



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 01:18 PM UTC

PDB ID : 5MML / pdb_00005mml
BMRB ID : 34075
Title : HYL-20k
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Deposited on : 2016-12-10

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

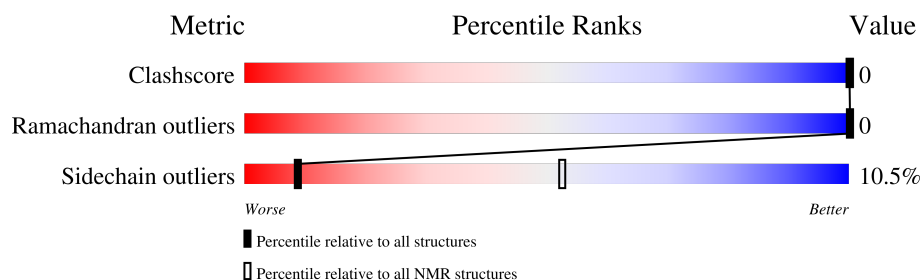
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 64%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	17	

2 Ensemble composition and analysis

This entry contains 30 models. Model 11 is the overall representative, medoid model (most similar to other models).

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:2-A:14 (13)	0.31	11

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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 5, 8, 10, 11, 12, 13, 14, 15, 21, 25, 28, 29, 30
2	3, 4, 6, 7, 9, 16, 19, 22
3	17, 18, 27
4	2, 23
5	24, 26
Single-model clusters	20

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 292 atoms, of which 163 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS.

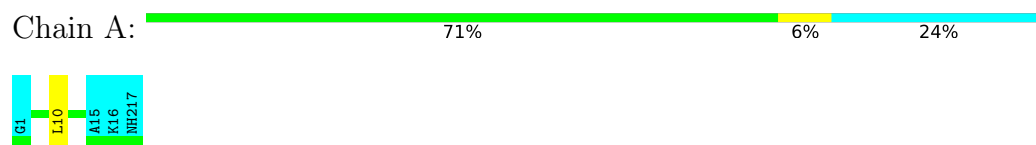
Mol	Chain	Residues	Atoms					Trace
1	A	17	Total	C	H	N	O	1
			292	88	163	23	18	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

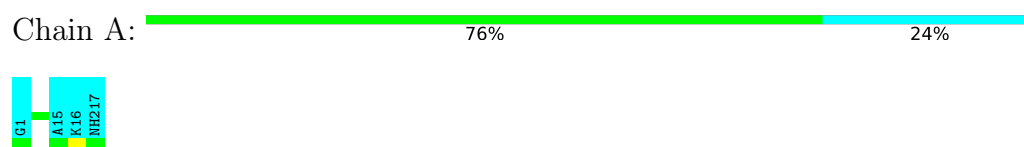


4.2 Scores per residue for each member of the ensemble

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

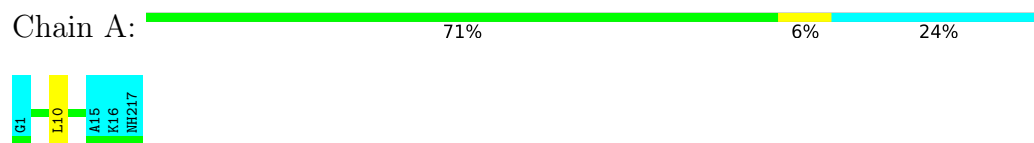
4.2.1 Score per residue for model 1

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



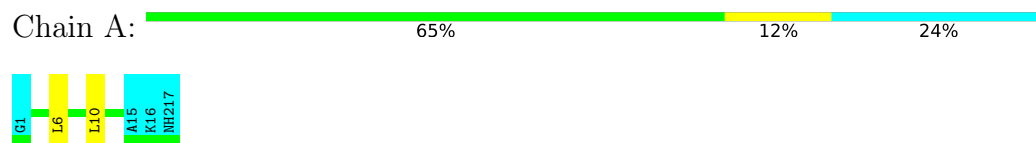
4.2.2 Score per residue for model 2

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



4.2.3 Score per residue for model 3

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



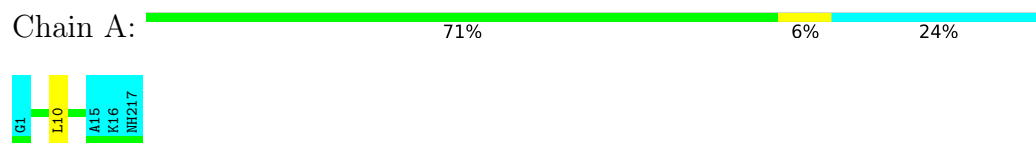
4.2.4 Score per residue for model 4

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



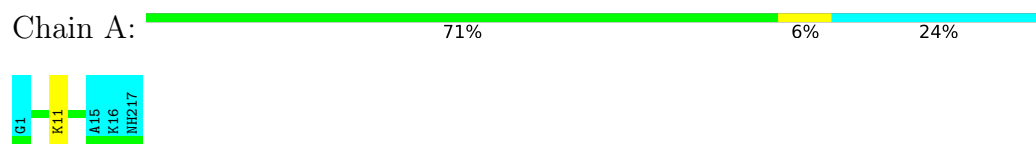
4.2.5 Score per residue for model 5

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



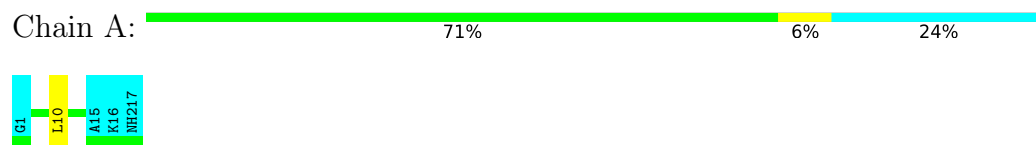
4.2.6 Score per residue for model 6

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



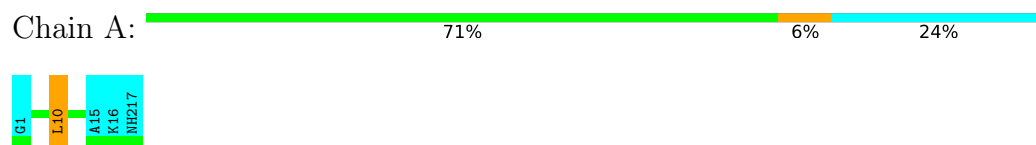
4.2.7 Score per residue for model 7

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



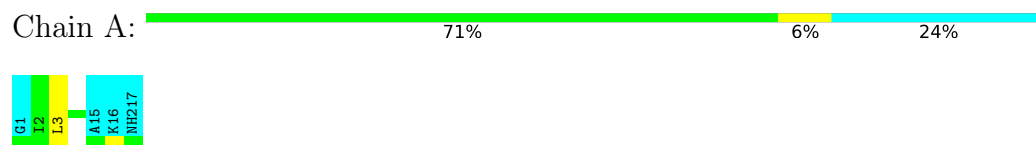
4.2.8 Score per residue for model 8

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



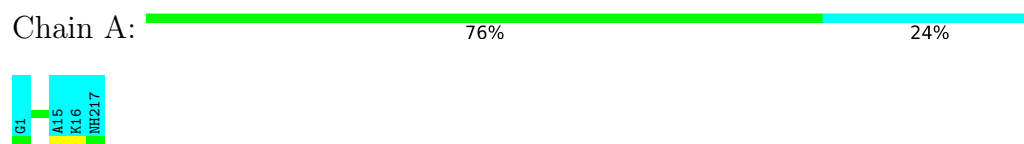
4.2.9 Score per residue for model 9

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



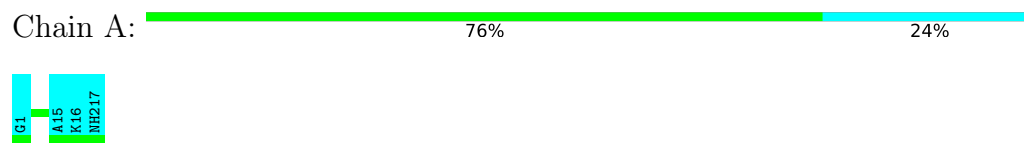
4.2.10 Score per residue for model 10

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



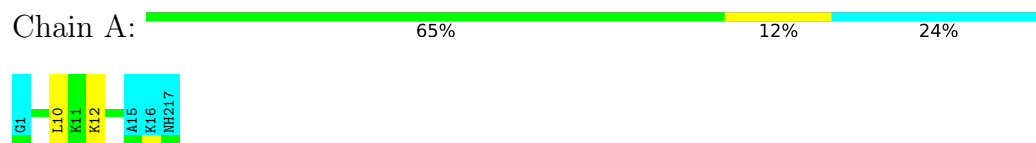
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



