wwPDB NMR Structure Validation Summary Report (i)

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Title	:	Bam_5924 docking domain
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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

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

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

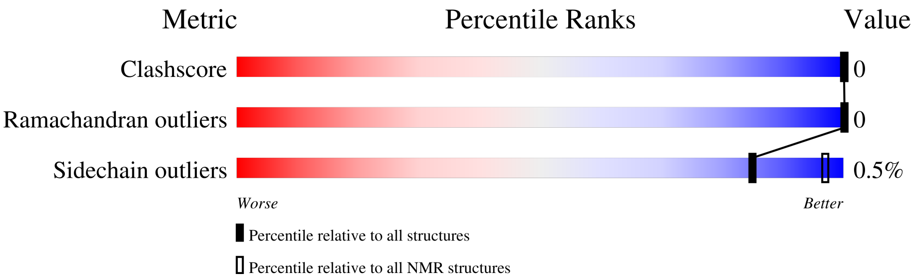
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 92%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	45	62% 38%
1	B	45	58% 42%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:14-A:41, B:115-B:140 (54)	0.30	10

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

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

The models can be grouped into 5 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1424 atoms, of which 722 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Beta-ketoacyl synthase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	45	712	216	361	64	69	2	0
1	B	45	712	216	361	64	69	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q0B304
A	2	PRO	-	expression tag	UNP Q0B304
A	3	GLY	-	expression tag	UNP Q0B304
A	4	SER	-	expression tag	UNP Q0B304
B	101	GLY	-	expression tag	UNP Q0B304
B	102	PRO	-	expression tag	UNP Q0B304
B	103	GLY	-	expression tag	UNP Q0B304
B	104	SER	-	expression tag	UNP Q0B304

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: Beta-ketoacyl synthase

- Molecule 1: Beta-ketoacyl synthase

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: Beta-ketoacyl synthase

- Molecule 1: Beta-ketoacyl synthase

5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 25 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1136
Number of shifts mapped to atoms	1136
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.67±0.01	0±0/239 (0.0± 0.0%)	1.01±0.02	0±0/319 (0.1± 0.2%)
1	B	0.63±0.01	0±0/214 (0.0± 0.0%)	0.96±0.03	0±0/284 (0.1± 0.2%)
All	All	0.65	0/11325 (0.0%)	0.99	15/15075 (0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	121	ARG	NE-CZ-NH1	7.10	123.85	120.30	11	4
1	A	21	ARG	NE-CZ-NH1	7.03	123.82	120.30	6	6
1	A	24	ARG	NE-CZ-NH1	5.33	122.97	120.30	13	3
1	B	124	ARG	NE-CZ-NH1	5.30	122.95	120.30	14	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	11225	12250	12250	-

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	28/45 (62%)	28±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	B	26/45 (58%)	26±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1350/2250 (60%)	1350 (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	26/39 (67%)	26±0 (100±1%)	0±0 (0±1%)	91	98
1	B	24/39 (62%)	24±0 (99±2%)	0±0 (1±2%)	77	96
All	All	1250/1950 (64%)	1244 (100%)	6 (0%)	85	97

5 of 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	B	118	TYR	1
1	B	125	LEU	1
1	A	40	GLN	1
1	B	128	ASN	1
1	B	121	ARG	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	1136
Number of shifts mapped to atoms	1136
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	90	-0.40 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	82	0.03 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	84	0.73 ± 0.11	Should be applied
^{15}N	84	-0.11 ± 0.19	None needed (< 0.5 ppm)

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 92%, i.e. 758 atoms were assigned a chemical shift out of a possible 821. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	270/270 (100%)	108/108 (100%)	108/108 (100%)	54/54 (100%)
Sidechain	464/521 (89%)	316/336 (94%)	139/156 (89%)	9/29 (31%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	24/30 (80%)	14/14 (100%)	9/15 (60%)	1/1 (100%)
Overall	758/821 (92%)	438/458 (96%)	256/279 (92%)	64/84 (76%)

