



Full wwPDB NMR Structure Validation Report ⓘ

Nov 8, 2023 – 03:03 AM EST

PDB ID : 6BVW
BMRB ID : 30381
Title : SFTI-HFRW-3
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Deposited on : 2017-12-14

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.36

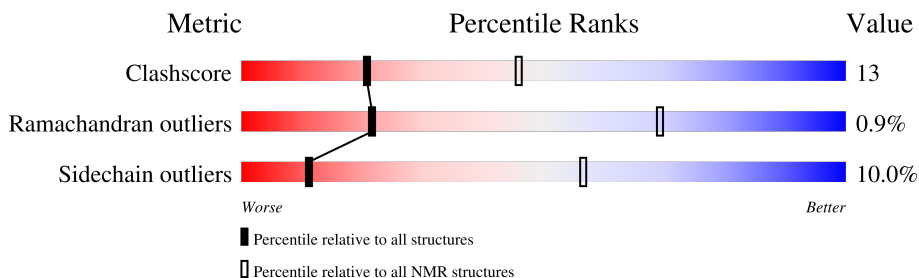
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 71%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	14	 57% 21% 21%

2 Ensemble composition and analysis

This entry contains 24 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:10, A:14-A:14 (11)	0.75	15

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. No single-model clusters were found.

Cluster number	Models
1	4, 6, 8, 9, 11, 13, 14, 15, 17, 19, 21, 24
2	1, 2, 12, 16, 18, 22
3	5, 7, 20
4	3, 10, 23

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 221 atoms, of which 102 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trypsin inhibitor 1 HFRW-3.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	14	221	78	102	23	16	2	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Trypsin inhibitor 1 HFRW-3

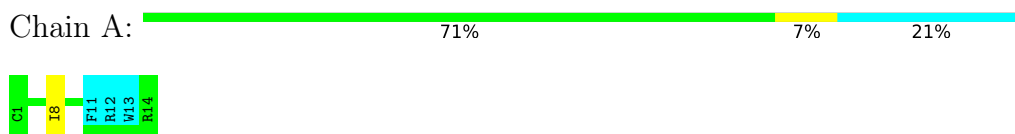


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.2 Score per residue for model 2

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.3 Score per residue for model 3

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.4 Score per residue for model 4

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.5 Score per residue for model 5

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.6 Score per residue for model 6

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.7 Score per residue for model 7

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.8 Score per residue for model 8

- Molecule 1: Trypsin inhibitor 1 HFRW-3



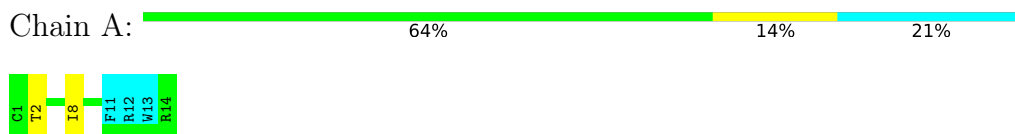
4.2.9 Score per residue for model 9

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.10 Score per residue for model 10

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.11 Score per residue for model 11

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.12 Score per residue for model 12

- Molecule 1: Trypsin inhibitor 1 HFRW-3



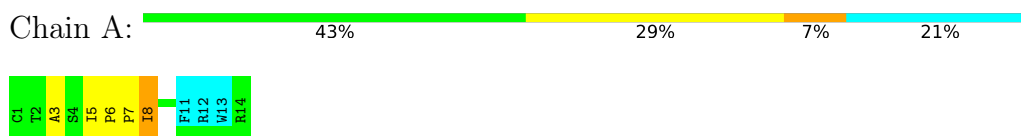
4.2.13 Score per residue for model 13

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.14 Score per residue for model 14

- Molecule 1: Trypsin inhibitor 1 HFRW-3



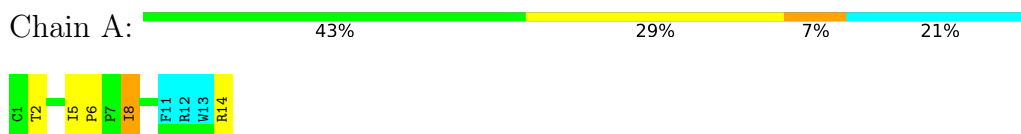
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.16 Score per residue for model 16

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.17 Score per residue for model 17

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.18 Score per residue for model 18

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.19 Score per residue for model 19

- Molecule 1: Trypsin inhibitor 1 HFRW-3



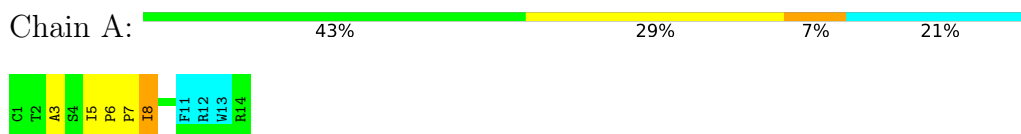
4.2.20 Score per residue for model 20

- Molecule 1: Trypsin inhibitor 1 HFRW-3



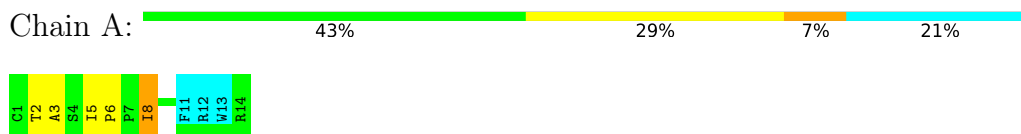
4.2.21 Score per residue for model 21

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.22 Score per residue for model 22

- Molecule 1: Trypsin inhibitor 1 HFRW-3



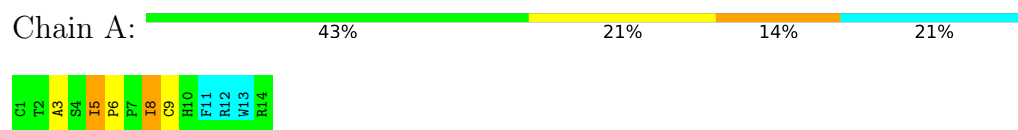
4.2.23 Score per residue for model 23

- Molecule 1: Trypsin inhibitor 1 HFRW-3



4.2.24 Score per residue for model 24

- Molecule 1: Trypsin inhibitor 1 HFRW-3



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 24 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	refinement	
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	135
Number of shifts mapped to atoms	135
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

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: E9M, DPN, MMO

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	81	66	81	2±2
All	All	1944	1584	1938	52

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ALA:HB3	1:A:8:ILE:HG22	0.72	1.59	19	4
1:A:5:ILE:HG23	1:A:5:ILE:O	0.68	1.89	23	3
1:A:5:ILE:HD12	1:A:7:PRO:HD3	0.66	1.65	14	5
1:A:8:ILE:HD13	1:A:9:CYS:N	0.60	2.11	24	1
1:A:3:ALA:HB3	1:A:8:ILE:CG2	0.56	2.31	19	3
1:A:5:ILE:O	1:A:5:ILE:CG2	0.56	2.54	23	1
1:A:5:ILE:C	1:A:5:ILE:HD13	0.55	2.22	23	1
1:A:2:THR:HG22	1:A:8:ILE:H	0.53	1.63	16	2
1:A:2:THR:HG22	1:A:8:ILE:HG13	0.51	1.81	10	1
1:A:5:ILE:C	1:A:5:ILE:CD1	0.50	2.80	23	1
1:A:2:THR:HG22	1:A:8:ILE:N	0.50	2.22	16	1
1:A:3:ALA:HB3	1:A:8:ILE:CG1	0.50	2.37	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:THR:HG22	1:A:8:ILE:HG12	0.48	1.84	23	1
1:A:5:ILE:HD13	1:A:6:PRO:N	0.48	2.24	23	1
1:A:5:ILE:HD12	1:A:7:PRO:CD	0.47	2.40	21	1
1:A:5:ILE:HA	1:A:6:PRO:C	0.46	2.31	12	17
1:A:8:ILE:O	1:A:8:ILE:CG2	0.45	2.64	24	1
1:A:8:ILE:O	1:A:8:ILE:HG23	0.43	2.11	19	1
1:A:3:ALA:HB3	1:A:8:ILE:HG12	0.43	1.90	17	1
1:A:4:SER:O	1:A:6:PRO:O	0.42	2.38	9	1
1:A:2:THR:CG2	1:A:3:ALA:N	0.42	2.83	22	1
1:A:8:ILE:O	1:A:8:ILE:HG22	0.41	2.15	22	1
1:A:5:ILE:O	1:A:5:ILE:HG23	0.40	2.16	24	1
1:A:4:SER:O	1:A:5:ILE:HD13	0.40	2.17	3	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	9/14 (64%)	8±1 (87±8%)	1±1 (12±9%)	0±0 (1±3%)	21	69
All	All	216/336 (64%)	187 (87%)	27 (12%)	2 (1%)	21	69