4.2.12 Score per residue for model 12

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



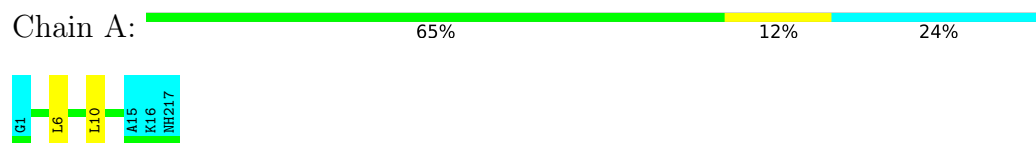
4.2.13 Score per residue for model 13

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



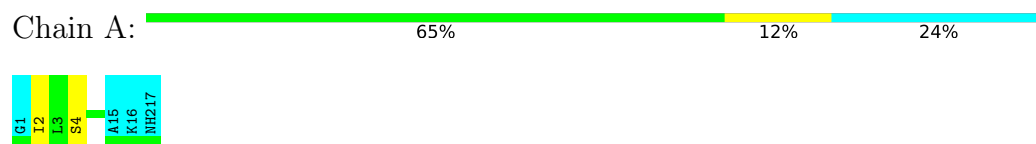
4.2.14 Score per residue for model 14

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



4.2.15 Score per residue for model 15

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



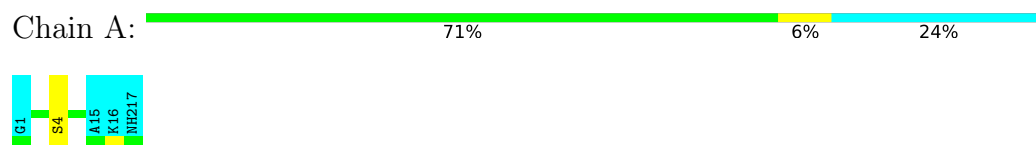
4.2.16 Score per residue for model 16

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



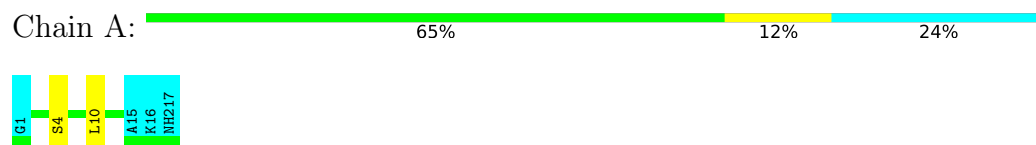
4.2.17 Score per residue for model 17

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



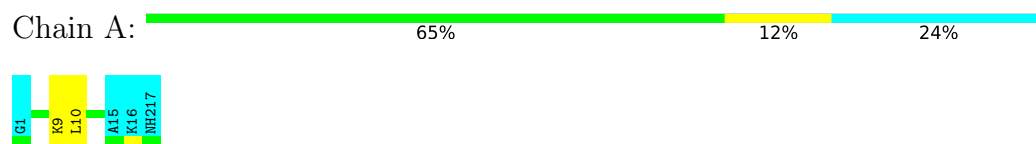
4.2.18 Score per residue for model 18

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



4.2.19 Score per residue for model 19

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



4.2.20 Score per residue for model 20

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS



4.2.21 Score per residue for model 21

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

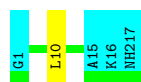
Chain A:  65% 12% 24%



4.2.22 Score per residue for model 22

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

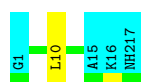
Chain A:  71% 6% 24%



4.2.23 Score per residue for model 23

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

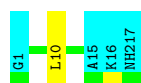
Chain A:  71% 6% 24%



4.2.24 Score per residue for model 24

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

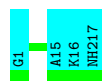
Chain A:  71% 6% 24%



4.2.25 Score per residue for model 25

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

Chain A:  76% 24%



4.2.26 Score per residue for model 26

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

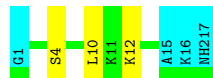
Chain A:  65% 12% 24%



4.2.27 Score per residue for model 27

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

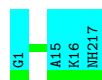
Chain A:  59% 18% 24%



4.2.28 Score per residue for model 28

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

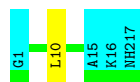
Chain A:  76% 24%



4.2.29 Score per residue for model 29

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

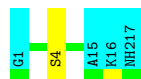
Chain A:  71% 6% 24%



4.2.30 Score per residue for model 30

- Molecule 1: GLY-ILE-LEU-SER-SER-LEU-TRP-LYS-LYS-LEU-LYS-LYS-ILE-ILE-ALA-LYS

Chain A:  71% 6% 24%



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 30 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
CYANA	structure calculation	

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	157
Number of shifts mapped to atoms	157
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	64%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	0.98±0.23	0±0/112 (0.1± 0.3%)	0.88±0.15	0±0/149 (0.0± 0.2%)
All	All	1.01	3/3360 (0.1%)	0.89	2/4470 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	14	ILE	CA-CB	6.14	1.61	1.54	13	1
1	A	9	LYS	C-O	-5.26	1.17	1.24	4	1
1	A	2	ILE	CA-CB	5.23	1.61	1.54	15	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	3	LEU	N-CA-C	-7.07	103.65	111.36	13	1
1	A	10	LEU	N-CA-C	-6.10	104.74	111.82	8	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	3300	4140	4140	-

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

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	13/17 (76%)	13±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	390/510 (76%)	390 (100%)	0 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	13/14 (93%)	12±1 (89±8%)	1±1 (11±8%)	9	52
All	All	390/420 (93%)	349 (89%)	41 (11%)	9	52

All 7 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	10	LEU	20
1	A	4	SER	9
1	A	12	LYS	4
1	A	6	LEU	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	3	LEU	3
1	A	11	LYS	1
1	A	9	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 63% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *lb10.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	157
Number of shifts mapped to atoms	157
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

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 64%, i.e. 138 atoms were assigned a chemical shift out of a possible 216. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	39/65 (60%)	26/26 (100%)	0/26 (0%)	13/13 (100%)
Sidechain	92/139 (66%)	92/92 (100%)	0/43 (0%)	0/4 (0%)
Aromatic	7/12 (58%)	6/6 (100%)	0/5 (0%)	1/1 (100%)
Overall	138/216 (64%)	124/124 (100%)	0/74 (0%)	14/18 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 63%, i.e. 157 atoms were assigned a chemical shift out of a possible 249. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	47/81 (58%)	32/33 (97%)	0/32 (0%)	15/16 (94%)
Sidechain	103/156 (66%)	103/103 (100%)	0/48 (0%)	0/5 (0%)
Aromatic	7/12 (58%)	6/6 (100%)	0/5 (0%)	1/1 (100%)
Overall	157/249 (63%)	141/142 (99%)	0/85 (0%)	16/22 (73%)

