0	1	0	0	1	21	52.5
0	0	0	0	0	0	22	55.0
0	0	0	1	0	1	23	57.5
0	0	0	0	0	0	24	60.0
0	0	0	1	0	1	25	62.5
0	0	1	0	0	1	26	65.0
0	0	0	0	0	0	27	67.5
0	0	0	0	0	0	28	70.0
0	0	0	0	0	0	29	72.5
0	0	0	0	0	0	30	75.0
0	0	0	0	0	0	31	77.5
0	0	0	0	0	0	32	80.0
0	0	0	0	0	0	33	82.5
0	0	0	0	0	0	34	85.0
0	0	0	0	0	0	35	87.5
0	0	0	0	0	0	36	90.0
0	0	0	0	0	0	37	92.5
0	0	0	0	0	0	38	95.0
0	0	0	0	0	0	39	97.5
0	0	0	0	0	0	40	100.0

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

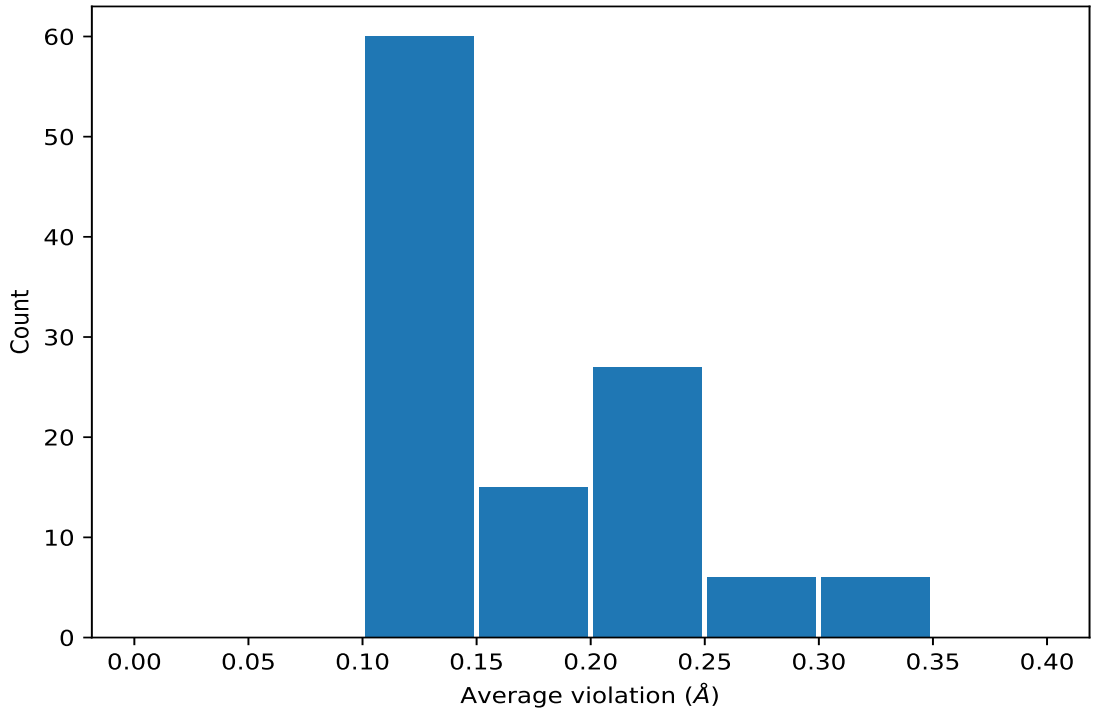
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of 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)
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	26	0.21	0.04	0.22
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	26	0.21	0.04	0.22
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	26	0.21	0.04	0.22
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	25	0.16	0.02	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	25	0.16	0.02	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	25	0.16	0.02	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	25	0.16	0.02	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	25	0.16	0.02	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	25	0.16	0.02	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	25	0.16	0.02	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	25	0.16	0.02	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	25	0.16	0.02	0.17
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	23	0.14	0.02	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	23	0.14	0.02	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	23	0.14	0.02	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	21	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	21	0.16	0.03	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	21	0.16	0.03	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	21	0.16	0.03	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	21	0.16	0.03	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	21	0.16	0.03	0.16
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	17	0.21	0.08	0.21
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	17	0.21	0.08	0.21
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	17	0.12	0.01	0.11
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	17	0.12	0.01	0.11
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	17	0.12	0.01	0.11
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	15	0.14	0.02	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	15	0.14	0.02	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	15	0.14	0.02	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	15	0.14	0.02	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	15	0.14	0.02	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	15	0.14	0.02	0.15
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	11	0.25	0.1	0.21
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	11	0.25	0.1	0.21
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	11	0.25	0.1	0.21
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	11	0.25	0.1	0.21
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	11	0.25	0.1	0.21
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	11	0.25	0.1	0.21
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	10	0.14	0.03	0.13
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	10	0.14	0.03	0.13
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	10	0.14	0.03	0.13
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	10	0.14	0.03	0.13
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	10	0.14	0.03	0.13
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	10	0.14	0.03	0.13
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	10	0.13	0.02	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	10	0.13	0.02	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	10	0.13	0.02	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	10	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	10	0.13	0.02	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	10	0.13	0.02	0.12
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG2	8	0.14	0.01	0.14
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG3	8	0.14	0.01	0.14
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG2	8	0.14	0.01	0.14
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG3	8	0.14	0.01	0.14
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG2	8	0.14	0.01	0.14
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG3	8	0.14	0.01	0.14
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG11	6	0.11	0.0	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG12	6	0.11	0.0	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG13	6	0.11	0.0	0.11
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG11	5	0.12	0.01	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG12	5	0.12	0.01	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG13	5	0.12	0.01	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG21	5	0.12	0.01	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG22	5	0.12	0.01	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG23	5	0.12	0.01	0.12
(1,1730)	1:A:28:LEU:HD11	1:A:32:LYS:H	4	0.13	0.01	0.13
(1,1730)	1:A:28:LEU:HD12	1:A:32:LYS:H	4	0.13	0.01	0.13
(1,1730)	1:A:28:LEU:HD13	1:A:32:LYS:H	4	0.13	0.01	0.13
(1,1730)	1:A:28:LEU:HD21	1:A:32:LYS:H	4	0.13	0.01	0.13
(1,1730)	1:A:28:LEU:HD22	1:A:32:LYS:H	4	0.13	0.01	0.13
(1,1730)	1:A:28:LEU:HD23	1:A:32:LYS:H	4	0.13	0.01	0.13
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD11	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD12	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD13	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD21	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD22	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD23	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD11	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD12	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD13	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD21	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD22	3	0.22	0.04	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD23	3	0.22	0.04	0.24
(1,1776)	1:A:32:LYS:HD2	1:A:65:LEU:HD11	2	0.32	0.02	0.32
(1,1776)	1:A:32:LYS:HD2	1:A:65:LEU:HD12	2	0.32	0.02	0.32
(1,1776)	1:A:32:LYS:HD2	1:A:65:LEU:HD13	2	0.32	0.02	0.32
(1,1776)	1:A:32:LYS:HD3	1:A:65:LEU:HD11	2	0.32	0.02	0.32
(1,1776)	1:A:32:LYS:HD3	1:A:65:LEU:HD12	2	0.32	0.02	0.32
(1,1776)	1:A:32:LYS:HD3	1:A:65:LEU:HD13	2	0.32	0.02	0.32
(1,1156)	1:A:12:MET:H	1:A:27:LEU:HD11	2	0.14	0.01	0.14