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	4	SER	2

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	10/10 (100%)	9±1 (90±10%)	1±1 (10±10%)	11	56
All	All	240/240 (100%)	216 (90%)	24 (10%)	11	56

All 6 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	8	ILE	12
1	A	5	ILE	4
1	A	14	ARG	4
1	A	4	SER	2
1	A	10	HIS	1
1	A	2	THR	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](#)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	E9M	A	13	1	14,16,17	0.69±0.01	0±0 (0±0%)
1	MMO	A	12	1	10,11,12	0.41±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	E9M	A	13	1	15,21,23	0.97±0.01	0±0 (0±0%)
1	MMO	A	12	1	8,12,14	0.86±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MMO	A	12	1	-	0±0,8,11,13	-
1	E9M	A	13	1	-	0±0,4,8,10	0±0,2,2,2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 71% for the well-defined parts and 71% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: AZ4_shifts.tbl

7.1.1 Bookkeeping i

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

Total number of shifts	135
Number of shifts mapped to atoms	135
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 i

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

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 71%, i.e. 101 atoms were assigned a chemical shift out of a possible 142. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	37/51 (73%)	19/20 (95%)	9/22 (41%)	9/9 (100%)
Sidechain	62/84 (74%)	37/56 (66%)	24/25 (96%)	1/3 (33%)
Aromatic	2/7 (29%)	2/4 (50%)	0/2 (0%)	0/1 (0%)
Overall	101/142 (71%)	58/80 (72%)	33/49 (67%)	10/13 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 101 atoms were assigned a chemical shift out of a possible 142. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	37/51 (73%)	19/20 (95%)	9/22 (41%)	9/9 (100%)
Sidechain	62/84 (74%)	37/56 (66%)	24/25 (96%)	1/3 (33%)
Aromatic	2/7 (29%)	2/4 (50%)	0/2 (0%)	0/1 (0%)
Overall	101/142 (71%)	58/80 (72%)	33/49 (67%)	10/13 (77%)

7.1.4 Statistically unusual chemical shifts [i](#)

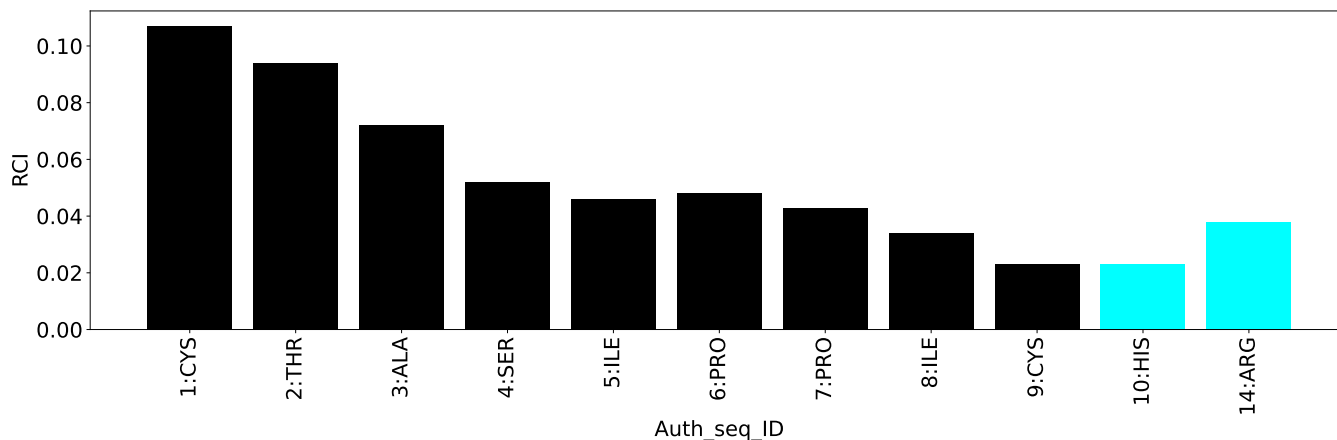
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	14	ARG	NE	119.26	76.53 – 92.65	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:



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	135
Intra-residue ($ i-j =0$)	48
Sequential ($ i-j =1$)	55
Medium range ($ i-j >1$ and $ i-j <5$)	20
Long range ($ i-j \geq 5$)	10
Inter-chain	0
Hydrogen bond restraints	2
Disulfide bond restraints	0
Total dihedral-angle restraints	13
Number of unmapped restraints	37
Number of restraints per residue	10.6
Number of long range restraints per residue ¹	0.9

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)	3.3	0.2
0.2-0.5 (Medium)	3.5	0.5
>0.5 (Large)	2.1	1.12

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)	1.0	4.5
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