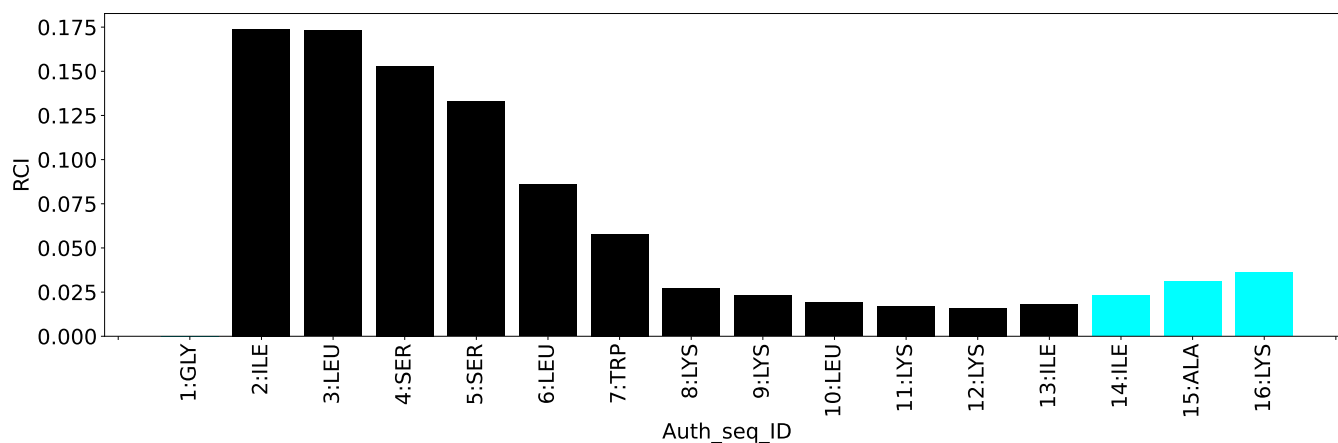
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	191
Intra-residue ($ i-j =0$)	77
Sequential ($ i-j =1$)	54
Medium range ($ i-j >1$ and $ i-j <5$)	60
Long range ($ i-j \geq 5$)	0
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	24
Number of unmapped restraints	0
Number of restraints per residue	12.6
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.9	0.2
0.2-0.5 (Medium)	1.0	0.5
>0.5 (Large)	1.9	5.61

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)	1.6	4.91
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

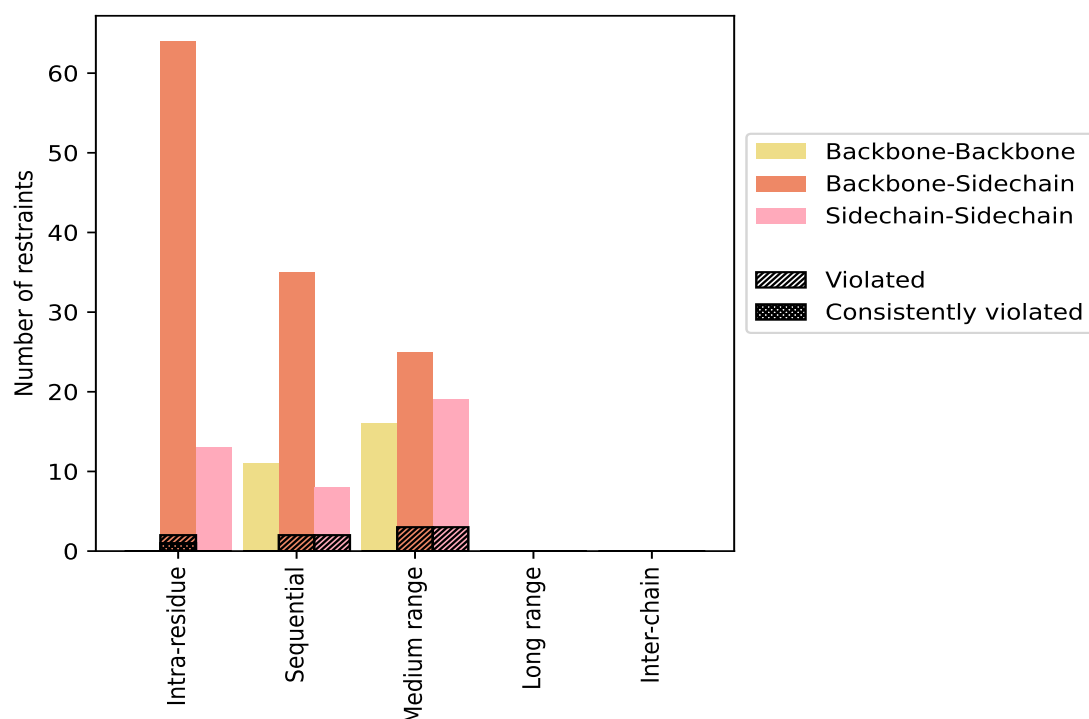
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	77	40.3	2	2.6	1.0	1	1.3	0.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	64	33.5	2	3.1	1.0	1	1.6	0.5
Sidechain-Sidechain	13	6.8	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	54	28.3	4	7.4	2.1	0	0.0	0.0
Backbone-Backbone	11	5.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	35	18.3	2	5.7	1.0	0	0.0	0.0
Sidechain-Sidechain	8	4.2	2	25.0	1.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	60	31.4	6	10.0	3.1	0	0.0	0.0
Backbone-Backbone	16	8.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	25	13.1	3	12.0	1.6	0	0.0	0.0
Sidechain-Sidechain	19	9.9	3	15.8	1.6	0	0.0	0.0
Long range ($i-j \geq 5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	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	191	100.0	12	6.3	6.3	1	0.5	0.5
Backbone-Backbone	27	14.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	124	64.9	7	5.6	3.7	1	0.8	0.5
Sidechain-Sidechain	40	20.9	5	12.5	2.6	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	1	3	0	0	5	1.45	4.17	1.65	0.21
2	1	0	2	0	0	3	0.51	1.14	0.44	0.22
3	1	1	2	0	0	4	1.18	3.06	1.15	0.74
4	2	0	1	0	0	3	1.54	2.31	1.02	2.22
5	1	1	2	0	0	4	0.59	1.51	0.55	0.34
6	1	1	2	0	0	4	1.37	3.0	1.18	1.14
7	1	0	2	0	0	3	2.93	5.6	2.24	3.07
8	1	1	3	0	0	5	1.14	2.94	1.12	0.3
9	1	0	2	0	0	3	2.35	3.84	1.48	2.87
10	1	0	2	0	0	3	2.51	4.71	1.83	2.59

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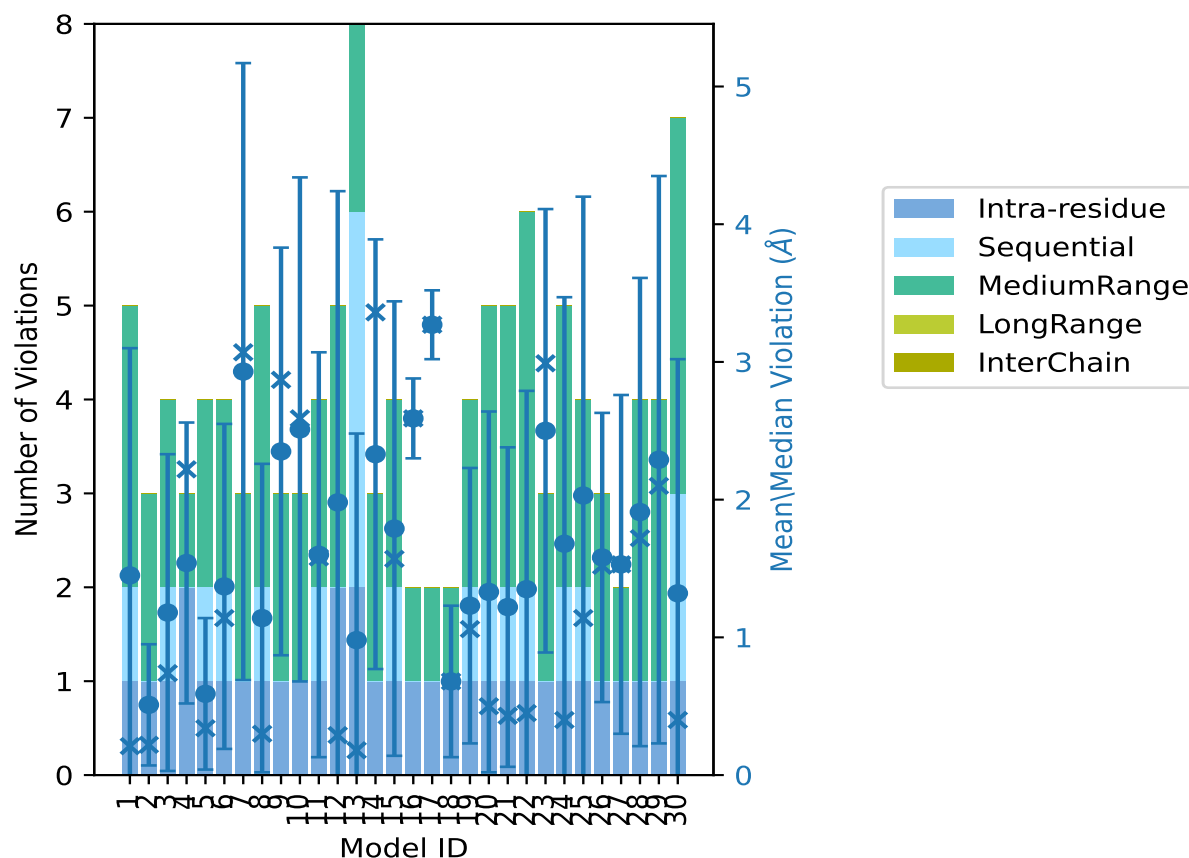
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	1	2	0	0	4	1.6	3.11	1.47	1.58
12	2	0	3	0	0	5	1.98	5.37	2.26	0.29
13	2	4	2	0	0	8	0.98	4.57	1.5	0.18
14	1	0	2	0	0	3	2.33	3.5	1.56	3.36
15	1	1	2	0	0	4	1.79	3.86	1.65	1.57
16	1	0	1	0	0	2	2.59	2.88	0.29	2.59
17	1	0	1	0	0	2	3.27	3.52	0.25	3.27
18	1	0	1	0	0	2	0.68	1.23	0.55	0.68
19	1	1	2	0	0	4	1.23	2.55	1.0	1.06
20	1	1	3	0	0	5	1.33	2.98	1.31	0.5
21	1	1	3	0	0	5	1.22	2.88	1.16	0.43
22	1	1	4	0	0	6	1.35	3.55	1.44	0.45
23	1	0	2	0	0	3	2.5	4.18	1.61	2.99
24	1	1	3	0	0	5	1.68	4.3	1.79	0.4
25	1	1	2	0	0	4	2.03	5.61	2.17	1.14
26	1	0	2	0	0	3	1.58	2.89	1.05	1.52
27	1	0	1	0	0	2	1.53	2.76	1.23	1.53
28	1	0	3	0	0	4	1.91	3.99	1.7	1.72
29	1	0	3	0	0	4	2.29	4.76	2.06	2.1
30	1	2	4	0	0	7	1.32	4.56	1.7	0.4