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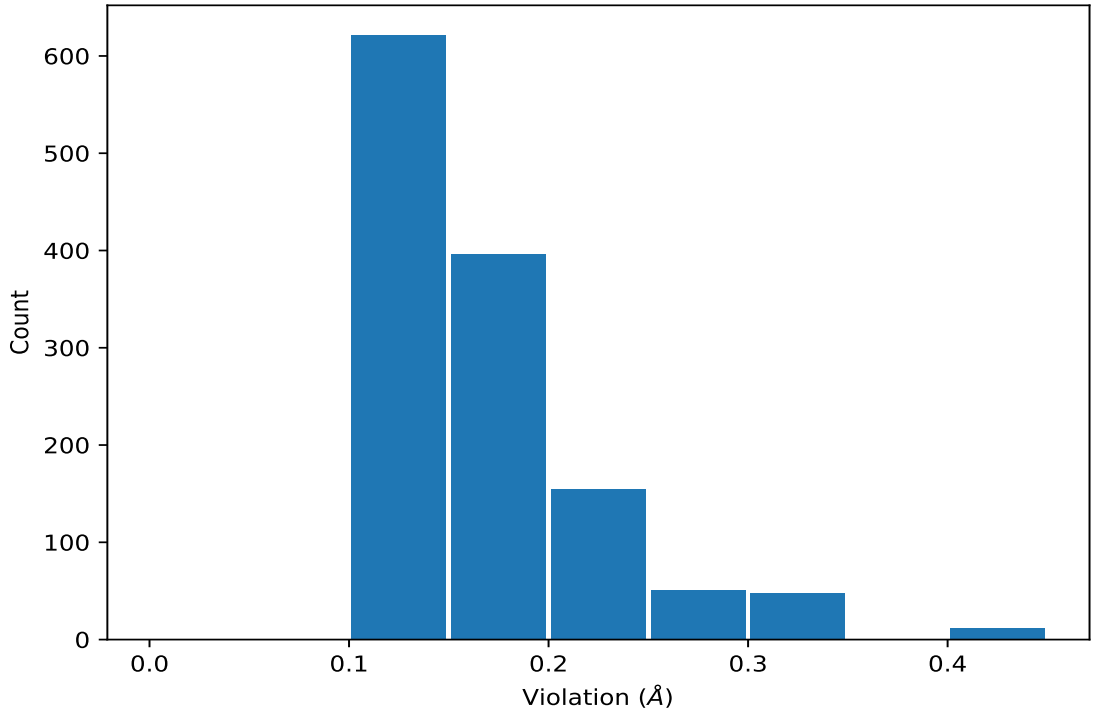
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1156)	1:A:12:MET:H	1:A:27:LEU:HD12	2	0.14	0.01	0.14
(1,1156)	1:A:12:MET:H	1:A:27:LEU:HD13	2	0.14	0.01	0.14
(1,978)	1:A:32:LYS:HE2	1:A:69:LEU:HD11	2	0.12	0.02	0.12
(1,978)	1:A:32:LYS:HE2	1:A:69:LEU:HD12	2	0.12	0.02	0.12
(1,978)	1:A:32:LYS:HE2	1:A:69:LEU:HD13	2	0.12	0.02	0.12
(1,978)	1:A:32:LYS:HE3	1:A:69:LEU:HD11	2	0.12	0.02	0.12
(1,978)	1:A:32:LYS:HE3	1:A:69:LEU:HD12	2	0.12	0.02	0.12
(1,978)	1:A:32:LYS:HE3	1:A:69:LEU:HD13	2	0.12	0.02	0.12
(1,1561)	1:A:6:VAL:HG11	1:A:10:LYS:HG2	2	0.12	0.0	0.12
(1,1561)	1:A:6:VAL:HG11	1:A:10:LYS:HG3	2	0.12	0.0	0.12
(1,1561)	1:A:6:VAL:HG12	1:A:10:LYS:HG2	2	0.12	0.0	0.12
(1,1561)	1:A:6:VAL:HG12	1:A:10:LYS:HG3	2	0.12	0.0	0.12
(1,1561)	1:A:6:VAL:HG13	1:A:10:LYS:HG2	2	0.12	0.0	0.12
(1,1561)	1:A:6:VAL:HG13	1:A:10:LYS:HG3	2	0.12	0.0	0.12