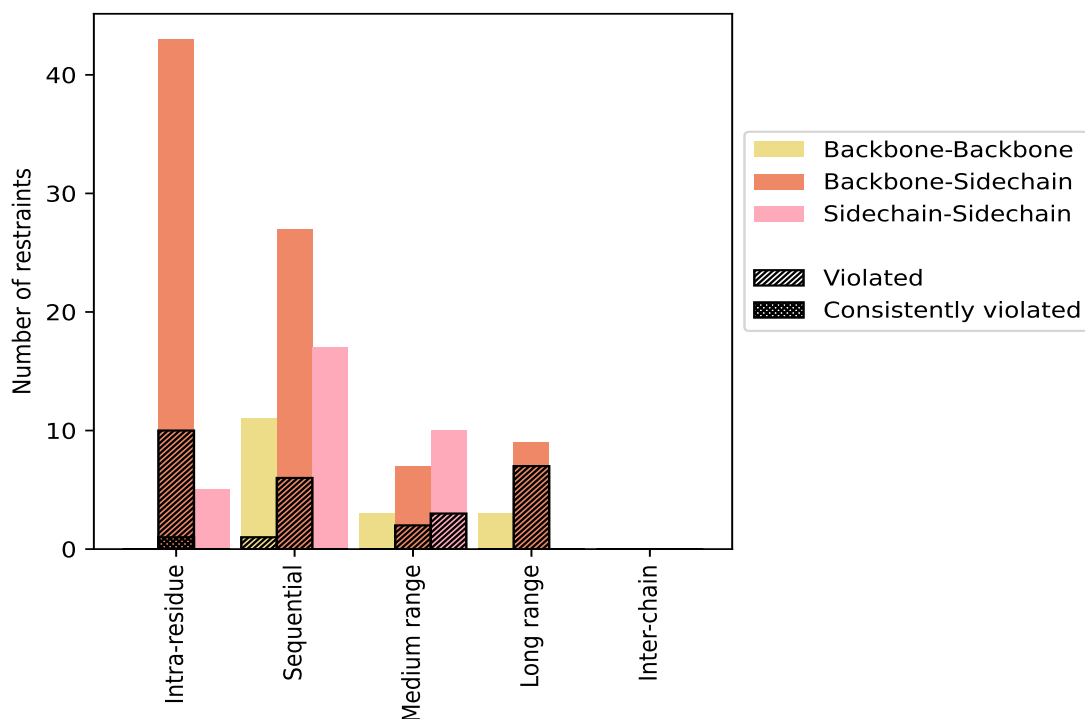
9.1 Summary of distance violations

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 ($i-j =0$)	48	35.6	10	20.8	7.4	1	2.1	0.7
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	43	31.9	10	23.3	7.4	1	2.3	0.7
Sidechain-Sidechain	5	3.7	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	55	40.7	7	12.7	5.2	0	0.0	0.0
Backbone-Backbone	11	8.1	1	9.1	0.7	0	0.0	0.0
Backbone-Sidechain	27	20.0	6	22.2	4.4	0	0.0	0.0
Sidechain-Sidechain	17	12.6	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	20	14.8	5	25.0	3.7	0	0.0	0.0
Backbone-Backbone	3	2.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	7	5.2	2	28.6	1.5	0	0.0	0.0
Sidechain-Sidechain	10	7.4	3	30.0	2.2	0	0.0	0.0
Long range ($i-j \geq 5$)	10	7.4	6	60.0	4.4	0	0.0	0.0
Backbone-Backbone	3	2.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	7	5.2	6	85.7	4.4	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	2	1.5	1	50.0	0.7	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	135	100.0	29	21.5	21.5	1	0.7	0.7
Backbone-Backbone	17	12.6	1	5.9	0.7	0	0.0	0.0
Backbone-Sidechain	86	63.7	25	29.1	18.5	1	1.2	0.7
Sidechain-Sidechain	32	23.7	3	9.4	2.2	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 disulfid 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	4	3	2	0	0	9	0.27	0.63	0.17	0.19
2	5	1	2	0	0	8	0.32	0.61	0.17	0.26
3	4	1	3	1	0	9	0.39	0.73	0.21	0.27
4	4	3	2	1	0	10	0.34	0.72	0.21	0.25
5	4	1	2	2	0	9	0.42	0.84	0.24	0.33
6	2	2	1	2	0	7	0.35	0.73	0.24	0.33
7	6	1	2	2	0	11	0.37	0.84	0.22	0.29
8	4	3	2	2	0	11	0.25	0.58	0.16	0.15
9	2	3	1	2	0	8	0.29	0.71	0.21	0.2
10	3	1	2	2	0	8	0.26	0.41	0.11	0.21
11	3	2	1	1	0	7	0.28	0.71	0.2	0.17

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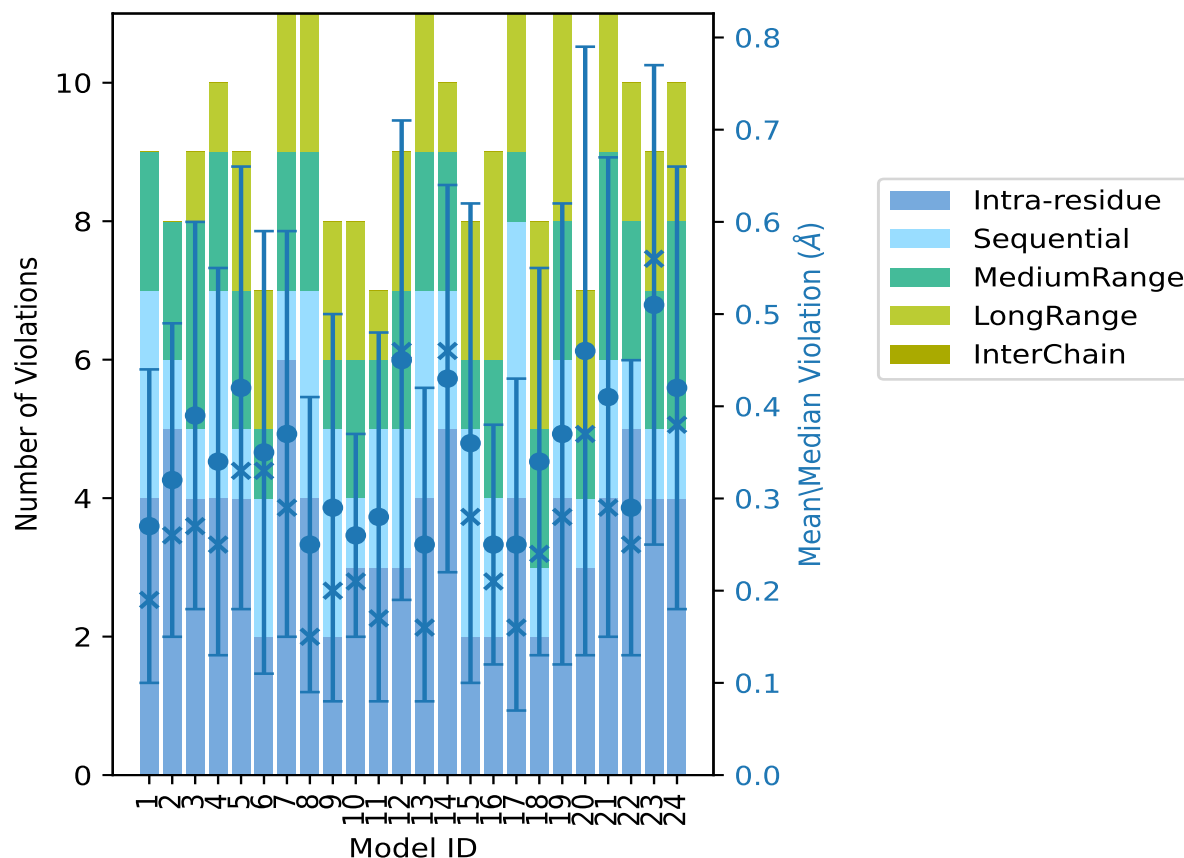
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	3	2	2	2	0	9	0.45	0.89	0.26	0.46
13	4	3	2	2	0	11	0.25	0.58	0.17	0.16
14	5	2	2	1	0	10	0.43	0.71	0.21	0.46
15	2	3	1	2	0	8	0.36	0.82	0.26	0.28
16	2	2	2	3	0	9	0.25	0.56	0.13	0.21
17	4	4	1	2	0	11	0.25	0.73	0.18	0.16
18	2	1	2	3	0	8	0.34	0.82	0.21	0.24
19	4	2	2	3	0	11	0.37	0.97	0.25	0.28
20	3	1	1	2	0	7	0.46	1.12	0.33	0.37
21	4	2	3	2	0	11	0.41	0.9	0.26	0.29
22	5	1	2	2	0	10	0.29	0.66	0.16	0.25
23	4	1	2	2	0	9	0.51	0.89	0.26	0.56
24	4	1	3	2	0	10	0.42	0.77	0.24	0.38

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, 105(IR:38, SQ:48, MR:15, LR:4, IC:0) restraints are not violated in the ensemble.