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 179(IR:75, SQ:50, MR:54, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	1	2	0	0	3	1	3.3
0	1	0	0	0	1	2	6.7
1	0	0	0	0	1	3	10.0
0	0	0	0	0	0	4	13.3
0	0	1	0	0	1	5	16.7
0	0	0	0	0	0	6	20.0

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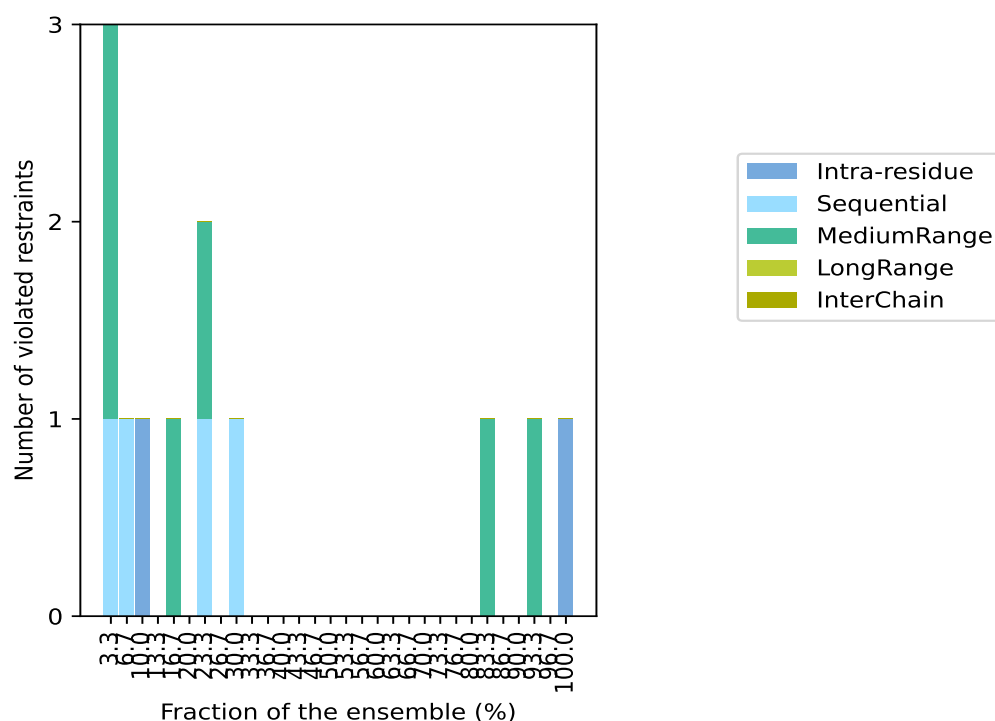
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	1	1	0	0	2	7	23.3
0	0	0	0	0	0	8	26.7
0	1	0	0	0	1	9	30.0
0	0	0	0	0	0	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	14	46.7
0	0	0	0	0	0	15	50.0
0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	24	80.0
0	0	1	0	0	1	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	1	0	0	1	28	93.3
0	0	0	0	0	0	29	96.7
1	0	0	0	0	1	30	100.0

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

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

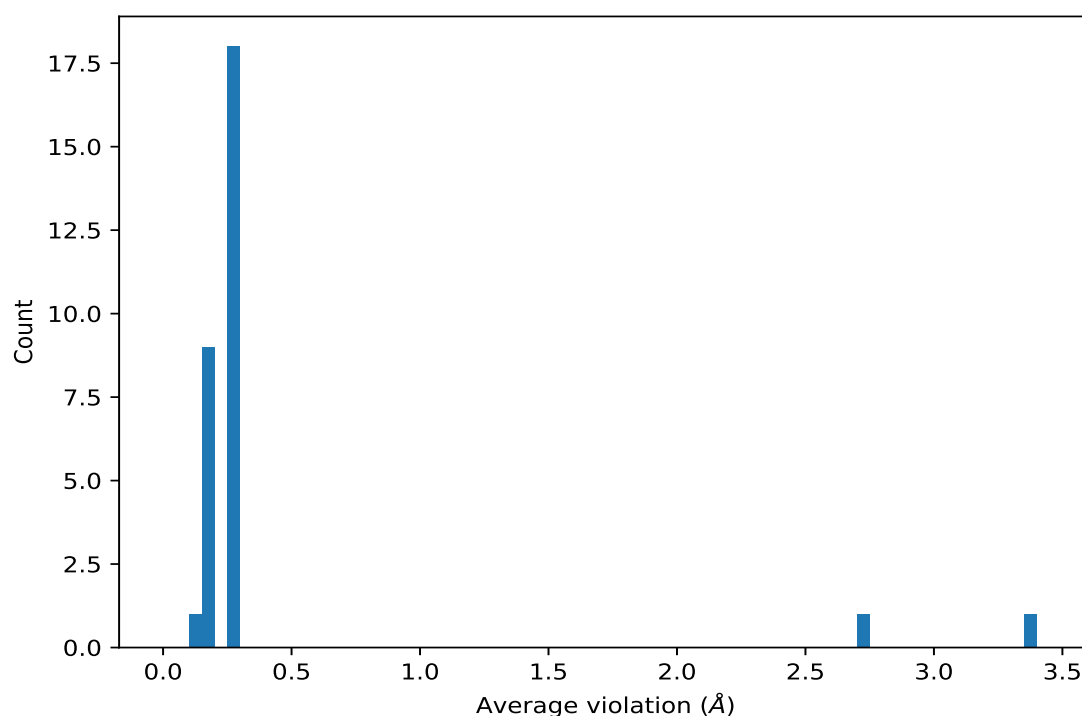
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	30	2.72	0.71	2.95
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	28	3.37	1.39	3.54
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	25	0.28	0.11	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	25	0.28	0.11	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	25	0.28	0.11	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	25	0.28	0.11	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	25	0.28	0.11	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	25	0.28	0.11	0.25
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD11	9	0.25	0.09	0.26
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD12	9	0.25	0.09	0.26
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD13	9	0.25	0.09	0.26
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD11	9	0.25	0.09	0.26
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD12	9	0.25	0.09	0.26
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD13	9	0.25	0.09	0.26
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD11	7	0.19	0.06	0.19
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD12	7	0.19	0.06	0.19