[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)
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	20	0.45
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	20	0.45
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	20	0.45
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	20	0.45
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	20	0.45
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	20	0.45
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	17	0.43
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	17	0.43
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	17	0.43
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	17	0.43
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	17	0.43
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	17	0.43
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	12	0.35
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	12	0.35
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	12	0.35
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	12	0.35
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	12	0.35
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	12	0.35
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	12	0.35
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	12	0.35
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	12	0.35
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	12	0.35
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	12	0.35
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	12	0.35
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	30	0.35
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	30	0.35
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	30	0.35
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	30	0.35
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	30	0.35
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	30	0.35
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	30	0.35
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	30	0.35
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	30	0.35
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	30	0.35
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	30	0.35
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	30	0.35
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	15	0.35
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	15	0.35
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	15	0.35
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	15	0.35
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	15	0.35
(1,1776)	1:A:32:LYS:HD2	1:A:65:LEU:HD11	3	0.34
(1,1776)	1:A:32:LYS:HD2	1:A:65:LEU:HD12	3	0.34
(1,1776)	1:A:32:LYS:HD2	1:A:65:LEU:HD13	3	0.34
(1,1776)	1:A:32:LYS:HD3	1:A:65:LEU:HD11	3	0.34
(1,1776)	1:A:32:LYS:HD3	1:A:65:LEU:HD12	3	0.34
(1,1776)	1:A:32:LYS:HD3	1:A:65:LEU:HD13	3	0.34
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	17	0.34
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	17	0.34
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	17	0.34
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	17	0.34
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	17	0.34
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	17	0.34
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	17	0.34
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	17	0.34
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	17	0.34
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	17	0.34
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	17	0.34
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	17	0.34
(1,1776)	1:A:32:LYS:HD2	1:A:65:LEU:HD11	24	0.3
(1,1776)	1:A:32:LYS:HD2	1:A:65:LEU:HD12	24	0.3
(1,1776)	1:A:32:LYS:HD2	1:A:65:LEU:HD13	24	0.3
(1,1776)	1:A:32:LYS:HD3	1:A:65:LEU:HD11	24	0.3
(1,1776)	1:A:32:LYS:HD3	1:A:65:LEU:HD12	24	0.3
(1,1776)	1:A:32:LYS:HD3	1:A:65:LEU:HD13	24	0.3
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	9	0.28
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	9	0.28
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	9	0.28
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	19	0.28
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	19	0.28
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	19	0.28
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	19	0.28
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	19	0.28
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	19	0.28
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	19	0.28
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	19	0.28
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	19	0.28
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	19	0.28
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	19	0.28
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	15	0.27
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	15	0.27
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	15	0.27
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD11	9	0.26
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD12	9	0.26
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD13	9	0.26
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD21	9	0.26
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD22	9	0.26
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD23	9	0.26
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD11	9	0.26
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD12	9	0.26
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD13	9	0.26
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD21	9	0.26
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD22	9	0.26
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD23	9	0.26
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	11	0.25
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	11	0.25
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	11	0.25
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	20	0.25
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	20	0.25
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	20	0.25
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	20	0.25
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	20	0.25
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	20	0.25
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	20	0.25
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	20	0.25
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	20	0.25
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	20	0.25
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	20	0.25
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	20	0.25
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	2	0.24
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	2	0.24
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	2	0.24
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	19	0.24
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	19	0.24
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	19	0.24
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	22	0.24
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	22	0.24
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	22	0.24
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	24	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	24	0.24
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	24	0.24
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	30	0.24
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	30	0.24
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	30	0.24
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	4	0.24
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	4	0.24
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	4	0.24
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	4	0.24
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	4	0.24
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	4	0.24
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	4	0.24
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	4	0.24
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	4	0.24
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	4	0.24
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	4	0.24
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	4	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD11	15	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD12	15	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD13	15	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD21	15	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD22	15	0.24
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD23	15	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD11	15	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD12	15	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD13	15	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD21	15	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD22	15	0.24
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD23	15	0.24
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	22	0.24
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	22	0.24
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	22	0.24
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	22	0.24
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	22	0.24
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	22	0.24
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	6	0.23
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	6	0.23
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	6	0.23
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	16	0.23
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	16	0.23
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	16	0.23
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	3	0.22
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	3	0.22
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	4	0.22
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	4	0.22
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	4	0.22
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	8	0.22
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	8	0.22
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	8	0.22
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	20	0.22
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	20	0.22
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	20	0.22
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	21	0.22
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	21	0.22
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	21	0.22
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	11	0.22
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	11	0.22
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	11	0.22
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	11	0.22
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	11	0.22
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	11	0.22
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	11	0.22
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	11	0.22
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	11	0.22
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	11	0.22
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	11	0.22
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	11	0.22
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	14	0.22
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	14	0.22
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	14	0.22
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	14	0.22
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	14	0.22
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	14	0.22
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	1	0.21
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	1	0.21
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	1	0.21
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	5	0.21
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	5	0.21
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	5	0.21
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	7	0.21
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	7	0.21
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	7	0.21
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	14	0.21
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	14	0.21
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	17	0.21
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	17	0.21
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	17	0.21
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	3	0.21
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	3	0.21
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	3	0.21
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	3	0.21
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	3	0.21
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	3	0.21
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	2	0.21
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	2	0.21
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	2	0.21
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	2	0.21
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	2	0.21
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	2	0.21
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	2	0.21
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	2	0.21
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	2	0.21
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	2	0.21
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	2	0.21
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	2	0.21
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	8	0.21
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	8	0.21
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	8	0.21
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	8	0.21
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	8	0.21
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	8	0.21
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	8	0.21
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	8	0.21
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	8	0.21
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	8	0.21
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	8	0.21
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	8	0.21
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	27	0.21
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	27	0.21
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	27	0.21
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	27	0.21
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	27	0.21
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	27	0.21
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	16	0.21
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	16	0.21
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	16	0.21
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	16	0.21
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	16	0.21
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	9	0.2
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	9	0.2
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	9	0.2
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	9	0.2
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	9	0.2
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	9	0.2
(1,1175)	1:A:14:LYS:HB2	1:A:15:MET:H	6	0.2
(1,1175)	1:A:14:LYS:HB3	1:A:15:MET:H	6	0.2
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	36	0.2
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	36	0.2
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	36	0.2
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	36	0.2
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	36	0.2
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	36	0.2
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	27	0.19
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	27	0.19
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	27	0.19
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	3	0.19
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	3	0.19
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	3	0.19
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	21	0.19
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	21	0.19
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	21	0.19
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	21	0.19
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	21	0.19
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	21	0.19
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	2	0.19
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	2	0.19
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	2	0.19
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	2	0.19
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	2	0.19
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	2	0.19
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	2	0.19
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	2	0.19
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	2	0.19
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	9	0.19
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	9	0.19
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	9	0.19
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	9	0.19
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	9	0.19
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	9	0.19
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	9	0.19
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	9	0.19
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	12	0.19
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	12	0.19
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	12	0.19
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	12	0.19
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	12	0.19
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	12	0.19
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	12	0.19
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	12	0.19
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	12	0.19
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	15	0.19
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	15	0.19
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	15	0.19
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	15	0.19
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	15	0.19
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	15	0.19
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	15	0.19
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	15	0.19
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	15	0.19
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	15	0.19
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	15	0.19
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	15	0.19
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	12	0.19
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	12	0.19
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	12	0.19
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	12	0.19
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	12	0.19
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	12	0.19
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	34	0.19
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	34	0.19
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	34	0.19
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	34	0.19
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	34	0.19
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	34	0.19
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	12	0.18
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	12	0.18
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	9	0.18
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	9	0.18
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	9	0.18
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	30	0.18
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	30	0.18
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	30	0.18
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	30	0.18
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	30	0.18
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	30	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	1	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	1	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	1	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	1	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	1	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	1	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	1	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	1	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	1	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	3	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	3	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	3	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	3	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	3	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	3	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	3	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	3	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	3	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	4	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	4	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	4	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	4	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	4	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	4	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	4	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	4	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	4	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	6	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	6	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	6	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	6	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	6	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	6	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	6	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	6	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	19	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	19	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	19	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	19	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	19	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	19	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	19	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	19	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	19	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	22	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	22	0.18
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	22	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	22	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	22	0.18
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	22	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	22	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	22	0.18
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	22	0.18
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	6	0.18
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	6	0.18
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	6	0.18
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	6	0.18
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	6	0.18
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	6	0.18
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	6	0.18
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	6	0.18
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	6	0.18
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	6	0.18
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	6	0.18
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	6	0.18
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	38	0.18
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	38	0.18
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	38	0.18
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	38	0.18
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	38	0.18
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	38	0.18
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	38	0.18
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	38	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	38	0.18
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	38	0.18
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	38	0.18
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	38	0.18