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

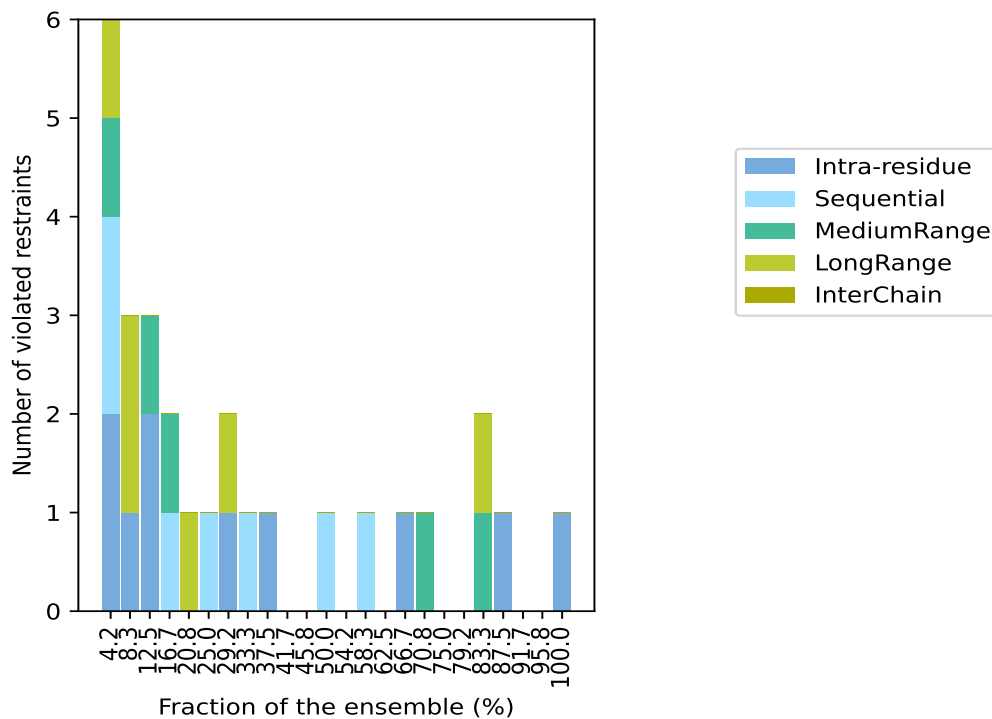
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	0	0	1	0	2	7	29.2
0	1	0	0	0	1	8	33.3
1	0	0	0	0	1	9	37.5
0	0	0	0	0	0	10	41.7
0	0	0	0	0	0	11	45.8
0	1	0	0	0	1	12	50.0
0	0	0	0	0	0	13	54.2
0	1	0	0	0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

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

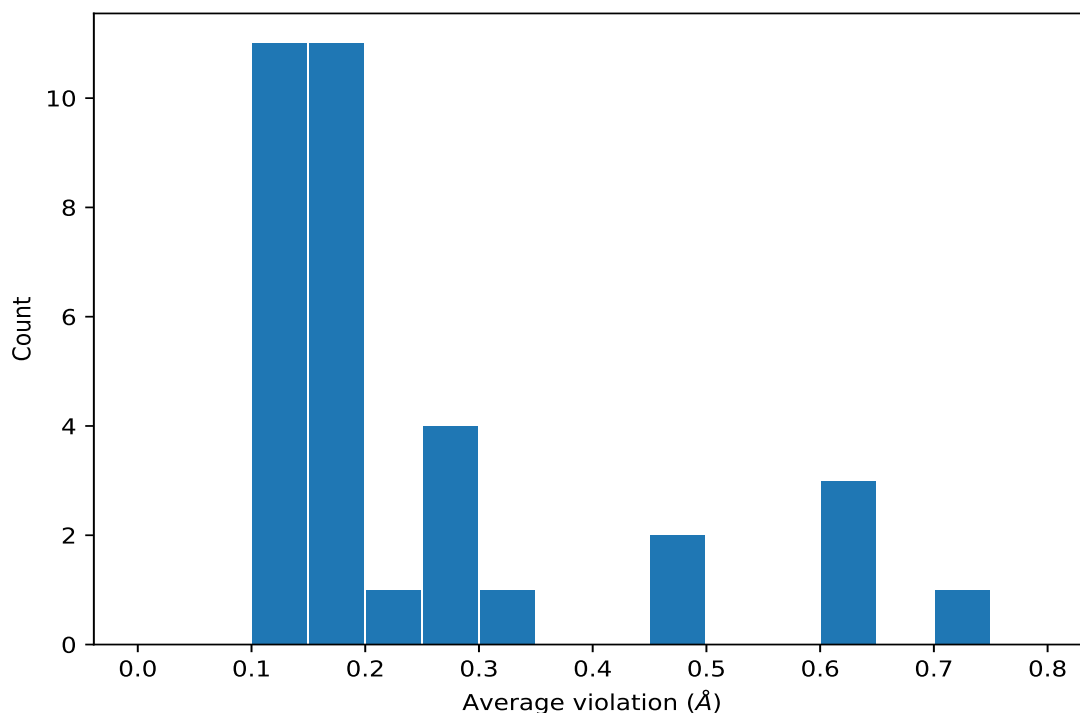
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	24	0.46	0.08	0.44
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	21	0.26	0.06	0.26
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	20	0.63	0.15	0.7
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	20	0.63	0.15	0.7
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	20	0.61	0.29	0.67
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	17	0.45	0.18	0.46
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	16	0.3	0.18	0.24
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	14	0.17	0.08	0.12
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	12	0.17	0.06	0.15
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	12	0.17	0.06	0.15
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	12	0.17	0.06	0.15
(1,54)	1:14:A:ARG:H	1:14:A:ARG:HG3	9	0.25	0.11	0.19
(1,100)	1:7:A:PRO:HB3	1:8:A:ILE:H	8	0.19	0.05	0.16
(1,101)	1:8:A:ILE:H	1:8:A:ILE:HG13	7	0.72	0.12	0.73
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG21	7	0.17	0.06	0.14
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG22	7	0.17	0.06	0.14