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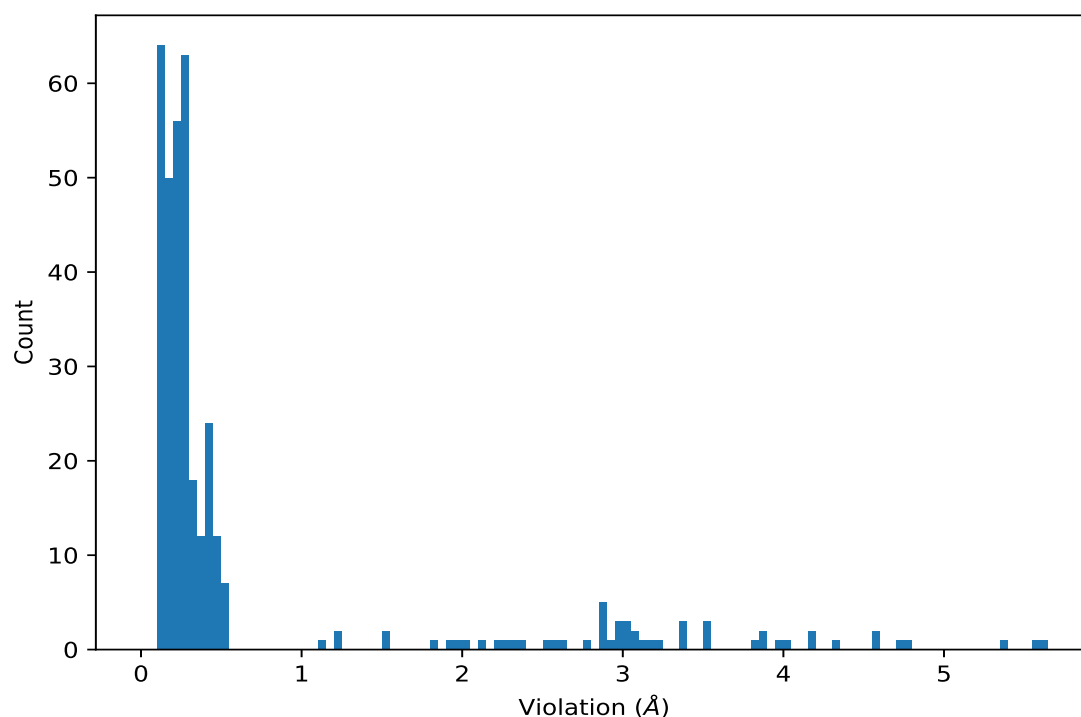
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD13	7	0.19	0.06	0.19
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD21	7	0.19	0.06	0.19
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD22	7	0.19	0.06	0.19
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD23	7	0.19	0.06	0.19
(1,60)	1:6:A:LEU:HB2	1:7:A:TRP:HD1	7	0.16	0.06	0.13
(1,60)	1:6:A:LEU:HB3	1:7:A:TRP:HD1	7	0.16	0.06	0.13
(1,170)	1:3:A:LEU:HD11	1:7:A:TRP:HE1	5	0.27	0.09	0.25
(1,170)	1:3:A:LEU:HD12	1:7:A:TRP:HE1	5	0.27	0.09	0.25
(1,170)	1:3:A:LEU:HD13	1:7:A:TRP:HE1	5	0.27	0.09	0.25
(1,170)	1:3:A:LEU:HD21	1:7:A:TRP:HE1	5	0.27	0.09	0.25
(1,170)	1:3:A:LEU:HD22	1:7:A:TRP:HE1	5	0.27	0.09	0.25
(1,170)	1:3:A:LEU:HD23	1:7:A:TRP:HE1	5	0.27	0.09	0.25
(1,11)	1:10:A:LEU:H	1:10:A:LEU:HG	3	0.12	0.02	0.12
(1,79)	1:7:A:TRP:HH2	1:8:A:LYS:HA	2	0.17	0.01	0.17