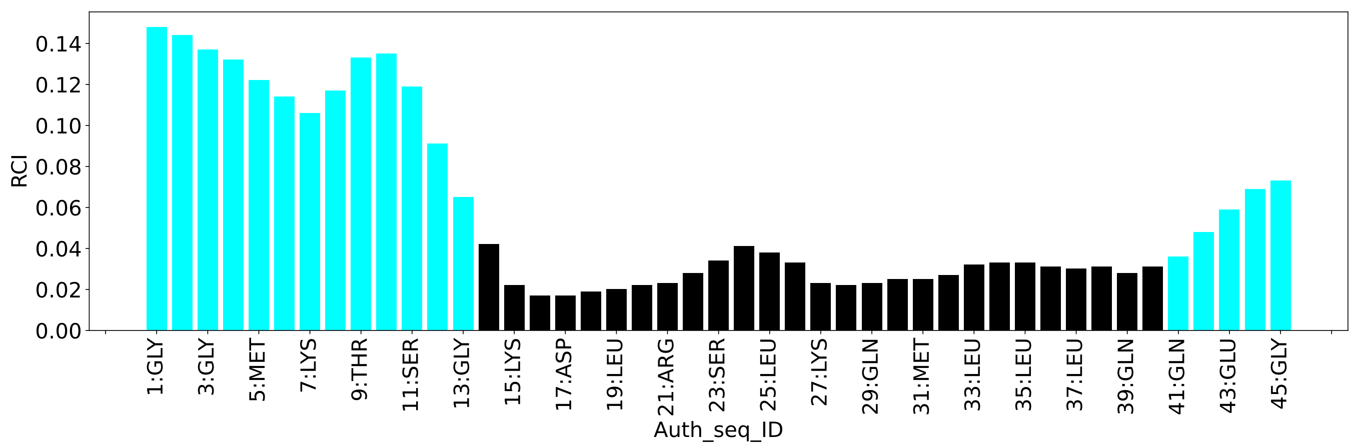
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

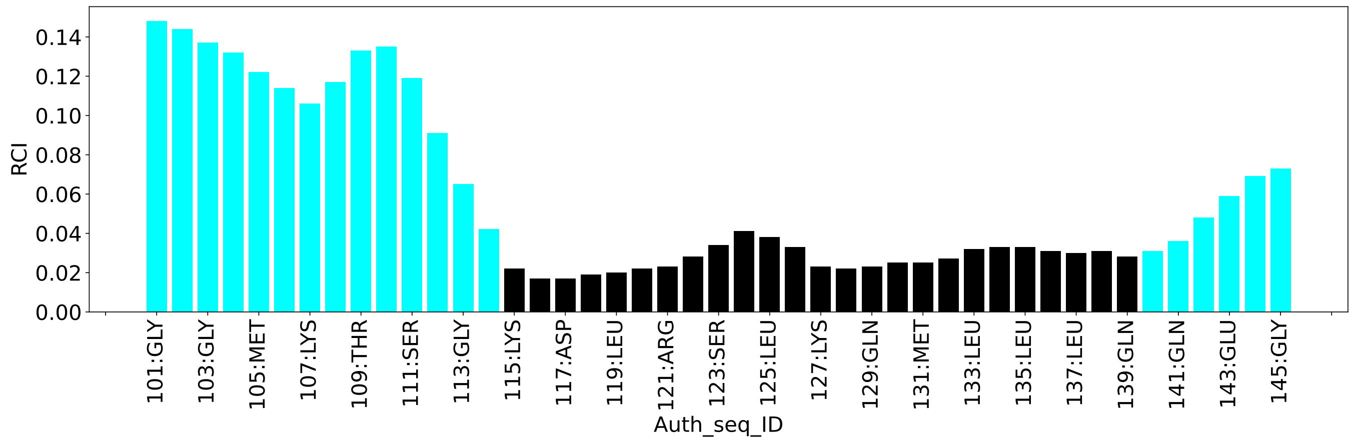
7.1.5 Random Coil Index (RCI) plots ⓘ

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:



Random coil index (RCI) for chain B:


RCI
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
101:GLY
103:GLY
105:MET
107:LYS
109:THR
111:SER
113:GLY
115:LYS
117:ASP
119:LEU
121:ARG
123:SER
125:LEU
127:LYS
129:GLN
131:MET
133:LEU
135:LEU
137:LEU
139:GLN
141:GLN
143:GLU
145:GLY
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	1812
Intra-residue (|i-j|=0)	519
Sequential (|i-j|=1)	466
Medium range (|i-j|>1 and |i-j|<5)	538
Long range (|i-j|≥5)	32
Inter-chain	257
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	116
Number of unmapped restraints	0
Number of restraints per residue	21.4
Number of long range restraints per residue[1]	0.4

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.1	0.15
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

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

Bins (°)	**Average number of violations per model**	**Max (°)**
1.0-10.0 (Small)	0.4	1.98
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

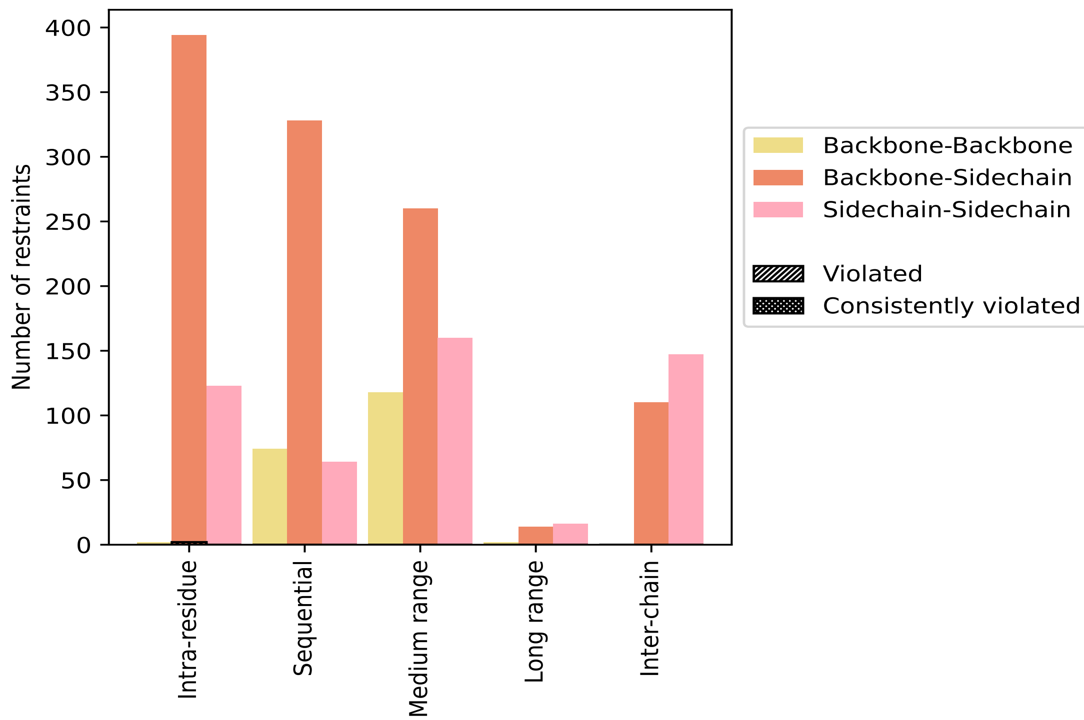
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	519	28.6	2	0.4	0.1	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	394	21.7	2	0.5	0.1	0	0.0	0.0