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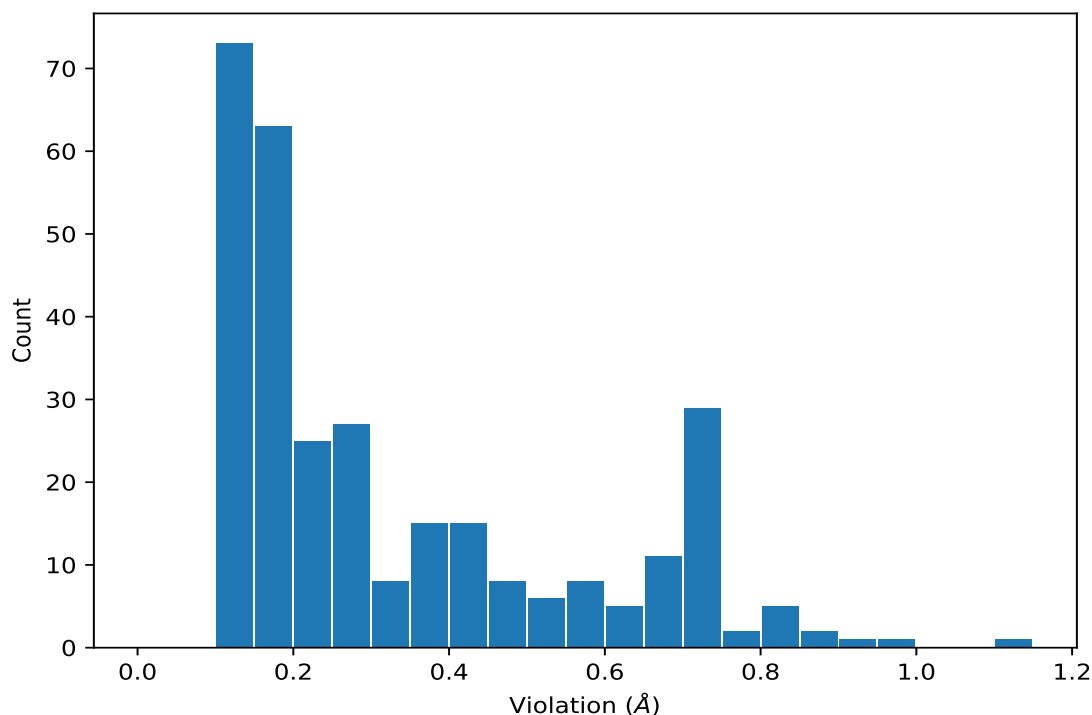
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG23	7	0.17	0.06	0.14
(1,96)	1:4:A:SER:HB3	1:5:A:ILE:H	6	0.32	0.16	0.29
(2,1)	1:2:A:THR:H	1:8:A:ILE:O	6	0.13	0.03	0.14
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD11	5	0.15	0.03	0.16
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD12	5	0.15	0.03	0.16
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD13	5	0.15	0.03	0.16
(1,25)	1:5:A:ILE:HB	1:7:A:PRO:HD3	4	0.15	0.03	0.14
(1,104)	1:9:A:CYS:HB3	1:10:A:HIS:H	4	0.15	0.02	0.14
(1,108)	1:9:A:CYS:HB3	1:13:A:E9M:HE3	3	0.3	0.15	0.28
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD11	3	0.16	0.0	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD12	3	0.16	0.0	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD13	3	0.16	0.0	0.16
(1,102)	1:8:A:ILE:HA	1:8:A:ILE:HG13	3	0.14	0.01	0.13
(1,92)	1:1:A:CYS:HA	1:9:A:CYS:HB3	2	0.2	0.02	0.2
(1,63)	1:14:A:ARG:HA	1:14:A:ARG:HG3	2	0.14	0.03	0.14
(1,62)	1:2:A:THR:H	1:8:A:ILE:HD11	2	0.11	0.0	0.11
(1,62)	1:2:A:THR:H	1:8:A:ILE:HD12	2	0.11	0.0	0.11
(1,62)	1:2:A:THR:H	1:8:A:ILE:HD13	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	20	1.12
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	19	0.97
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	21	0.9
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	12	0.89
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	23	0.89
(1,101)	1:8:A:ILE:H	1:8:A:ILE:HG13	5	0.84
(1,101)	1:8:A:ILE:H	1:8:A:ILE:HG13	7	0.84
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	15	0.82
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	18	0.82
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	23	0.8
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	24	0.77
(1,101)	1:8:A:ILE:H	1:8:A:ILE:HG13	21	0.76
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	6	0.73
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	6	0.73
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	15	0.73
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	15	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	17	0.73
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	17	0.73
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	19	0.73
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	19	0.73
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	21	0.73
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	21	0.73
(1,101)	1:8:A:ILE:H	1:8:A:ILE:HG13	3	0.73
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	4	0.72
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	5	0.71
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	5	0.71
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	7	0.71
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	7	0.71
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	9	0.71
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	9	0.71
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	11	0.71
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	11	0.71
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	23	0.71
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	23	0.71
(1,101)	1:8:A:ILE:H	1:8:A:ILE:HG13	14	0.71
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	20	0.71
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	14	0.71
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	3	0.7
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	3	0.7
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	4	0.7
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	4	0.7
(1,101)	1:8:A:ILE:H	1:8:A:ILE:HG13	24	0.69
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	14	0.68
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	14	0.68
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	24	0.68
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	23	0.67
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	5	0.66
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	22	0.66
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	6	0.66
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	12	0.65
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	12	0.65
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	12	0.65
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	24	0.63
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	24	0.63
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	1	0.63
(1,96)	1:4:A:SER:HB3	1:5:A:ILE:H	12	0.62
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	2	0.61
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	8	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	8	0.58
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	2	0.58
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	13	0.58
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	13	0.56
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	13	0.56
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	16	0.56
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	23	0.56
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	14	0.54
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	18	0.54
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	14	0.51
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	1	0.5
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	3	0.5
(1,108)	1:9:A:CYS:HB3	1:13:A:E9M:HE3	21	0.5
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	3	0.49
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	9	0.48
(1,101)	1:8:A:ILE:H	1:8:A:ILE:HG13	19	0.47
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	8	0.47
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	12	0.46
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	21	0.46
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	7	0.45
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	19	0.45
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	5	0.44
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	20	0.44
(1,54)	1:14:A:ARG:H	1:14:A:ARG:HG3	7	0.44
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	7	0.42
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	4	0.42
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	10	0.41
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	17	0.41
(1,96)	1:4:A:SER:HB3	1:5:A:ILE:H	14	0.41
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	6	0.4
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	9	0.4
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	11	0.4
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	15	0.4
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	22	0.4
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	24	0.4
(1,54)	1:14:A:ARG:H	1:14:A:ARG:HG3	16	0.4
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	10	0.39
(1,2)	1:2:A:THR:H	1:2:A:THR:HG21	22	0.39
(1,2)	1:2:A:THR:H	1:2:A:THR:HG22	22	0.39
(1,2)	1:2:A:THR:H	1:2:A:THR:HG23	22	0.39
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	15	0.38
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	23	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	4	0.37
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	20	0.37
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	2	0.37
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	2	0.37
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	8	0.37
(1,103)	1:9:A:CYS:H	1:9:A:CYS:HB3	13	0.37
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	10	0.37
(1,96)	1:4:A:SER:HB3	1:5:A:ILE:H	17	0.36
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	24	0.35
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	8	0.34
(1,54)	1:14:A:ARG:H	1:14:A:ARG:HG3	6	0.33
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	5	0.33
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	5	0.33
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	5	0.33
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	23	0.32
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	1	0.3
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	1	0.3
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	19	0.29
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	18	0.29
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	21	0.29
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	7	0.29
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG21	22	0.29
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG22	22	0.29
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG23	22	0.29
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	11	0.28
(1,108)	1:9:A:CYS:HB3	1:13:A:E9M:HE3	19	0.28
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	7	0.28
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	7	0.28
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	7	0.28
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	1	0.27
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	9	0.27
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	17	0.27
(1,100)	1:7:A:PRO:HB3	1:8:A:ILE:H	18	0.27
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	2	0.27
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	12	0.27
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	3	0.27
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	2	0.26
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	3	0.26
(1,100)	1:7:A:PRO:HB3	1:8:A:ILE:H	22	0.26
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	16	0.26
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	12	0.25
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	3	0.25
(1,54)	1:14:A:ARG:H	1:14:A:ARG:HG3	4	0.25
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	20	0.24
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	21	0.24
(1,100)	1:7:A:PRO:HB3	1:8:A:ILE:H	19	0.24
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	4	0.24
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	8	0.24
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	13	0.24
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	14	0.24
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	22	0.24
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	5	0.23
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	10	0.23
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	5	0.23
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	21	0.23
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	17	0.23
(1,96)	1:4:A:SER:HB3	1:5:A:ILE:H	16	0.22
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	5	0.22
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG21	18	0.22
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG22	18	0.22
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG23	18	0.22
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE1	22	0.21
(1,107)	1:9:A:CYS:HB3	1:11:A:DPN:HE2	22	0.21
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	3	0.21
(1,92)	1:1:A:CYS:HA	1:9:A:CYS:HB3	16	0.21
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	13	0.2
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	14	0.2
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	16	0.2
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	10	0.19
(1,96)	1:4:A:SER:HB3	1:5:A:ILE:H	1	0.19
(1,95)	1:4:A:SER:H	1:4:A:SER:HB3	7	0.19
(1,54)	1:14:A:ARG:H	1:14:A:ARG:HG3	2	0.19
(1,54)	1:14:A:ARG:H	1:14:A:ARG:HG3	14	0.19
(1,25)	1:5:A:ILE:HB	1:7:A:PRO:HD3	18	0.19
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	24	0.19
(1,92)	1:1:A:CYS:HA	1:9:A:CYS:HB3	18	0.18
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	7	0.17
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	18	0.17
(1,104)	1:9:A:CYS:HB3	1:10:A:HIS:H	16	0.17
(1,63)	1:14:A:ARG:HA	1:14:A:ARG:HG3	24	0.17
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD11	7	0.17
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD12	7	0.17
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD13	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD11	19	0.17
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD12	19	0.17
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD13	19	0.17
(1,54)	1:14:A:ARG:H	1:14:A:ARG:HG3	11	0.17
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	15	0.17
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	15	0.17
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	15	0.17
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	21	0.17
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	21	0.17
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	21	0.17
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	19	0.17
(2,1)	1:2:A:THR:H	1:8:A:ILE:O	19	0.16
(2,1)	1:2:A:THR:H	1:8:A:ILE:O	21	0.16
(1,133)	1:14:A:ARG:H	1:14:A:ARG:HB3	22	0.16
(1,100)	1:7:A:PRO:HB3	1:8:A:ILE:H	13	0.16
(1,100)	1:7:A:PRO:HB3	1:8:A:ILE:H	14	0.16
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	1	0.16
(1,94)	1:2:A:THR:H	1:7:A:PRO:HB3	10	0.16
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD11	24	0.16
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD12	24	0.16
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD13	24	0.16
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG21	20	0.16
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG22	20	0.16
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG23	20	0.16
(1,54)	1:14:A:ARG:H	1:14:A:ARG:HG3	19	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD11	1	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD12	1	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD13	1	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD11	2	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD12	2	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD13	2	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD11	23	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD12	23	0.16
(1,16)	1:8:A:ILE:HA	1:8:A:ILE:HD13	23	0.16
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	11	0.16
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	11	0.16
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	11	0.16
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	17	0.16
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	17	0.16
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	17	0.16
(2,1)	1:2:A:THR:H	1:8:A:ILE:O	15	0.15
(1,102)	1:8:A:ILE:HA	1:8:A:ILE:HG13	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,100)	1:7:A:PRO:HB3	1:8:A:ILE:H	4	0.15
(1,100)	1:7:A:PRO:HB3	1:8:A:ILE:H	8	0.15
(1,97)	1:5:A:ILE:H	1:5:A:ILE:HG13	7	0.15
(1,96)	1:4:A:SER:HB3	1:5:A:ILE:H	15	0.15
(1,93)	1:1:A:CYS:HB3	1:2:A:THR:H	20	0.15
(1,25)	1:5:A:ILE:HB	1:7:A:PRO:HD3	10	0.15
(1,104)	1:9:A:CYS:HB3	1:10:A:HIS:H	1	0.14
(1,104)	1:9:A:CYS:HB3	1:10:A:HIS:H	2	0.14
(1,100)	1:7:A:PRO:HB3	1:8:A:ILE:H	17	0.14
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG21	10	0.14
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG22	10	0.14
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG23	10	0.14
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG21	23	0.14
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG22	23	0.14
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG23	23	0.14
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	4	0.14
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	4	0.14
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	4	0.14
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	9	0.14
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	9	0.14
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	9	0.14
(2,1)	1:2:A:THR:H	1:8:A:ILE:O	11	0.13
(1,108)	1:9:A:CYS:HB3	1:13:A:E9M:HE3	13	0.13
(1,104)	1:9:A:CYS:HB3	1:10:A:HIS:H	12	0.13
(1,102)	1:8:A:ILE:HA	1:8:A:ILE:HG13	8	0.13
(1,102)	1:8:A:ILE:HA	1:8:A:ILE:HG13	13	0.13
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	6	0.13
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	6	0.13
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	6	0.13
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	8	0.13
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	8	0.13
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	8	0.13
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	13	0.13
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	13	0.13
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	13	0.13
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	6	0.13
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	8	0.13
(1,77)	1:2:A:THR:HG21	1:8:A:ILE:H	9	0.12
(1,77)	1:2:A:THR:HG22	1:8:A:ILE:H	9	0.12
(1,77)	1:2:A:THR:HG23	1:8:A:ILE:H	9	0.12
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD11	22	0.12
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD12	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD13	22	0.12
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG21	12	0.12
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG22	12	0.12
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG23	12	0.12
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG21	16	0.12
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG22	16	0.12
(1,55)	1:3:A:ALA:H	1:8:A:ILE:HG23	16	0.12
(1,54)	1:14:A:ARG:H	1:14:A:ARG:HG3	22	0.12
(1,25)	1:5:A:ILE:HB	1:7:A:PRO:HD3	3	0.12
(1,25)	1:5:A:ILE:HB	1:7:A:PRO:HD3	16	0.12
(1,11)	1:2:A:THR:HG21	1:3:A:ALA:H	1	0.12
(1,11)	1:2:A:THR:HG22	1:3:A:ALA:H	1	0.12
(1,11)	1:2:A:THR:HG23	1:3:A:ALA:H	1	0.12
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	4	0.12
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	9	0.12
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	13	0.12
(1,110)	1:10:A:HIS:H	1:14:A:ARG:HB3	8	0.11
(1,63)	1:14:A:ARG:HA	1:14:A:ARG:HG3	17	0.11
(1,62)	1:2:A:THR:H	1:8:A:ILE:HD11	8	0.11
(1,62)	1:2:A:THR:H	1:8:A:ILE:HD12	8	0.11
(1,62)	1:2:A:THR:H	1:8:A:ILE:HD13	8	0.11
(1,62)	1:2:A:THR:H	1:8:A:ILE:HD11	13	0.11
(1,62)	1:2:A:THR:H	1:8:A:ILE:HD12	13	0.11
(1,62)	1:2:A:THR:H	1:8:A:ILE:HD13	13	0.11
(1,58)	1:10:A:HIS:H	1:14:A:ARG:HB3	24	0.11
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD11	5	0.11
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD12	5	0.11
(1,56)	1:3:A:ALA:H	1:8:A:ILE:HD13	5	0.11
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	11	0.11
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	17	0.11
(2,1)	1:2:A:THR:H	1:8:A:ILE:O	6	0.1
(2,1)	1:2:A:THR:H	1:8:A:ILE:O	17	0.1
(1,40)	1:8:A:ILE:HD11	1:9:A:CYS:H	9	0.1
(1,40)	1:8:A:ILE:HD12	1:9:A:CYS:H	9	0.1
(1,40)	1:8:A:ILE:HD13	1:9:A:CYS:H	9	0.1
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	15	0.1
(1,10)	1:2:A:THR:HA	1:3:A:ALA:H	21	0.1