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	25	5.61
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	7	5.6
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	12	5.37
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	29	4.76
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	10	4.71
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	13	4.57
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	30	4.56
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	24	4.3
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	23	4.18
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	1	4.17
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	12	4.03
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	28	3.99
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	29	3.89
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	15	3.86
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	9	3.84
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	22	3.55
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	17	3.52
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	14	3.5
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	24	3.39
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	14	3.36
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	30	3.35
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	22	3.22
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	28	3.16
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	11	3.11
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	7	3.07
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	3	3.06
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	11	3.02
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	17	3.02
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	6	3.0
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	23	2.99
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	20	2.98
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	15	2.96
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	8	2.94
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	26	2.89
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	16	2.88
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	21	2.88
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	20	2.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	9	2.87
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	27	2.76
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	1	2.6
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	10	2.59
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	19	2.55
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	21	2.37
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	4	2.31
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	16	2.3
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	4	2.22
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	13	2.13
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	6	2.0
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	8	1.98
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	25	1.91
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	19	1.84
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	26	1.52
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	5	1.51
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	18	1.23
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	3	1.21
(1,49)	1:16:A:LYS:H	1:16:A:LYS:HE3	2	1.14
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	5	0.51
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	20	0.5
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	20	0.5
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	20	0.5
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	20	0.5
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	20	0.5
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	20	0.5
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	22	0.48
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	22	0.48
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	22	0.48
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	22	0.48
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	22	0.48
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	22	0.48
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	30	0.46
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	30	0.46
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	30	0.46
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	30	0.46
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	30	0.46
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	30	0.46
(1,170)	1:3:A:LEU:HD11	1:7:A:TRP:HE1	22	0.43
(1,170)	1:3:A:LEU:HD12	1:7:A:TRP:HE1	22	0.43
(1,170)	1:3:A:LEU:HD13	1:7:A:TRP:HE1	22	0.43
(1,170)	1:3:A:LEU:HD21	1:7:A:TRP:HE1	22	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:3:A:LEU:HD22	1:7:A:TRP:HE1	22	0.43
(1,170)	1:3:A:LEU:HD23	1:7:A:TRP:HE1	22	0.43
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	21	0.43
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	21	0.43
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	21	0.43
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	21	0.43
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	21	0.43
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	21	0.43
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD11	30	0.4
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD12	30	0.4
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD13	30	0.4
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD11	30	0.4
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD12	30	0.4
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD13	30	0.4
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	24	0.4
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	24	0.4
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	24	0.4
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	24	0.4
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	24	0.4
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	24	0.4
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	13	0.37
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	13	0.37
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	13	0.37
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	13	0.37
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	13	0.37
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	13	0.37
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD11	25	0.36
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD12	25	0.36
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD13	25	0.36
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD11	25	0.36
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD12	25	0.36
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD13	25	0.36
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	9	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	9	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	9	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	9	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	9	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	9	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	23	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	23	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	23	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	23	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	23	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	23	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	26	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	26	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	26	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	26	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	26	0.33
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	26	0.33
(2,1)	1:13:A:ILE:HA	1:16:A:LYS:HE3	27	0.3
(1,60)	1:6:A:LEU:HB2	1:7:A:TRP:HD1	8	0.3
(1,60)	1:6:A:LEU:HB3	1:7:A:TRP:HD1	8	0.3
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	29	0.3
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	29	0.3
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	29	0.3
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	29	0.3
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	29	0.3
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	29	0.3
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	12	0.29
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	12	0.29
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	12	0.29
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	12	0.29
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	12	0.29
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	12	0.29
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD11	6	0.28
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD12	6	0.28
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD13	6	0.28
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD11	6	0.28
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD12	6	0.28
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD13	6	0.28
(1,170)	1:3:A:LEU:HD11	1:7:A:TRP:HE1	28	0.28
(1,170)	1:3:A:LEU:HD12	1:7:A:TRP:HE1	28	0.28
(1,170)	1:3:A:LEU:HD13	1:7:A:TRP:HE1	28	0.28
(1,170)	1:3:A:LEU:HD21	1:7:A:TRP:HE1	28	0.28
(1,170)	1:3:A:LEU:HD22	1:7:A:TRP:HE1	28	0.28
(1,170)	1:3:A:LEU:HD23	1:7:A:TRP:HE1	28	0.28
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD11	21	0.28
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD12	21	0.28
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD13	21	0.28
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD21	21	0.28
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD22	21	0.28
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD23	21	0.28
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD11	19	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD12	19	0.27
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD13	19	0.27
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD11	19	0.27
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD12	19	0.27
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD13	19	0.27
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD11	3	0.26
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD12	3	0.26
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD13	3	0.26
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD11	3	0.26
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD12	3	0.26
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD13	3	0.26
(1,170)	1:3:A:LEU:HD11	1:7:A:TRP:HE1	8	0.25
(1,170)	1:3:A:LEU:HD12	1:7:A:TRP:HE1	8	0.25
(1,170)	1:3:A:LEU:HD13	1:7:A:TRP:HE1	8	0.25
(1,170)	1:3:A:LEU:HD21	1:7:A:TRP:HE1	8	0.25
(1,170)	1:3:A:LEU:HD22	1:7:A:TRP:HE1	8	0.25
(1,170)	1:3:A:LEU:HD23	1:7:A:TRP:HE1	8	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	8	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	8	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	8	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	8	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	8	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	8	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	19	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	19	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	19	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	19	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	19	0.25
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	19	0.25
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD11	22	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD12	22	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD13	22	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD21	22	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD22	22	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD23	22	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD11	30	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD12	30	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD13	30	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD21	30	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD22	30	0.24
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD23	30	0.24
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	10	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	10	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	10	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	10	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	10	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	25	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	25	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	25	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	25	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	25	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	25	0.23
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	2	0.22
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	2	0.22
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	2	0.22
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	2	0.22
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	2	0.22
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	2	0.22
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	1	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	1	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	1	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	1	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	1	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	1	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	3	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	3	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	3	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	3	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	3	0.21
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	3	0.21
(1,170)	1:3:A:LEU:HD11	1:7:A:TRP:HE1	29	0.2
(1,170)	1:3:A:LEU:HD12	1:7:A:TRP:HE1	29	0.2
(1,170)	1:3:A:LEU:HD13	1:7:A:TRP:HE1	29	0.2
(1,170)	1:3:A:LEU:HD21	1:7:A:TRP:HE1	29	0.2
(1,170)	1:3:A:LEU:HD22	1:7:A:TRP:HE1	29	0.2
(1,170)	1:3:A:LEU:HD23	1:7:A:TRP:HE1	29	0.2
(1,60)	1:6:A:LEU:HB2	1:7:A:TRP:HD1	22	0.2
(1,60)	1:6:A:LEU:HB3	1:7:A:TRP:HD1	22	0.2
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	6	0.2
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	6	0.2
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	6	0.2
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	6	0.2
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	6	0.2
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD11	13	0.19
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD12	13	0.19
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD13	13	0.19
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD11	13	0.19
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD12	13	0.19
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD13	13	0.19
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD11	24	0.19
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD12	24	0.19
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD13	24	0.19
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD21	24	0.19
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD22	24	0.19
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD23	24	0.19
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	28	0.19
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	28	0.19
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	28	0.19
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	28	0.19
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	28	0.19
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	28	0.19
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD11	5	0.18
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD12	5	0.18
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD13	5	0.18
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD11	5	0.18
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD12	5	0.18
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD13	5	0.18
(1,170)	1:3:A:LEU:HD11	1:7:A:TRP:HE1	2	0.18
(1,170)	1:3:A:LEU:HD12	1:7:A:TRP:HE1	2	0.18
(1,170)	1:3:A:LEU:HD13	1:7:A:TRP:HE1	2	0.18
(1,170)	1:3:A:LEU:HD21	1:7:A:TRP:HE1	2	0.18
(1,170)	1:3:A:LEU:HD22	1:7:A:TRP:HE1	2	0.18
(1,170)	1:3:A:LEU:HD23	1:7:A:TRP:HE1	2	0.18
(1,79)	1:7:A:TRP:HH2	1:8:A:LYS:HA	13	0.18
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	15	0.18
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	15	0.18
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	15	0.18
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	15	0.18
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	15	0.18
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	15	0.18
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD11	20	0.17
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD12	20	0.17
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD13	20	0.17
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD11	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD12	20	0.17
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD13	20	0.17
(1,79)	1:7:A:TRP:HH2	1:8:A:LYS:HA	15	0.16
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD11	1	0.16
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD12	1	0.16
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD13	1	0.16
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD21	1	0.16
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD22	1	0.16
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD23	1	0.16
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	5	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	5	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	5	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	5	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	5	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	5	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	11	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	11	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	11	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	11	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	11	0.15
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	11	0.15
(1,11)	1:10:A:LEU:H	1:10:A:LEU:HG	13	0.14
(1,177)	1:6:A:LEU:HD11	1:10:A:LEU:H	18	0.13
(1,177)	1:6:A:LEU:HD12	1:10:A:LEU:H	18	0.13
(1,177)	1:6:A:LEU:HD13	1:10:A:LEU:H	18	0.13
(1,177)	1:6:A:LEU:HD21	1:10:A:LEU:H	18	0.13
(1,177)	1:6:A:LEU:HD22	1:10:A:LEU:H	18	0.13
(1,177)	1:6:A:LEU:HD23	1:10:A:LEU:H	18	0.13
(1,60)	1:6:A:LEU:HB2	1:7:A:TRP:HD1	1	0.13
(1,60)	1:6:A:LEU:HB3	1:7:A:TRP:HD1	1	0.13
(1,60)	1:6:A:LEU:HB2	1:7:A:TRP:HD1	21	0.13
(1,60)	1:6:A:LEU:HB3	1:7:A:TRP:HD1	21	0.13
(1,60)	1:6:A:LEU:HB2	1:7:A:TRP:HD1	30	0.13
(1,60)	1:6:A:LEU:HB3	1:7:A:TRP:HD1	30	0.13
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	7	0.13
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	7	0.13
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	7	0.13
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	7	0.13
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	7	0.13
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	7	0.13
(1,138)	1:8:A:LYS:HA	1:11:A:LYS:HD2	30	0.12
(1,138)	1:8:A:LYS:HA	1:11:A:LYS:HD3	30	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD11	20	0.12
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD12	20	0.12
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD13	20	0.12
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD21	20	0.12
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD22	20	0.12
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD23	20	0.12
(1,60)	1:6:A:LEU:HB2	1:7:A:TRP:HD1	13	0.12
(1,60)	1:6:A:LEU:HB3	1:7:A:TRP:HD1	13	0.12
(1,60)	1:6:A:LEU:HB2	1:7:A:TRP:HD1	24	0.12
(1,60)	1:6:A:LEU:HB3	1:7:A:TRP:HD1	24	0.12
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD11	14	0.12
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD12	14	0.12
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD13	14	0.12
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD21	14	0.12
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD22	14	0.12
(1,52)	1:7:A:TRP:HZ3	1:10:A:LEU:HD23	14	0.12
(1,11)	1:10:A:LEU:H	1:10:A:LEU:HG	12	0.12
(1,160)	1:14:A:ILE:HB	1:15:A:ALA:H	13	0.11
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD11	11	0.1
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD12	11	0.1
(1,186)	1:12:A:LYS:HG2	1:13:A:ILE:HD13	11	0.1
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD11	11	0.1
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD12	11	0.1
(1,186)	1:12:A:LYS:HG3	1:13:A:ILE:HD13	11	0.1
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD11	12	0.1
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD12	12	0.1
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD13	12	0.1
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD21	12	0.1
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD22	12	0.1
(1,70)	1:7:A:TRP:HE3	1:10:A:LEU:HD23	12	0.1
(1,11)	1:10:A:LEU:H	1:10:A:LEU:HG	4	0.1