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	10	0.17
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	10	0.17
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	10	0.17
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	4	0.17
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	4	0.17
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	4	0.17
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	11	0.17
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	11	0.17
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	11	0.17
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	24	0.17
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	24	0.17
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	24	0.17
(1,314)	1:A:11:LYS:HE2	1:A:27:LEU:HD11	6	0.17
(1,314)	1:A:11:LYS:HE2	1:A:27:LEU:HD12	6	0.17
(1,314)	1:A:11:LYS:HE2	1:A:27:LEU:HD13	6	0.17
(1,314)	1:A:11:LYS:HE3	1:A:27:LEU:HD11	6	0.17
(1,314)	1:A:11:LYS:HE3	1:A:27:LEU:HD12	6	0.17
(1,314)	1:A:11:LYS:HE3	1:A:27:LEU:HD13	6	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	1	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	1	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	1	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	1	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	1	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	1	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	5	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	5	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	5	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	5	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	5	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	5	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	10	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	10	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	10	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	10	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	10	0.17
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	10	0.17
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	17	0.17
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	17	0.17
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	17	0.17
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	17	0.17
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	17	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	5	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	5	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	5	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	5	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	5	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	5	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	5	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	5	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	5	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	8	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	8	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	8	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	8	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	8	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	8	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	8	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	8	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	8	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	11	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	11	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	11	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	11	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	11	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	11	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	11	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	11	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	11	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	20	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	20	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	20	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	20	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	20	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	20	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	20	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	20	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	20	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	21	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	21	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	21	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	21	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	21	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	21	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	21	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	21	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	21	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	27	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	27	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	27	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	27	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	27	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	27	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	27	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	27	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	27	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	30	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	30	0.17
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	30	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	30	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	30	0.17
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	30	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	30	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	30	0.17
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	30	0.17
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	39	0.17
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	39	0.17
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	39	0.17
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	39	0.17
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	39	0.17
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	39	0.17
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	39	0.17
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	39	0.17
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	39	0.17
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	39	0.17
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	39	0.17
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	39	0.17
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	22	0.17
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	22	0.17
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	22	0.17
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	22	0.17
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	22	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	22	0.17
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD11	36	0.17
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD12	36	0.17
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD13	36	0.17
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD21	36	0.17
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD22	36	0.17
(1,1576)	1:A:8:PHE:HE1	1:A:27:LEU:HD23	36	0.17
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD11	36	0.17
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD12	36	0.17
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD13	36	0.17
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD21	36	0.17
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD22	36	0.17
(1,1576)	1:A:8:PHE:HE2	1:A:27:LEU:HD23	36	0.17
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	31	0.16
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	31	0.16
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	31	0.16
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	12	0.16
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	12	0.16
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	12	0.16
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	15	0.16
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	15	0.16
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	15	0.16
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG2	27	0.16
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG3	27	0.16
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG2	27	0.16
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG3	27	0.16
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG2	27	0.16
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG3	27	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	4	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	4	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	4	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	4	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	4	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	4	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	8	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	8	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	8	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	8	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	8	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	8	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	15	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	15	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	15	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	15	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	15	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	27	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	27	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	27	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	27	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	27	0.16
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	27	0.16
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	15	0.16
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	15	0.16
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	15	0.16
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	15	0.16
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	15	0.16
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	15	0.16
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	10	0.16
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	10	0.16
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	10	0.16
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	10	0.16
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	10	0.16
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	10	0.16
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	10	0.16
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	10	0.16
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	10	0.16
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	15	0.16
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	15	0.16
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	15	0.16
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	15	0.16
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	15	0.16
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	15	0.16
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	15	0.16
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	15	0.16
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	15	0.16
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	24	0.16
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	24	0.16
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	24	0.16
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	24	0.16
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	24	0.16
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	24	0.16
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	24	0.16
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	24	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	24	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	4	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	4	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	4	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	4	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	4	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	4	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	5	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	5	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	5	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	5	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	5	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	5	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	6	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	6	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	6	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	6	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	6	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	6	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	15	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	15	0.16
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	15	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	15	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	15	0.16
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	15	0.16
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	11	0.16
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	11	0.16
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	11	0.16
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	11	0.16
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	11	0.16
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	11	0.16
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE2	24	0.16
(1,1021)	1:A:70:ILE:HG21	1:A:74:LYS:HE3	24	0.16
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE2	24	0.16
(1,1021)	1:A:70:ILE:HG22	1:A:74:LYS:HE3	24	0.16
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE2	24	0.16
(1,1021)	1:A:70:ILE:HG23	1:A:74:LYS:HE3	24	0.16
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	8	0.15
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	8	0.15
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	8	0.15
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	10	0.15
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	10	0.15
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG2	7	0.15
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG3	7	0.15
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG2	7	0.15
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG3	7	0.15
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG2	7	0.15
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG3	7	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	12	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	12	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	12	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	12	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	12	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	12	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	22	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	22	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	22	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	22	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	22	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	22	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	24	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	24	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	24	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	24	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	24	0.15
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	24	0.15
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	5	0.15
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	5	0.15
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	5	0.15
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	5	0.15
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	5	0.15
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	5	0.15
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	14	0.15
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	14	0.15
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	14	0.15
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	14	0.15
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	14	0.15
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	14	0.15
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	14	0.15
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	14	0.15
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	14	0.15
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	16	0.15
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	16	0.15
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	16	0.15
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	16	0.15
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	16	0.15
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	16	0.15
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	16	0.15
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	16	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	2	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	2	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	2	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	2	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	2	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	2	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	21	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	21	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	21	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	21	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	21	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	21	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	24	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	24	0.15
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	24	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	24	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	24	0.15
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	24	0.15
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	12	0.15
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	12	0.15
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	12	0.15
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	12	0.15
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	12	0.15
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	12	0.15
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	19	0.15
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	19	0.15
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	19	0.15
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	19	0.15
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	19	0.15
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	19	0.15
(1,1156)	1:A:12:MET:H	1:A:27:LEU:HD11	9	0.15
(1,1156)	1:A:12:MET:H	1:A:27:LEU:HD12	9	0.15
(1,1156)	1:A:12:MET:H	1:A:27:LEU:HD13	9	0.15
(1,978)	1:A:32:LYS:HE2	1:A:69:LEU:HD11	4	0.14
(1,978)	1:A:32:LYS:HE2	1:A:69:LEU:HD12	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,978)	1:A:32:LYS:HE2	1:A:69:LEU:HD13	4	0.14
(1,978)	1:A:32:LYS:HE3	1:A:69:LEU:HD11	4	0.14
(1,978)	1:A:32:LYS:HE3	1:A:69:LEU:HD12	4	0.14
(1,978)	1:A:32:LYS:HE3	1:A:69:LEU:HD13	4	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	7	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	7	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	7	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	12	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	12	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	12	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	16	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	16	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	16	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	17	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	17	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	17	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	19	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	19	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	19	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	20	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	20	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	20	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	30	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	30	0.14
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	30	0.14
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG2	21	0.14
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG3	21	0.14
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG2	21	0.14
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG3	21	0.14
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG2	21	0.14
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG3	21	0.14
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG2	22	0.14
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG3	22	0.14
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG2	22	0.14
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG3	22	0.14
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG2	22	0.14
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG3	22	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	6	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	6	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	6	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	6	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	6	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	14	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	14	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	14	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	14	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	14	0.14
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	14	0.14
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	11	0.14
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	11	0.14
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	11	0.14
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	11	0.14
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	11	0.14
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	11	0.14
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	7	0.14
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	7	0.14
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	7	0.14
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	7	0.14
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	7	0.14
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	7	0.14
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	7	0.14
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	7	0.14
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	7	0.14
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	17	0.14
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	17	0.14
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	17	0.14
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	17	0.14
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	17	0.14
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	17	0.14
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	17	0.14
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	17	0.14
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	17	0.14
(1,1730)	1:A:28:LEU:HD11	1:A:32:LYS:H	21	0.14
(1,1730)	1:A:28:LEU:HD12	1:A:32:LYS:H	21	0.14
(1,1730)	1:A:28:LEU:HD13	1:A:32:LYS:H	21	0.14
(1,1730)	1:A:28:LEU:HD21	1:A:32:LYS:H	21	0.14
(1,1730)	1:A:28:LEU:HD22	1:A:32:LYS:H	21	0.14
(1,1730)	1:A:28:LEU:HD23	1:A:32:LYS:H	21	0.14
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	7	0.14
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	7	0.14
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	7	0.14
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	7	0.14
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	7	0.14
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	11	0.14
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	11	0.14
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	11	0.14
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	11	0.14
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	11	0.14
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	11	0.14
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	14	0.14
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	14	0.14
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	14	0.14
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	14	0.14
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	14	0.14