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

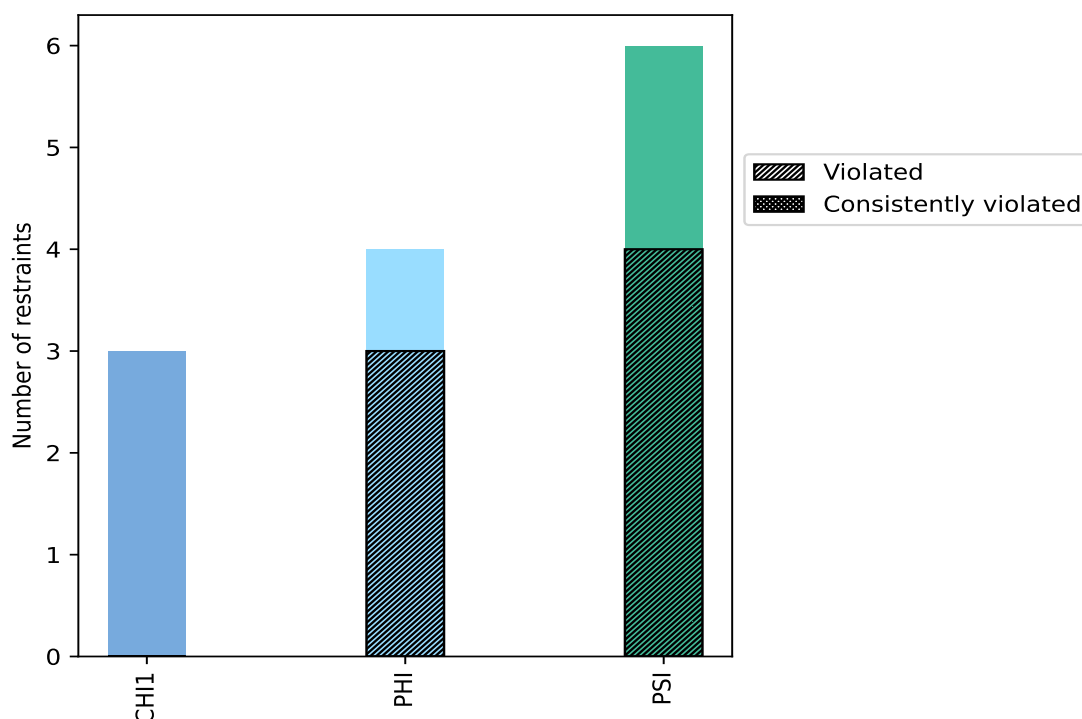
10.1 Summary of dihedral-angle violations [i](#)