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

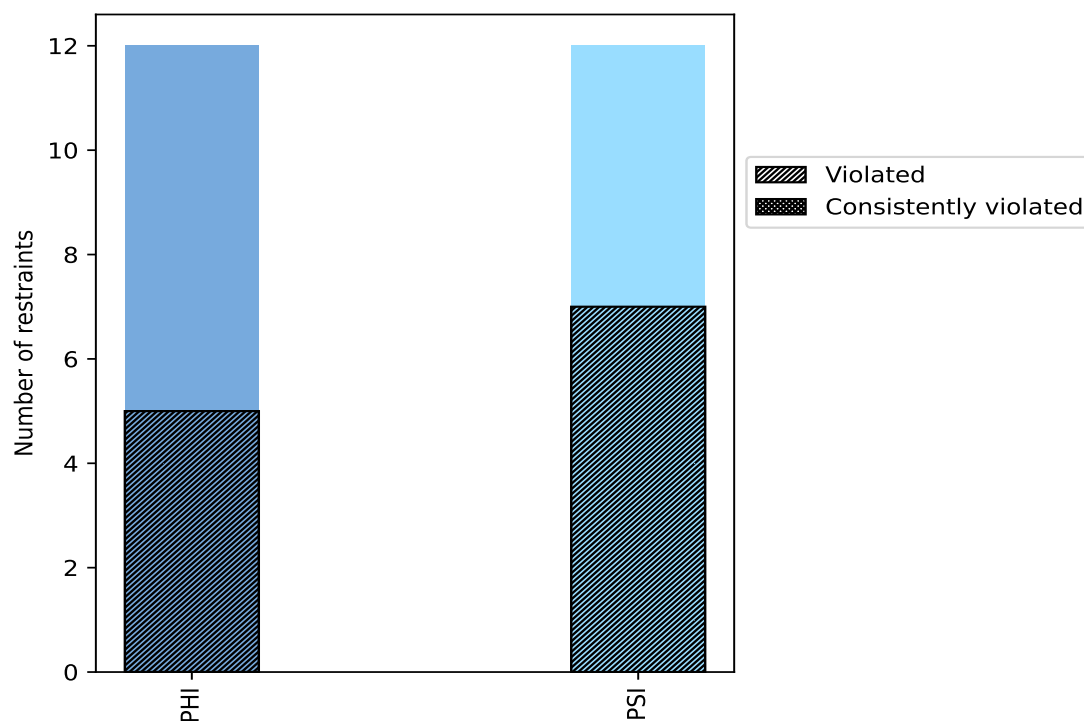
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	12	50.0	5	41.7	20.8	0	0.0	0.0
PSI	12	50.0	7	58.3	29.2	0	0.0	0.0
Total	24	100.0	12	50.0	50.0	0	0.0	0.0

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

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



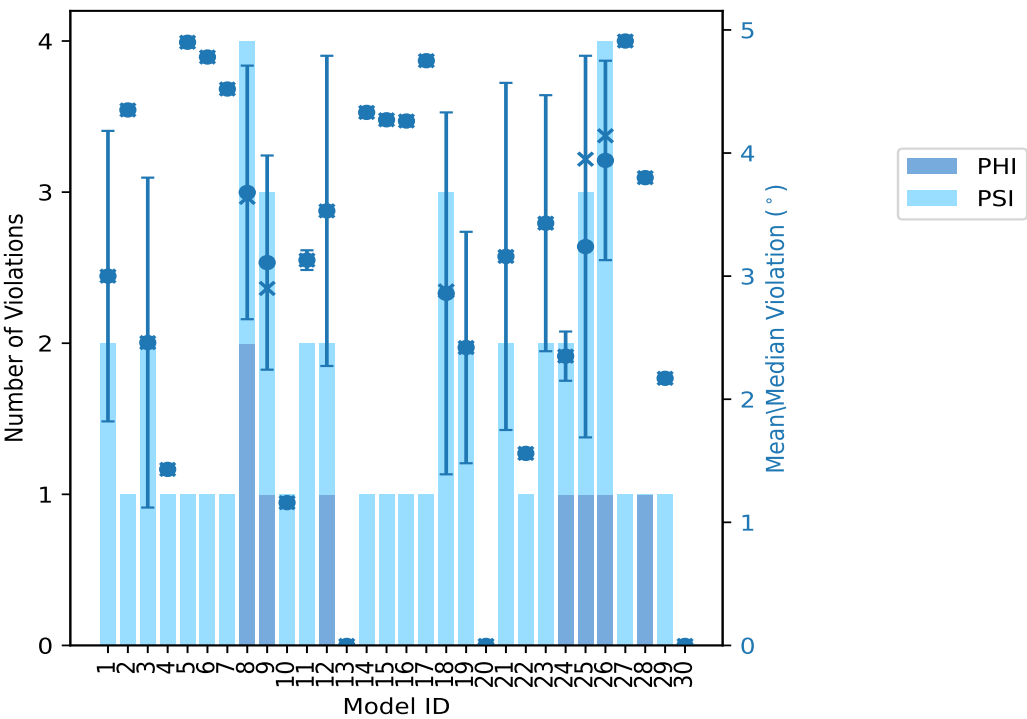
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	2	2	3.0	4.18	1.18	3.0
2	0	1	1	4.35	4.35	0.0	4.35
3	0	2	2	2.46	3.8	1.34	2.46
4	0	1	1	1.43	1.43	0.0	1.43
5	0	1	1	4.9	4.9	0.0	4.9
6	0	1	1	4.78	4.78	0.0	4.78
7	0	1	1	4.52	4.52	0.0	4.52
8	2	2	4	3.68	4.85	1.03	3.64
9	1	2	3	3.11	4.26	0.87	2.9
10	0	1	1	1.16	1.16	0.0	1.16
11	0	2	2	3.13	3.21	0.08	3.13
12	1	1	2	3.53	4.79	1.26	3.53
13	0	0	0	0.0	0.0	0.0	0.0
14	0	1	1	4.33	4.33	0.0	4.33
15	0	1	1	4.27	4.27	0.0	4.27
16	0	1	1	4.26	4.26	0.0	4.26
17	0	1	1	4.75	4.75	0.0	4.75
18	0	3	3	2.86	4.65	1.47	2.88
19	0	2	2	2.42	3.37	0.94	2.42
20	0	0	0	0.0	0.0	0.0	0.0
21	0	2	2	3.16	4.57	1.41	3.16
22	0	1	1	1.56	1.56	0.0	1.56
23	0	2	2	3.43	4.47	1.04	3.43
24	1	1	2	2.35	2.55	0.2	2.35
25	1	2	3	3.24	4.68	1.55	3.95
26	1	3	4	3.94	4.76	0.81	4.14
27	0	1	1	4.91	4.91	0.0	4.91
28	1	0	1	3.8	3.8	0.0	3.8
29	0	1	1	2.17	2.17	0.0	2.17
30	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
3	1	4	1	3.3
1	2	3	2	6.7
1	1	2	3	10.0
0	1	1	4	13.3
0	0	0	5	16.7
0	0	0	6	20.0
0	0	0	7	23.3
0	0	0	8	26.7
0	0	0	9	30.0
0	1	1	10	33.3
0	0	0	11	36.7

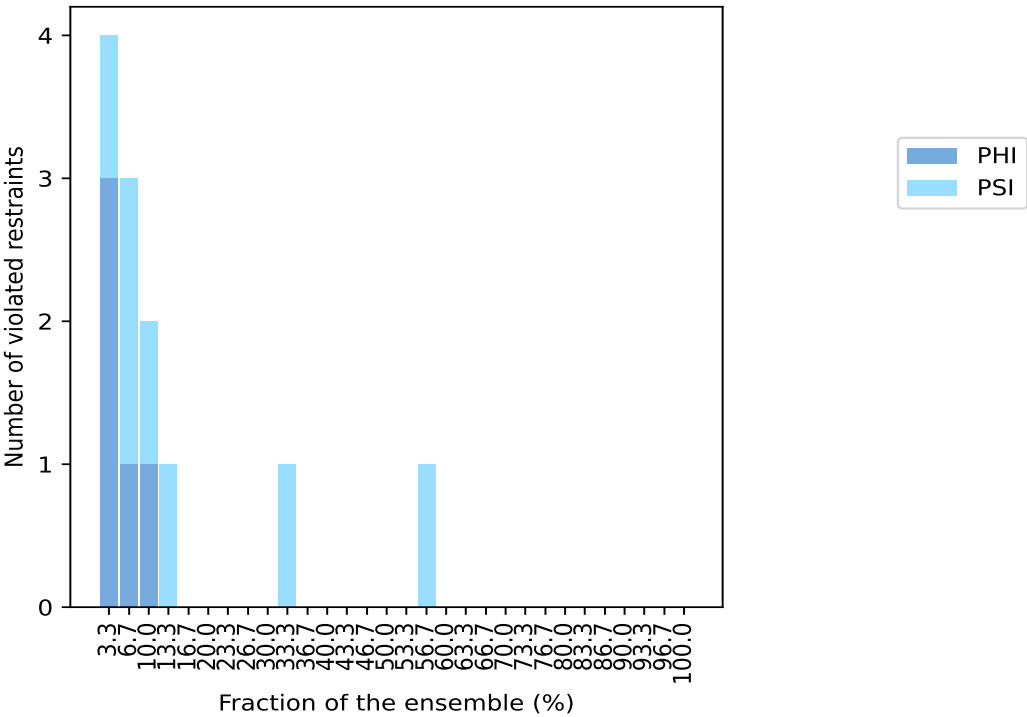
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	40.0
0	0	0	13	43.3
0	0	0	14	46.7
0	0	0	15	50.0
0	0	0	16	53.3
0	1	1	17	56.7
0	0	0	18	60.0
0	0	0	19	63.3
0	0	0	20	66.7
0	0	0	21	70.0
0	0	0	22	73.3
0	0	0	23	76.7
0	0	0	24	80.0
0	0	0	25	83.3
0	0	0	26	86.7
0	0	0	27	90.0
0	0	0	28	93.3
0	0	0	29	96.7
0	0	0	30	100.0