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	14	0.14
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG11	27	0.14
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG12	27	0.14
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG13	27	0.14
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG21	27	0.14
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG22	27	0.14
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG23	27	0.14
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	34	0.13
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	34	0.13
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	34	0.13
(1,945)	1:A:65:LEU:HD21	1:A:69:LEU:HA	36	0.13
(1,945)	1:A:65:LEU:HD22	1:A:69:LEU:HA	36	0.13
(1,945)	1:A:65:LEU:HD23	1:A:69:LEU:HA	36	0.13
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	3	0.13
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	3	0.13
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	3	0.13
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	15	0.13
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	15	0.13
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	15	0.13
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	27	0.13
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	27	0.13
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	27	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	1	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	1	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	1	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	5	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	5	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	5	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	6	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	6	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	14	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	14	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	14	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	22	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	22	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	22	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	27	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	27	0.13
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	27	0.13
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG2	2	0.13
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG3	2	0.13
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG2	2	0.13
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG3	2	0.13
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG2	2	0.13
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG3	2	0.13
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG2	20	0.13
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG3	20	0.13
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG2	20	0.13
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG3	20	0.13
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG2	20	0.13
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG3	20	0.13
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG2	24	0.13
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG3	24	0.13
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG2	24	0.13
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG3	24	0.13
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG2	24	0.13
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG3	24	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	7	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	7	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	7	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	7	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	7	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	7	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	17	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	17	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	17	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	17	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	17	0.13
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	17	0.13
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	3	0.13
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	3	0.13
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	3	0.13
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	3	0.13
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	3	0.13
(1,1730)	1:A:28:LEU:HD11	1:A:32:LYS:H	9	0.13
(1,1730)	1:A:28:LEU:HD12	1:A:32:LYS:H	9	0.13
(1,1730)	1:A:28:LEU:HD13	1:A:32:LYS:H	9	0.13
(1,1730)	1:A:28:LEU:HD21	1:A:32:LYS:H	9	0.13
(1,1730)	1:A:28:LEU:HD22	1:A:32:LYS:H	9	0.13
(1,1730)	1:A:28:LEU:HD23	1:A:32:LYS:H	9	0.13
(1,1730)	1:A:28:LEU:HD11	1:A:32:LYS:H	14	0.13
(1,1730)	1:A:28:LEU:HD12	1:A:32:LYS:H	14	0.13
(1,1730)	1:A:28:LEU:HD13	1:A:32:LYS:H	14	0.13
(1,1730)	1:A:28:LEU:HD21	1:A:32:LYS:H	14	0.13
(1,1730)	1:A:28:LEU:HD22	1:A:32:LYS:H	14	0.13
(1,1730)	1:A:28:LEU:HD23	1:A:32:LYS:H	14	0.13
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG11	21	0.13
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG12	21	0.13
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG13	21	0.13
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG21	21	0.13
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG22	21	0.13
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG23	21	0.13
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	2	0.13
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	2	0.13
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	2	0.13
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	2	0.13
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	2	0.13
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	2	0.13
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	3	0.13
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	3	0.13
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	3	0.13
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	3	0.13
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	3	0.13
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	3	0.13
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	9	0.13
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	9	0.13
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	9	0.13
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	9	0.13
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	9	0.13
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	9	0.13
(1,1156)	1:A:12:MET:H	1:A:27:LEU:HD11	15	0.13
(1,1156)	1:A:12:MET:H	1:A:27:LEU:HD12	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:A:12:MET:H	1:A:27:LEU:HD13	15	0.13
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	6	0.12
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	6	0.12
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	6	0.12
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	19	0.12
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	19	0.12
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	19	0.12
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	21	0.12
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	21	0.12
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	21	0.12
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	24	0.12
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	24	0.12
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	24	0.12
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG11	1	0.12
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG12	1	0.12
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG13	1	0.12
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG11	16	0.12
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG12	16	0.12
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG13	16	0.12
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG2	8	0.12
(1,1933)	1:A:52:ALA:HB1	1:A:56:GLN:HG3	8	0.12
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG2	8	0.12
(1,1933)	1:A:52:ALA:HB2	1:A:56:GLN:HG3	8	0.12
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG2	8	0.12
(1,1933)	1:A:52:ALA:HB3	1:A:56:GLN:HG3	8	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	2	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	2	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	2	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	2	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	2	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	2	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	11	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	11	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	11	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	11	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	11	0.12
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	11	0.12
(1,1886)	1:A:42:GLN:HE21	1:A:77:LEU:HD11	11	0.12
(1,1886)	1:A:42:GLN:HE21	1:A:77:LEU:HD12	11	0.12
(1,1886)	1:A:42:GLN:HE21	1:A:77:LEU:HD13	11	0.12
(1,1886)	1:A:42:GLN:HE21	1:A:77:LEU:HD21	11	0.12
(1,1886)	1:A:42:GLN:HE21	1:A:77:LEU:HD22	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1886)	1:A:42:GLN:HE21	1:A:77:LEU:HD23	11	0.12
(1,1886)	1:A:42:GLN:HE22	1:A:77:LEU:HD11	11	0.12
(1,1886)	1:A:42:GLN:HE22	1:A:77:LEU:HD12	11	0.12
(1,1886)	1:A:42:GLN:HE22	1:A:77:LEU:HD13	11	0.12
(1,1886)	1:A:42:GLN:HE22	1:A:77:LEU:HD21	11	0.12
(1,1886)	1:A:42:GLN:HE22	1:A:77:LEU:HD22	11	0.12
(1,1886)	1:A:42:GLN:HE22	1:A:77:LEU:HD23	11	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	10	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	10	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	10	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	10	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	10	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	10	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	12	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	12	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	12	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	12	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	12	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	12	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	24	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	24	0.12
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	24	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	24	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	24	0.12
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	24	0.12
(1,1730)	1:A:28:LEU:HD11	1:A:32:LYS:H	6	0.12
(1,1730)	1:A:28:LEU:HD12	1:A:32:LYS:H	6	0.12
(1,1730)	1:A:28:LEU:HD13	1:A:32:LYS:H	6	0.12
(1,1730)	1:A:28:LEU:HD21	1:A:32:LYS:H	6	0.12
(1,1730)	1:A:28:LEU:HD22	1:A:32:LYS:H	6	0.12
(1,1730)	1:A:28:LEU:HD23	1:A:32:LYS:H	6	0.12
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	8	0.12
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	8	0.12
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	8	0.12
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	8	0.12
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	8	0.12
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	8	0.12
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	27	0.12
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	27	0.12
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	27	0.12
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	27	0.12
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	27	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	27	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG11	22	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG12	22	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG13	22	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG21	22	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG22	22	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG23	22	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG11	24	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG12	24	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG13	24	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG21	24	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG22	24	0.12
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG23	24	0.12
(1,1561)	1:A:6:VAL:HG11	1:A:10:LYS:HG2	12	0.12
(1,1561)	1:A:6:VAL:HG11	1:A:10:LYS:HG3	12	0.12
(1,1561)	1:A:6:VAL:HG12	1:A:10:LYS:HG2	12	0.12
(1,1561)	1:A:6:VAL:HG12	1:A:10:LYS:HG3	12	0.12
(1,1561)	1:A:6:VAL:HG13	1:A:10:LYS:HG2	12	0.12
(1,1561)	1:A:6:VAL:HG13	1:A:10:LYS:HG3	12	0.12
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	15	0.12
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	15	0.12
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	15	0.12
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	15	0.12
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	15	0.12
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	15	0.12
(1,981)	1:A:32:LYS:HG2	1:A:69:LEU:HD11	12	0.11
(1,981)	1:A:32:LYS:HG2	1:A:69:LEU:HD12	12	0.11
(1,981)	1:A:32:LYS:HG2	1:A:69:LEU:HD13	12	0.11
(1,981)	1:A:32:LYS:HG3	1:A:69:LEU:HD11	12	0.11
(1,981)	1:A:32:LYS:HG3	1:A:69:LEU:HD12	12	0.11
(1,981)	1:A:32:LYS:HG3	1:A:69:LEU:HD13	12	0.11
(1,978)	1:A:32:LYS:HE2	1:A:69:LEU:HD11	19	0.11
(1,978)	1:A:32:LYS:HE2	1:A:69:LEU:HD12	19	0.11
(1,978)	1:A:32:LYS:HE2	1:A:69:LEU:HD13	19	0.11
(1,978)	1:A:32:LYS:HE3	1:A:69:LEU:HD11	19	0.11
(1,978)	1:A:32:LYS:HE3	1:A:69:LEU:HD12	19	0.11
(1,978)	1:A:32:LYS:HE3	1:A:69:LEU:HD13	19	0.11
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	2	0.11
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	2	0.11
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	2	0.11
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	4	0.11
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	4	0.11
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	5	0.11
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	5	0.11
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	5	0.11
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	8	0.11
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	8	0.11
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	8	0.11
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	11	0.11
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	11	0.11
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	11	0.11
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	14	0.11
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	14	0.11
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	14	0.11
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	20	0.11
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	20	0.11
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	20	0.11
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	22	0.11
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	22	0.11
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	22	0.11
(1,944)	1:A:31:LEU:HD11	1:A:69:LEU:HA	30	0.11
(1,944)	1:A:31:LEU:HD12	1:A:69:LEU:HA	30	0.11
(1,944)	1:A:31:LEU:HD13	1:A:69:LEU:HA	30	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG11	2	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG12	2	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG13	2	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG11	6	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG12	6	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG13	6	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG11	14	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG12	14	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG13	14	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG11	22	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG12	22	0.11
(1,819)	1:A:23:GLY:HA2	1:A:62:VAL:HG13	22	0.11
(1,774)	1:A:16:VAL:HG11	1:A:56:GLN:HB3	3	0.11
(1,774)	1:A:16:VAL:HG12	1:A:56:GLN:HB3	3	0.11
(1,774)	1:A:16:VAL:HG13	1:A:56:GLN:HB3	3	0.11
(1,738)	1:A:21:ALA:H	1:A:53:ILE:HG21	5	0.11
(1,738)	1:A:21:ALA:H	1:A:53:ILE:HG22	5	0.11
(1,738)	1:A:21:ALA:H	1:A:53:ILE:HG23	5	0.11
(1,502)	1:A:37:THR:HG21	1:A:40:LEU:HD21	12	0.11
(1,502)	1:A:37:THR:HG21	1:A:40:LEU:HD22	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:A:37:THR:HG21	1:A:40:LEU:HD23	12	0.11
(1,502)	1:A:37:THR:HG22	1:A:40:LEU:HD21	12	0.11
(1,502)	1:A:37:THR:HG22	1:A:40:LEU:HD22	12	0.11
(1,502)	1:A:37:THR:HG22	1:A:40:LEU:HD23	12	0.11
(1,502)	1:A:37:THR:HG23	1:A:40:LEU:HD21	12	0.11
(1,502)	1:A:37:THR:HG23	1:A:40:LEU:HD22	12	0.11
(1,502)	1:A:37:THR:HG23	1:A:40:LEU:HD23	12	0.11
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	2	0.11
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	2	0.11
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	2	0.11
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD21	21	0.11
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD22	21	0.11
(1,388)	1:A:30:GLU:H	1:A:65:LEU:HD23	21	0.11
(1,237)	1:A:21:ALA:HB1	1:A:24:ALA:HA	11	0.11
(1,237)	1:A:21:ALA:HB2	1:A:24:ALA:HA	11	0.11
(1,237)	1:A:21:ALA:HB3	1:A:24:ALA:HA	11	0.11
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG11	31	0.11
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG12	31	0.11
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG13	31	0.11
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG21	31	0.11
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG22	31	0.11
(1,1898)	1:A:47:GLY:HA3	1:A:50:VAL:HG23	31	0.11
(1,1774)	1:A:32:LYS:HG2	1:A:69:LEU:HD11	12	0.11
(1,1774)	1:A:32:LYS:HG2	1:A:69:LEU:HD12	12	0.11
(1,1774)	1:A:32:LYS:HG2	1:A:69:LEU:HD13	12	0.11
(1,1774)	1:A:32:LYS:HG2	1:A:69:LEU:HD21	12	0.11
(1,1774)	1:A:32:LYS:HG2	1:A:69:LEU:HD22	12	0.11
(1,1774)	1:A:32:LYS:HG2	1:A:69:LEU:HD23	12	0.11
(1,1774)	1:A:32:LYS:HG3	1:A:69:LEU:HD11	12	0.11
(1,1774)	1:A:32:LYS:HG3	1:A:69:LEU:HD12	12	0.11
(1,1774)	1:A:32:LYS:HG3	1:A:69:LEU:HD13	12	0.11
(1,1774)	1:A:32:LYS:HG3	1:A:69:LEU:HD21	12	0.11
(1,1774)	1:A:32:LYS:HG3	1:A:69:LEU:HD22	12	0.11
(1,1774)	1:A:32:LYS:HG3	1:A:69:LEU:HD23	12	0.11
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	14	0.11
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	14	0.11
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	14	0.11
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	14	0.11
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	14	0.11
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	14	0.11
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD11	16	0.11
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD12	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:A:29:LYS:HE2	1:A:65:LEU:HD13	16	0.11
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD11	16	0.11
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD12	16	0.11
(1,1755)	1:A:29:LYS:HE3	1:A:65:LEU:HD13	16	0.11
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	31	0.11
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	31	0.11
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	31	0.11
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	31	0.11
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	31	0.11
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	31	0.11
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	31	0.11
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	31	0.11
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	31	0.11
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG21	34	0.11
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG22	34	0.11
(1,175)	1:A:12:MET:HE1	1:A:46:ILE:HG23	34	0.11
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG21	34	0.11
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG22	34	0.11
(1,175)	1:A:12:MET:HE2	1:A:46:ILE:HG23	34	0.11
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG21	34	0.11
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG22	34	0.11
(1,175)	1:A:12:MET:HE3	1:A:46:ILE:HG23	34	0.11
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	9	0.11
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	9	0.11
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	9	0.11
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	9	0.11
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	9	0.11
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	9	0.11
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	9	0.11
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	9	0.11
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	9	0.11
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	9	0.11
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	9	0.11
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	9	0.11
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	10	0.11
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	10	0.11
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	10	0.11
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	10	0.11
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	10	0.11
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	10	0.11
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	10	0.11
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	10	0.11
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	10	0.11
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	10	0.11
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	10	0.11
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	33	0.11
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	33	0.11
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	33	0.11
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	33	0.11
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	33	0.11
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	33	0.11
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	33	0.11
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	33	0.11
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	33	0.11
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	33	0.11
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	33	0.11
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	33	0.11
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE21	37	0.11
(1,1664)	1:A:16:VAL:HG11	1:A:56:GLN:HE22	37	0.11
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE21	37	0.11
(1,1664)	1:A:16:VAL:HG12	1:A:56:GLN:HE22	37	0.11
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE21	37	0.11
(1,1664)	1:A:16:VAL:HG13	1:A:56:GLN:HE22	37	0.11
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE21	37	0.11
(1,1664)	1:A:16:VAL:HG21	1:A:56:GLN:HE22	37	0.11
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE21	37	0.11
(1,1664)	1:A:16:VAL:HG22	1:A:56:GLN:HE22	37	0.11
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE21	37	0.11
(1,1664)	1:A:16:VAL:HG23	1:A:56:GLN:HE22	37	0.11
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	16	0.11
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	16	0.11
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	16	0.11
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	16	0.11
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	16	0.11
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	16	0.11
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG21	20	0.11
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG22	20	0.11
(1,1641)	1:A:15:MET:HG2	1:A:53:ILE:HG23	20	0.11
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG21	20	0.11
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG22	20	0.11
(1,1641)	1:A:15:MET:HG3	1:A:53:ILE:HG23	20	0.11
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG11	8	0.11
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG12	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG13	8	0.11
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG21	8	0.11
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG22	8	0.11
(1,1631)	1:A:15:MET:HB2	1:A:16:VAL:HG23	8	0.11
(1,1561)	1:A:6:VAL:HG11	1:A:10:LYS:HG2	2	0.11
(1,1561)	1:A:6:VAL:HG11	1:A:10:LYS:HG3	2	0.11
(1,1561)	1:A:6:VAL:HG12	1:A:10:LYS:HG2	2	0.11
(1,1561)	1:A:6:VAL:HG12	1:A:10:LYS:HG3	2	0.11
(1,1561)	1:A:6:VAL:HG13	1:A:10:LYS:HG2	2	0.11
(1,1561)	1:A:6:VAL:HG13	1:A:10:LYS:HG3	2	0.11
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	11	0.11
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	11	0.11
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	11	0.11
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	11	0.11
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	11	0.11
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	11	0.11
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	17	0.11
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	17	0.11
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	17	0.11
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	17	0.11
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	17	0.11
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	17	0.11
(1,1535)	1:A:5:VAL:HG11	1:A:8:PHE:HA	24	0.11
(1,1535)	1:A:5:VAL:HG12	1:A:8:PHE:HA	24	0.11
(1,1535)	1:A:5:VAL:HG13	1:A:8:PHE:HA	24	0.11
(1,1535)	1:A:5:VAL:HG21	1:A:8:PHE:HA	24	0.11
(1,1535)	1:A:5:VAL:HG22	1:A:8:PHE:HA	24	0.11
(1,1535)	1:A:5:VAL:HG23	1:A:8:PHE:HA	24	0.11