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
CHI1	3	23.1	0	0.0	0.0	0	0.0	0.0
PHI	4	30.8	3	75.0	23.1	0	0.0	0.0
PSI	6	46.2	4	66.7	30.8	0	0.0	0.0
Total	13	100.0	7	53.8	53.8	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 [i](#)



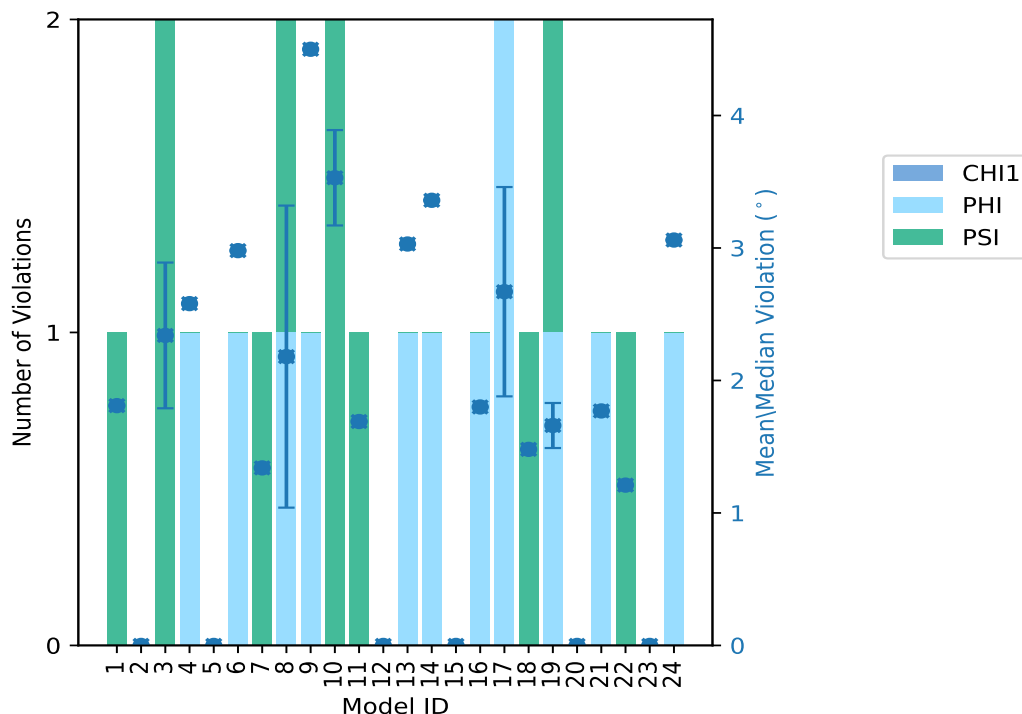
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	CHI1	PHI	PSI	Total				
1	0	0	1	1	1.81	1.81	0.0	1.81
2	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	2	2	2.34	2.9	0.55	2.34
4	0	1	0	1	2.58	2.58	0.0	2.58
5	0	0	0	0	0.0	0.0	0.0	0.0
6	0	1	0	1	2.98	2.98	0.0	2.98
7	0	0	1	1	1.34	1.34	0.0	1.34
8	0	1	1	2	2.18	3.32	1.14	2.18
9	0	1	0	1	4.5	4.5	0.0	4.5
10	0	0	2	2	3.53	3.89	0.36	3.53
11	0	0	1	1	1.69	1.69	0.0	1.69
12	0	0	0	0	0.0	0.0	0.0	0.0
13	0	1	0	1	3.03	3.03	0.0	3.03
14	0	1	0	1	3.36	3.36	0.0	3.36
15	0	0	0	0	0.0	0.0	0.0	0.0
16	0	1	0	1	1.8	1.8	0.0	1.8
17	0	2	0	2	2.67	3.46	0.79	2.67
18	0	0	1	1	1.48	1.48	0.0	1.48
19	0	1	1	2	1.66	1.83	0.17	1.66
20	0	0	0	0	0.0	0.0	0.0	0.0
21	0	1	0	1	1.77	1.77	0.0	1.77
22	0	0	1	1	1.21	1.21	0.0	1.21
23	0	0	0	0	0.0	0.0	0.0	0.0
24	0	1	0	1	3.06	3.06	0.0	3.06

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	
CHI1	PHI	PSI	Total	Count ¹	%
0	2	0	2	1	4.2
0	0	2	2	2	8.3
0	0	1	1	3	12.5
0	0	1	1	4	16.7
0	0	0	0	5	20.8
0	0	0	0	6	25.0
0	0	0	0	7	29.2
0	0	0	0	8	33.3
0	0	0	0	9	37.5
0	1	0	1	10	41.7
0	0	0	0	11	45.8

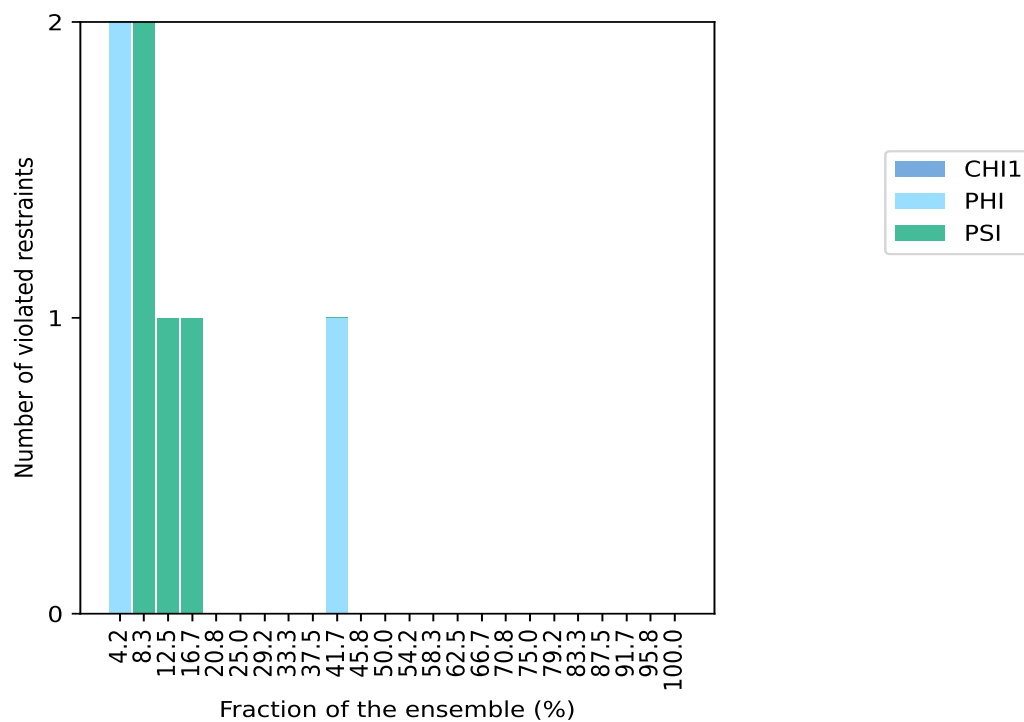
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Number of violated restraints				Fraction of the ensemble	
CHI1	PHI	PSI	Total	Count ¹	%
0	0	0	0	12	50.0
0	0	0	0	13	54.2
0	0	0	0	14	58.3
0	0	0	0	15	62.5
0	0	0	0	16	66.7
0	0	0	0	17	70.8
0	0	0	0	18	75.0
0	0	0	0	19	79.2
0	0	0	0	20	83.3
0	0	0	0	21	87.5
0	0	0	0	22	91.7
0	0	0	0	23	95.8
0	0	0	0	24	100.0