¹ Number of models with violations

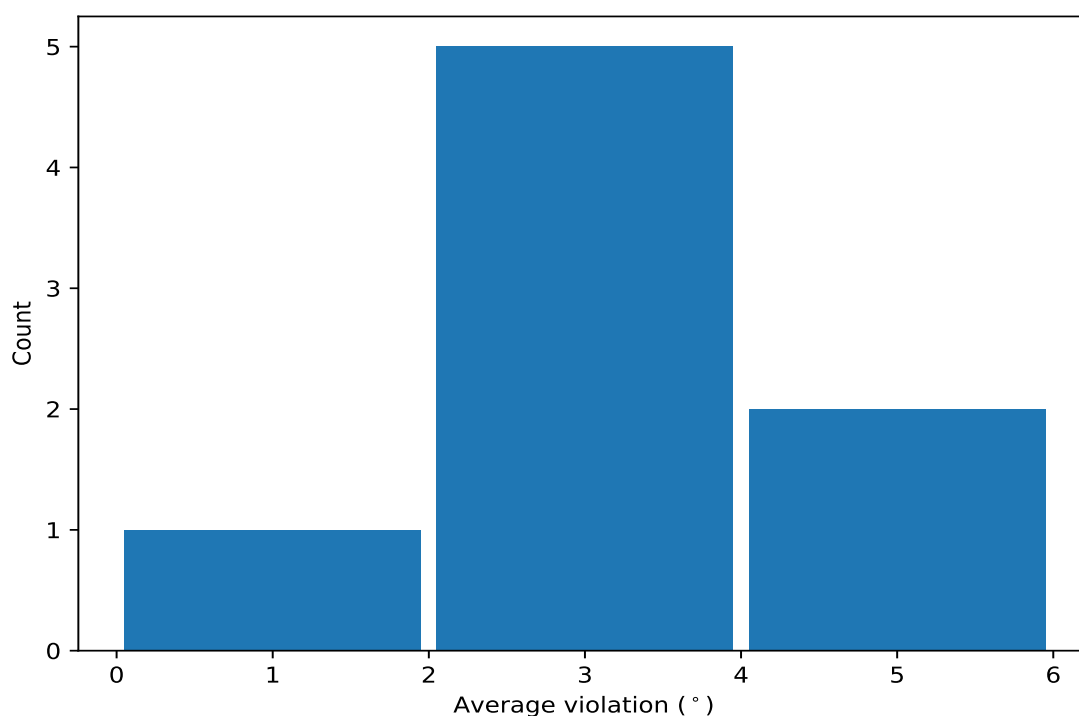
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

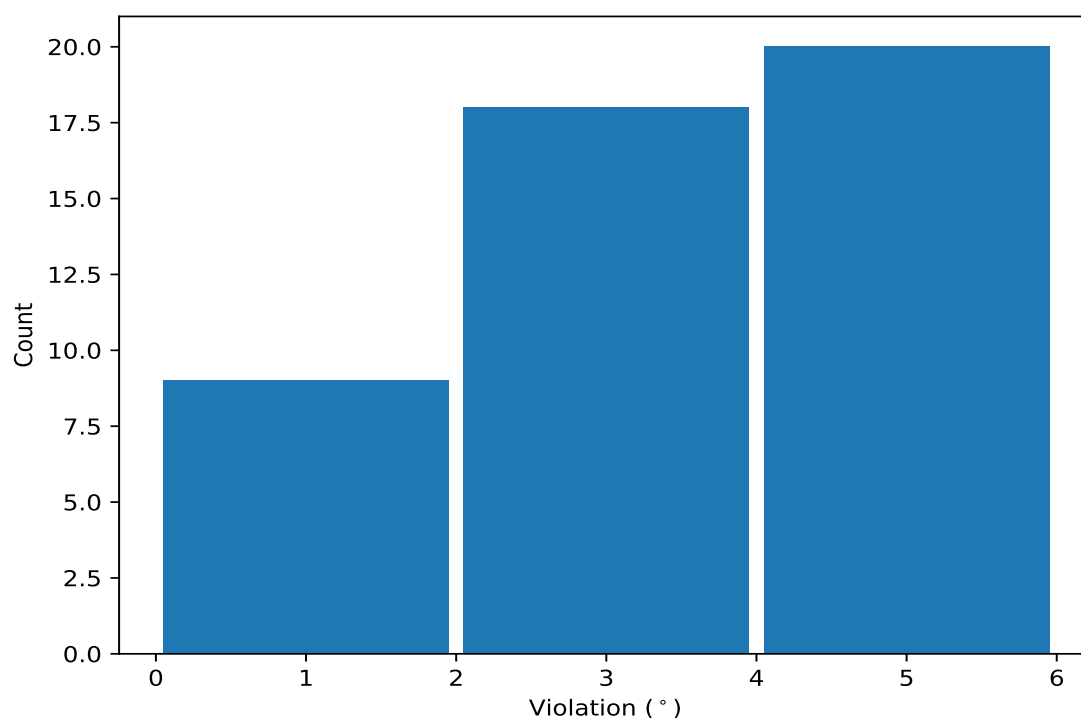
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	17	3.21	1.31	3.21
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	10	3.81	0.84	4.22
(1,20)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:LYS:N	4	4.03	0.85	4.24
(1,8)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LEU:N	3	2.81	0.63	2.62
(1,13)	1:7:A:TRP:C	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	3	2.09	0.75	2.27
(1,17)	1:9:A:LYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	2	4.21	0.41	4.21
(1,18)	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	1:11:A:LYS:N	2	2.86	1.71	2.86
(1,16)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	2	1.08	0.03	1.08

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	27	4.91
(1,20)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:LYS:N	5	4.9
(1,3)	1:2:A:ILE:C	1:3:A:LEU:N	1:3:A:LEU:CA	1:3:A:LEU:C	8	4.85
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	12	4.79
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	6	4.78
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	26	4.76
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	17	4.75
(1,20)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:LYS:N	25	4.68
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	18	4.65
(1,17)	1:9:A:LYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	26	4.62
(1,23)	1:12:A:LYS:C	1:13:A:ILE:N	1:13:A:ILE:CA	1:13:A:ILE:C	8	4.57
(1,18)	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	1:11:A:LYS:N	21	4.57
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	7	4.52
(1,4)	1:3:A:LEU:N	1:3:A:LEU:CA	1:3:A:LEU:C	1:4:A:SER:N	23	4.47
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	2	4.35
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	14	4.33
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	15	4.27
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	9	4.26
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	16	4.26
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	1	4.18
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	25	3.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,20)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:LYS:N	3	3.8
(1,17)	1:9:A:LYS:C	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	28	3.8
(1,8)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LEU:N	26	3.65
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	19	3.37
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	11	3.21
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	11	3.05
(1,13)	1:7:A:TRP:C	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	9	2.9
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	18	2.88
(1,20)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:LYS:N	26	2.75
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	8	2.7
(1,8)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LEU:N	8	2.62
(1,1)	1:1:A:GLY:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	24	2.55
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	23	2.39
(1,13)	1:7:A:TRP:C	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	12	2.27
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	29	2.17
(1,14)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:LYS:N	9	2.17
(1,8)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LEU:N	24	2.15
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	1	1.81
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	21	1.75
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	22	1.56
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	19	1.48
(1,22)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ILE:N	4	1.43
(1,18)	1:10:A:LEU:N	1:10:A:LEU:CA	1:10:A:LEU:C	1:11:A:LYS:N	10	1.16
(1,16)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	3	1.11
(1,13)	1:7:A:TRP:C	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	25	1.09
(1,16)	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1:10:A:LEU:N	18	1.05