10 Dihedral-angle violation analysis

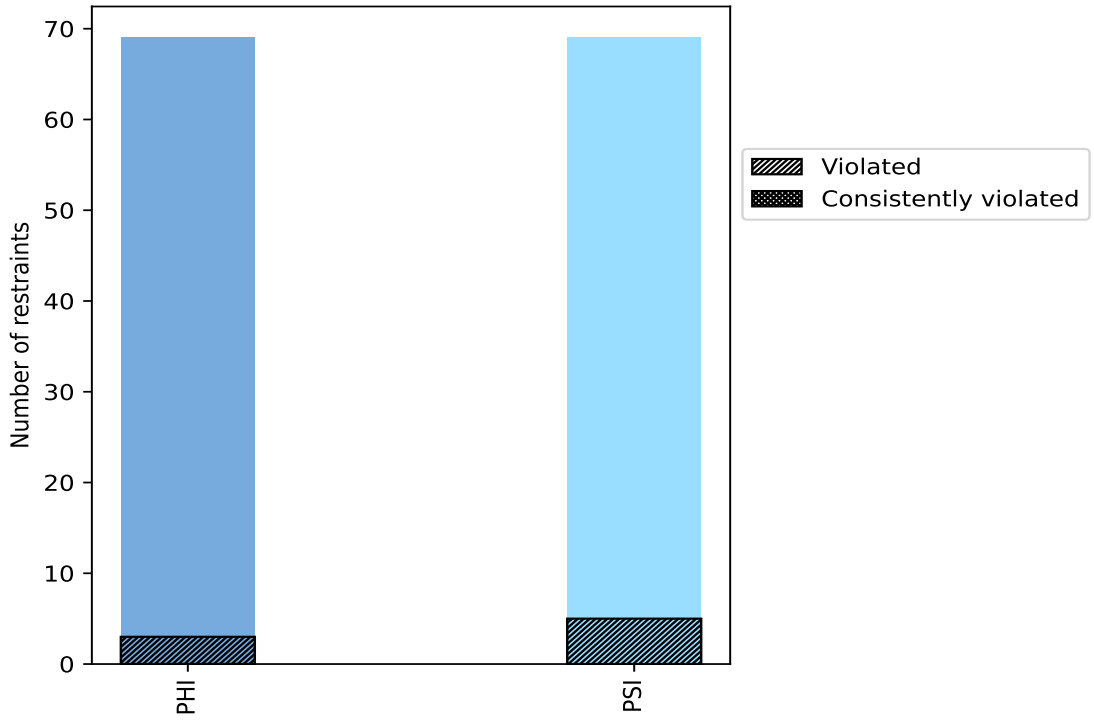
10.1 Summary of dihedral-angle violations

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	69	50.0	3	4.3	2.2	0	0.0	0.0
PSI	69	50.0	5	7.2	3.6	0	0.0	0.0
Total	138	100.0	8	5.8	5.8	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