Sidechain-Sidechain	123	6.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	466	25.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	74	4.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	328	18.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	64	3.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	538	29.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	118	6.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	260	14.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	160	8.8	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	32	1.8	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	14	0.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	16	0.9	0	0.0	0.0	0	0.0	0.0
Inter-chain	257	14.2	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	110	6.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	147	8.1	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	1812	100.0	2	0.1	0.1	0	0.0	0.0
Backbone-Backbone	196	10.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1106	61.0	2	0.2	0.1	0	0.0	0.0
Sidechain-Sidechain	510	28.1	0	0.0	0.0	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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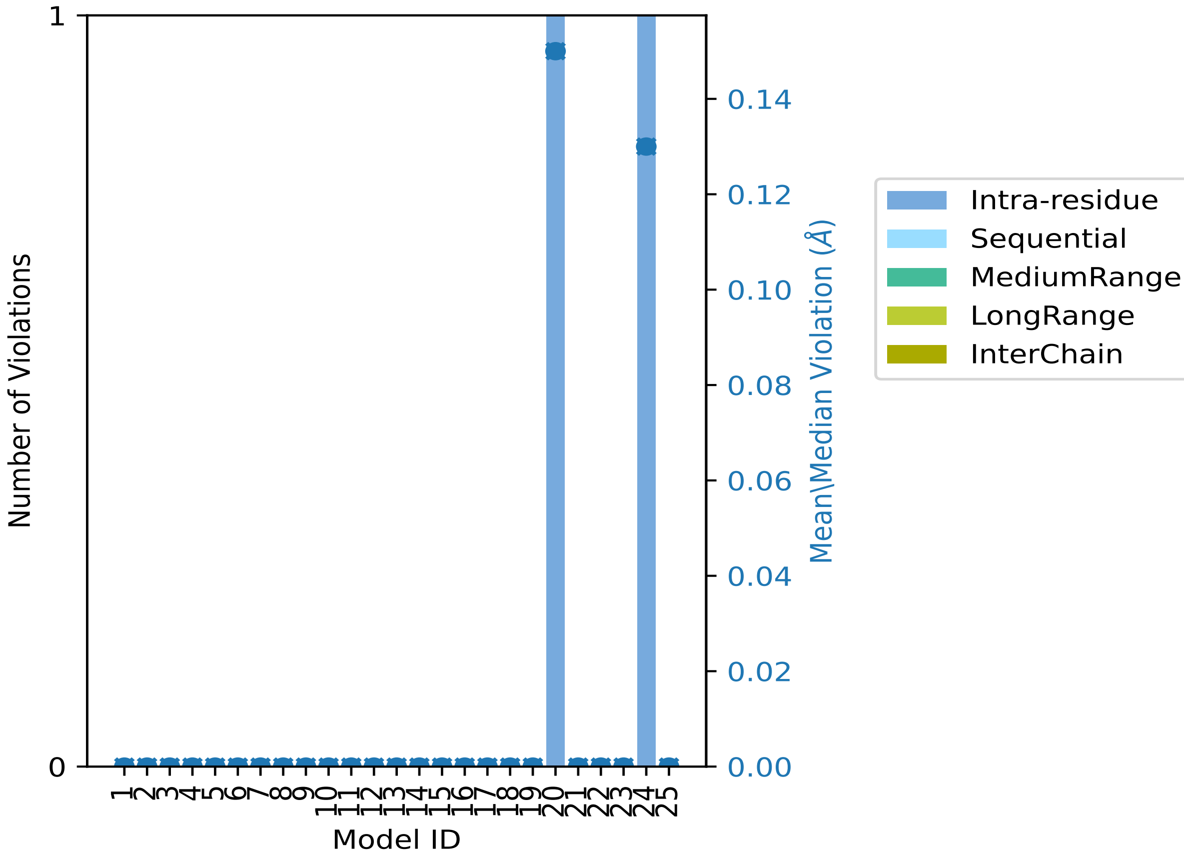
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	1	0	0	0	0	1	0.15	0.15	0.0	0.15
21	0	0	0	0	0	0	0.0	0.0	0.0	0.0
22	0	0	0	0	0	0	0.0	0.0	0.0	0.0
23	0	0	0	0	0	0	0.0	0.0	0.0	0.0
24	1	0	0	0	0	1	0.13	0.13	0.0	0.13
25	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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