¹ Number of models with violations

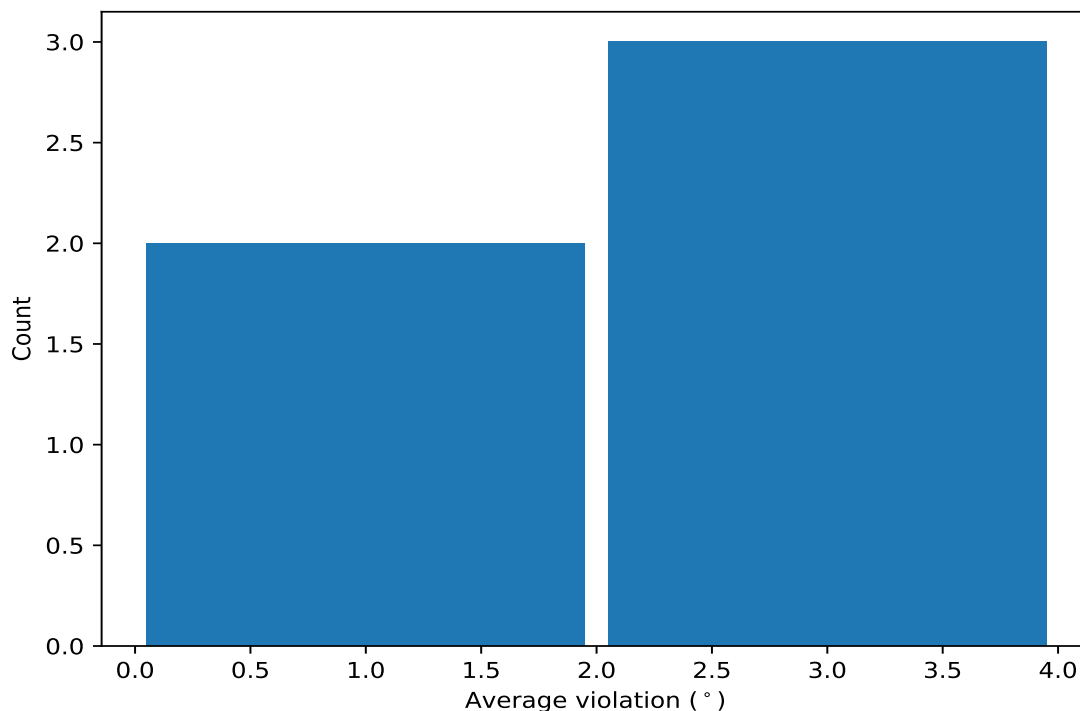
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

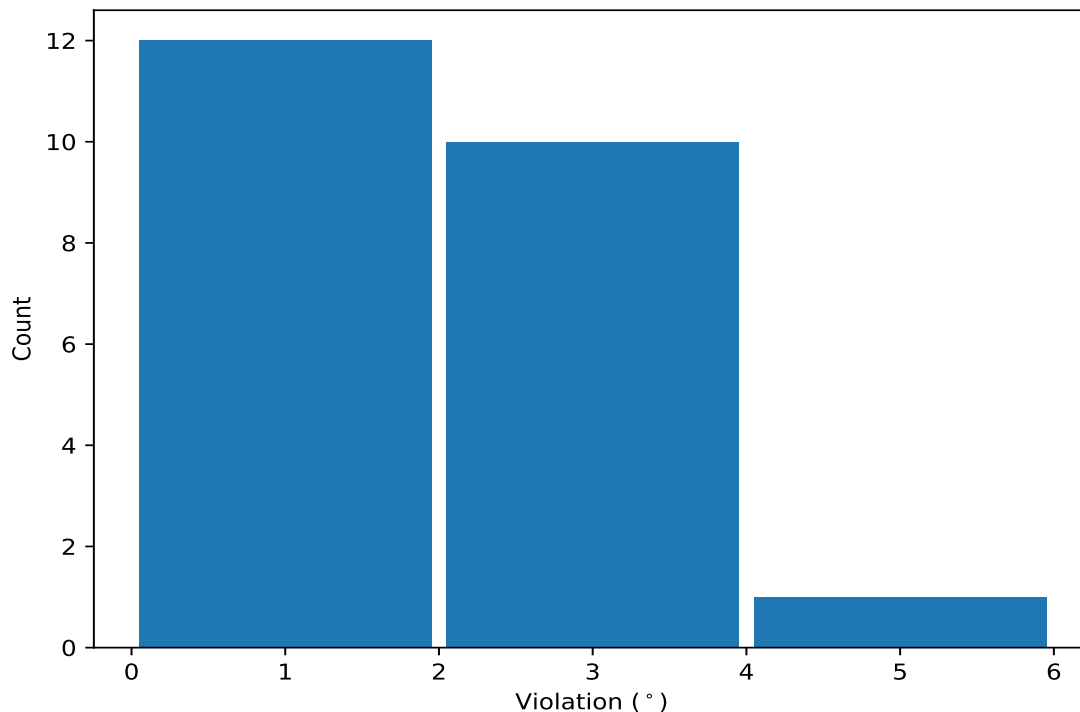
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	10	2.95	0.82	3.04
(1,5)	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	1:6:A:PRO:N	4	2.3	0.75	2.36
(1,3)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:ILE:N	3	2.46	1.01	1.79
(1,9)	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	1:9:A:CYS:N	2	1.44	0.4	1.44
(1,7)	1:7:A:PRO:N	1:7:A:PRO:CA	1:7:A:PRO:C	1:8:A:ILE:N	2	1.34	0.14	1.34

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 (°)
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	9	4.5
(1,3)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:ILE:N	10	3.89
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	17	3.46
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	14	3.36
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	8	3.32
(1,5)	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	1:6:A:PRO:N	10	3.16
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	24	3.06
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	13	3.03
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	6	2.98
(1,5)	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	1:6:A:PRO:N	3	2.9
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	4	2.58
(1,10)	1:8:A:ILE:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	17	1.88
(1,9)	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	1:9:A:CYS:N	19	1.83
(1,5)	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	1:6:A:PRO:N	1	1.81

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:7:A:PRO:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	16	1.8
(1,3)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:ILE:N	3	1.79
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	21	1.77
(1,3)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:ILE:N	11	1.69
(1,4)	1:4:A:SER:C	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	19	1.49
(1,7)	1:7:A:PRO:N	1:7:A:PRO:CA	1:7:A:PRO:C	1:8:A:ILE:N	18	1.48
(1,5)	1:5:A:ILE:N	1:5:A:ILE:CA	1:5:A:ILE:C	1:6:A:PRO:N	7	1.34
(1,7)	1:7:A:PRO:N	1:7:A:PRO:CA	1:7:A:PRO:C	1:8:A:ILE:N	22	1.21
(1,9)	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	1:9:A:CYS:N	8	1.04