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	1	2	3	3.3	4.9	1.44	3.6
2	0	1	1	4.1	4.1	0.0	4.1
3	0	1	1	4.9	4.9	0.0	4.9
4	0	1	1	4.8	4.8	0.0	4.8
5	1	2	3	4.07	4.7	0.53	4.1
6	0	2	2	3.75	5.1	1.35	3.75
7	0	2	2	2.7	3.3	0.6	2.7
8	1	1	2	3.2	4.9	1.7	3.2
9	0	3	3	2.7	4.2	1.1	2.3
10	0	1	1	5.1	5.1	0.0	5.1
11	0	1	1	4.8	4.8	0.0	4.8
12	2	1	3	3.17	4.5	0.97	2.8
13	0	0	0	0.0	0.0	0.0	0.0
14	0	2	2	4.95	5.0	0.05	4.95
15	1	1	2	3.4	4.3	0.9	3.4
16	0	2	2	4.25	4.7	0.45	4.25
17	0	2	2	2.9	3.2	0.3	2.9
18	0	0	0	0.0	0.0	0.0	0.0
19	0	2	2	3.2	4.2	1.0	3.2
20	1	1	2	1.85	2.4	0.55	1.85
21	0	1	1	4.7	4.7	0.0	4.7
22	0	1	1	4.8	4.8	0.0	4.8
23	0	0	0	0.0	0.0	0.0	0.0
24	1	1	2	3.15	4.5	1.35	3.15
25	0	0	0	0.0	0.0	0.0	0.0
26	0	0	0	0.0	0.0	0.0	0.0
27	0	1	1	4.8	4.8	0.0	4.8
28	0	0	0	0.0	0.0	0.0	0.0
29	0	0	0	0.0	0.0	0.0	0.0
30	0	2	2	4.0	4.4	0.4	4.0
31	0	1	1	5.0	5.0	0.0	5.0
32	0	1	1	4.5	4.5	0.0	4.5
33	0	0	0	0.0	0.0	0.0	0.0
34	0	1	1	4.8	4.8	0.0	4.8
35	0	1	1	3.5	3.5	0.0	3.5
36	0	0	0	0.0	0.0	0.0	0.0
37	0	0	0	0.0	0.0	0.0	0.0
38	0	0	0	0.0	0.0	0.0	0.0

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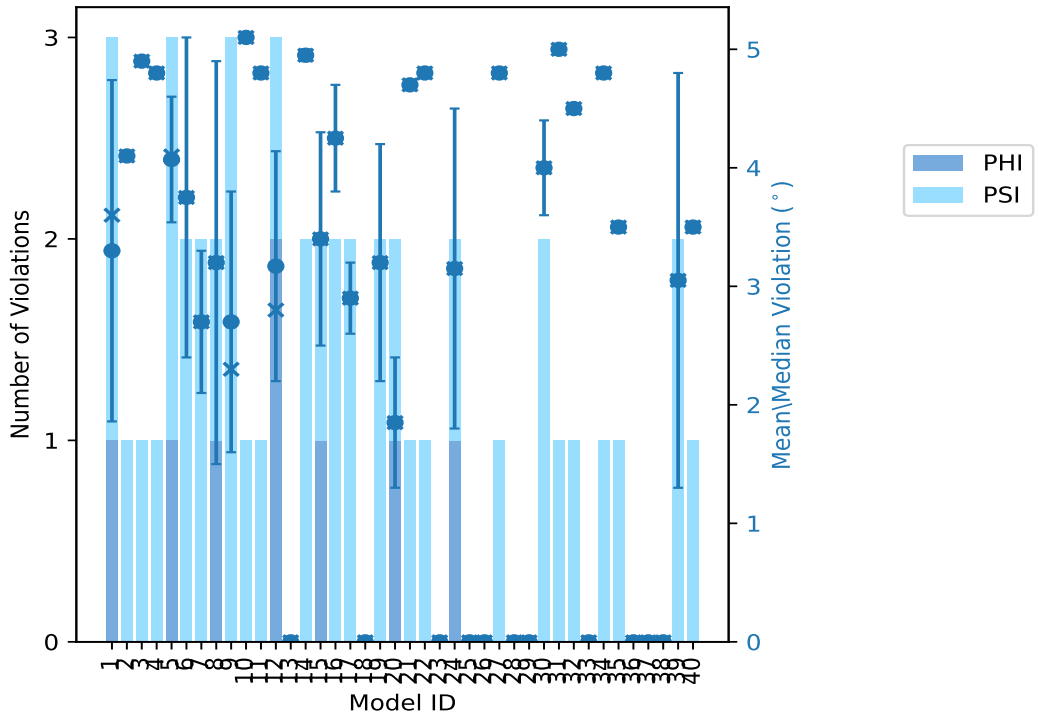
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
39	0	2	2	3.05	4.8	1.75	3.05
40	0	1	1	3.5	3.5	0.0	3.5

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]	%
2	2	4	1	2.5
0	1	1	2	5.0
0	0	0	3	7.5
0	0	0	4	10.0

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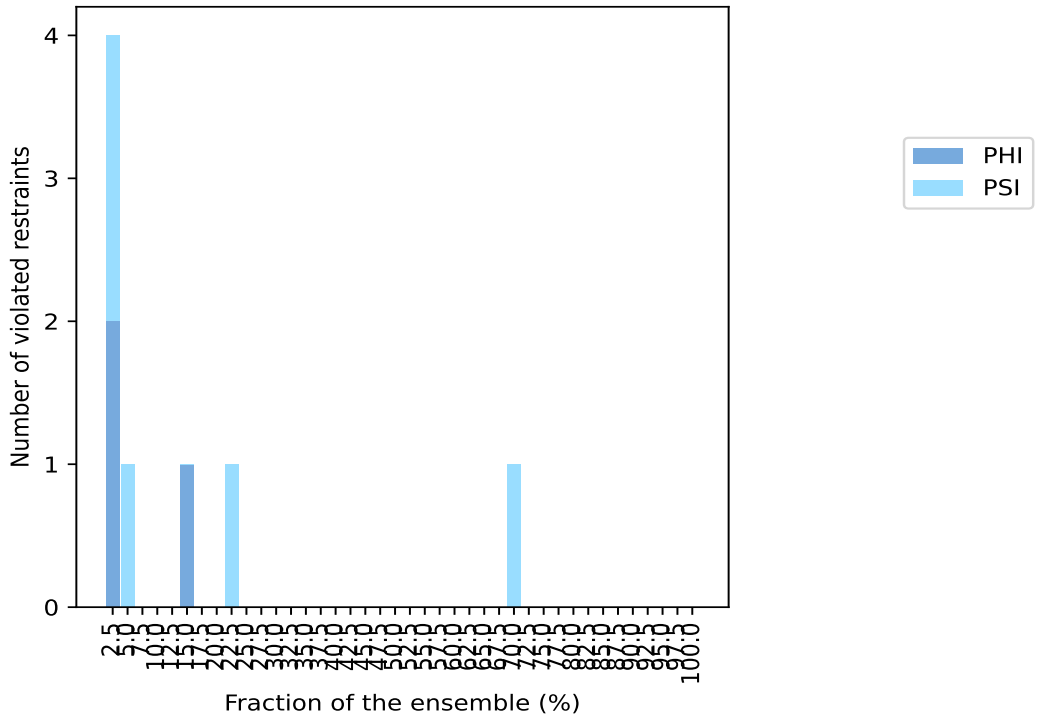
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	5	12.5
1	0	1	6	15.0
0	0	0	7	17.5
0	0	0	8	20.0
0	1	1	9	22.5
0	0	0	10	25.0
0	0	0	11	27.5
0	0	0	12	30.0
0	0	0	13	32.5
0	0	0	14	35.0
0	0	0	15	37.5
0	0	0	16	40.0
0	0	0	17	42.5
0	0	0	18	45.0
0	0	0	19	47.5
0	0	0	20	50.0
0	0	0	21	52.5
0	0	0	22	55.0
0	0	0	23	57.5
0	0	0	24	60.0
0	0	0	25	62.5
0	0	0	26	65.0
0	0	0	27	67.5
0	1	1	28	70.0
0	0	0	29	72.5
0	0	0	30	75.0
0	0	0	31	77.5
0	0	0	32	80.0
0	0	0	33	82.5
0	0	0	34	85.0
0	0	0	35	87.5
0	0	0	36	90.0
0	0	0	37	92.5
0	0	0	38	95.0
0	0	0	39	97.5
0	0	0	40	100.0

[1] Number of models with violations

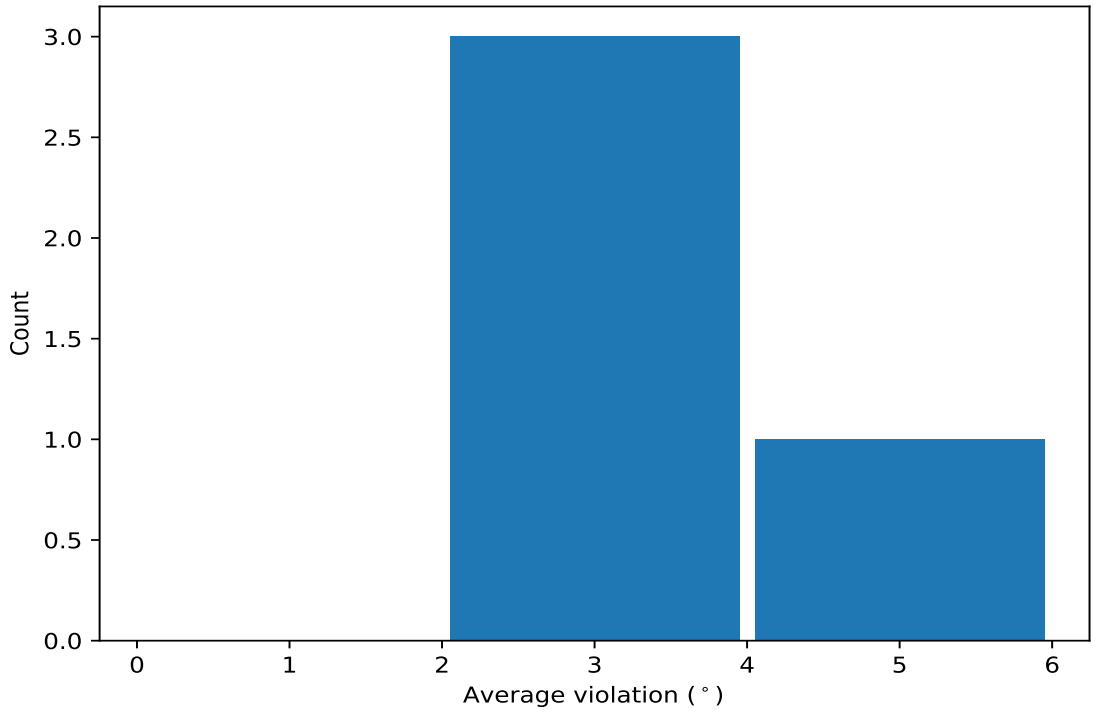
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



10.4.2 Table: Most violated dihedral-angle restraints

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

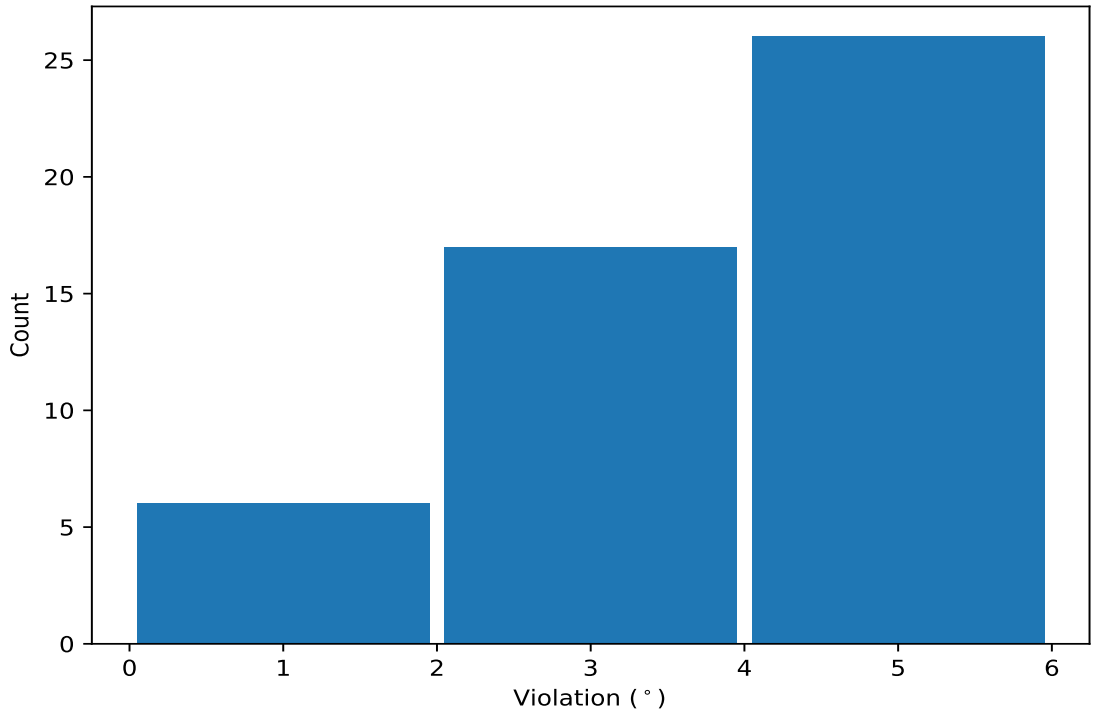
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	28	4.3	0.81	4.6
(1,26)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:MET:N	9	3.52	1.12	3.6
(1,135)	1:A:76:LEU:C	1:A:77:LEU:N	1:A:77:LEU:CA	1:A:77:LEU:C	6	2.45	1.13	2.15
(1,98)	1:A:55:LYS:N	1:A:55:LYS:CA	1:A:55:LYS:C	1:A:56:GLN:N	2	2.0	0.4	2.0

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	6	5.1
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	10	5.1
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	14	5.0
(1,26)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:MET:N	31	5.0
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	1	4.9
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	3	4.9
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	8	4.9
(1,26)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:MET:N	14	4.9
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	4	4.8
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	11	4.8
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	22	4.8
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	27	4.8
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	34	4.8
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	39	4.8
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	16	4.7
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	21	4.7
(1,135)	1:A:76:LEU:C	1:A:77:LEU:N	1:A:77:LEU:CA	1:A:77:LEU:C	5	4.7
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	12	4.5
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	24	4.5
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	32	4.5
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	30	4.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	15	4.3
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	9	4.2
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	19	4.2
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	2	4.1
(1,26)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:MET:N	5	4.1
(1,26)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:MET:N	16	3.8
(1,26)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:MET:N	1	3.6
(1,26)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:MET:N	30	3.6
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	35	3.5
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	40	3.5
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	5	3.4
(1,138)	1:A:78:ASP:N	1:A:78:ASP:CA	1:A:78:ASP:C	1:A:79:GLY:N	7	3.3
(1,26)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:MET:N	17	3.2
(1,135)	1:A:76:LEU:C	1:A:77:LEU:N	1:A:77:LEU:CA	1:A:77:LEU:C	12	2.8
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	17	2.6
(1,135)	1:A:76:LEU:C	1:A:77:LEU:N	1:A:77:LEU:CA	1:A:77:LEU:C	15	2.5
(1,98)	1:A:55:LYS:N	1:A:55:LYS:CA	1:A:55:LYS:C	1:A:56:GLN:N	6	2.4
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	20	2.4
(1,44)	1:A:24:ALA:N	1:A:24:ALA:CA	1:A:24:ALA:C	1:A:25:LEU:N	9	2.3
(1,26)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:MET:N	19	2.2
(1,125)	1:A:71:LYS:C	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	12	2.2
(1,42)	1:A:23:GLY:N	1:A:23:GLY:CA	1:A:23:GLY:C	1:A:24:ALA:N	7	2.1
(1,135)	1:A:76:LEU:C	1:A:77:LEU:N	1:A:77:LEU:CA	1:A:77:LEU:C	24	1.8
(1,98)	1:A:55:LYS:N	1:A:55:LYS:CA	1:A:55:LYS:C	1:A:56:GLN:N	9	1.6
(1,135)	1:A:76:LEU:C	1:A:77:LEU:N	1:A:77:LEU:CA	1:A:77:LEU:C	8	1.5
(1,135)	1:A:76:LEU:C	1:A:77:LEU:N	1:A:77:LEU:CA	1:A:77:LEU:C	1	1.4
(1,26)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:MET:N	39	1.3
(1,25)	1:A:13:ASP:C	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	20	1.3