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



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

9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1810(IR:517, SQ:466, MR:538, LR:32, IC:257) 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	0	0	0	0	2	1	4.0
0	0	0	0	0	0	2	8.0
0	0	0	0	0	0	3	12.0
0	0	0	0	0	0	4	16.0
0	0	0	0	0	0	5	20.0
0	0	0	0	0	0	6	24.0

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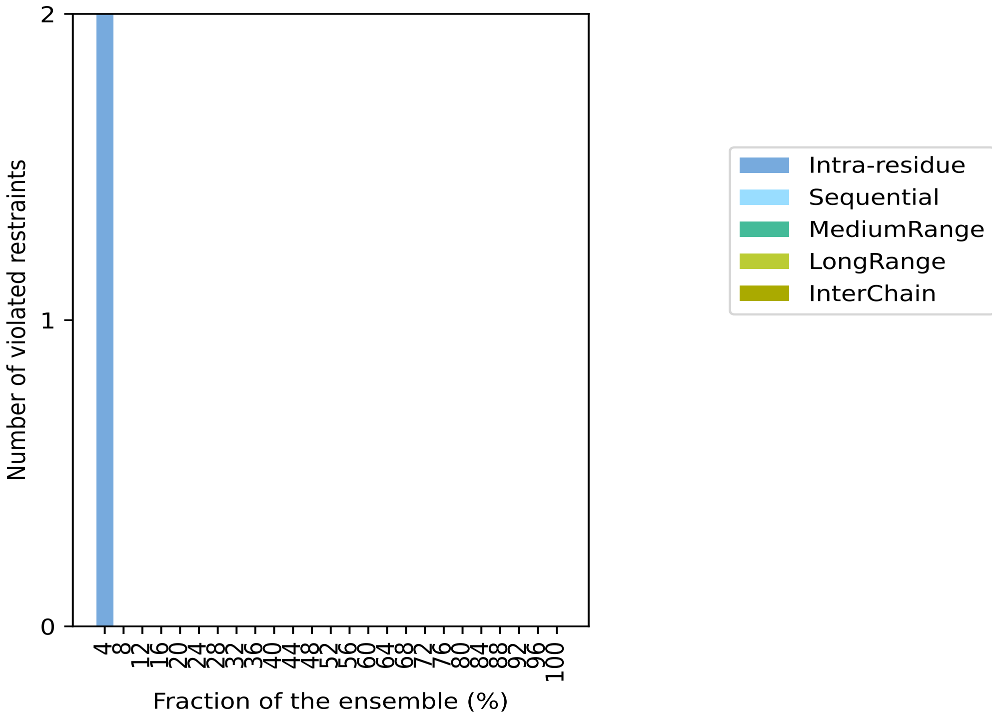
Number of violated restraints						**Fraction of the ensemble**	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	7	28.0
0	0	0	0	0	0	8	32.0
0	0	0	0	0	0	9	36.0
0	0	0	0	0	0	10	40.0
0	0	0	0	0	0	11	44.0
0	0	0	0	0	0	12	48.0
0	0	0	0	0	0	13	52.0
0	0	0	0	0	0	14	56.0
0	0	0	0	0	0	15	60.0
0	0	0	0	0	0	16	64.0
0	0	0	0	0	0	17	68.0
0	0	0	0	0	0	18	72.0
0	0	0	0	0	0	19	76.0
0	0	0	0	0	0	20	80.0
0	0	0	0	0	0	21	84.0
0	0	0	0	0	0	22	88.0
0	0	0	0	0	0	23	92.0
0	0	0	0	0	0	24	96.0
0	0	0	0	0	0	25	100.0

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

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



9.4 Most violated distance restraints in the ensemble (i)

No violations found

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.
Data insufficient to plot histogram

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)
(1,190)	1:121:B:ARG:HA	1:121:B:ARG:HD2	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:21:A:ARG:HA	1:21:A:ARG:HD2	24	0.13

10 Dihedral-angle violation analysis (i)

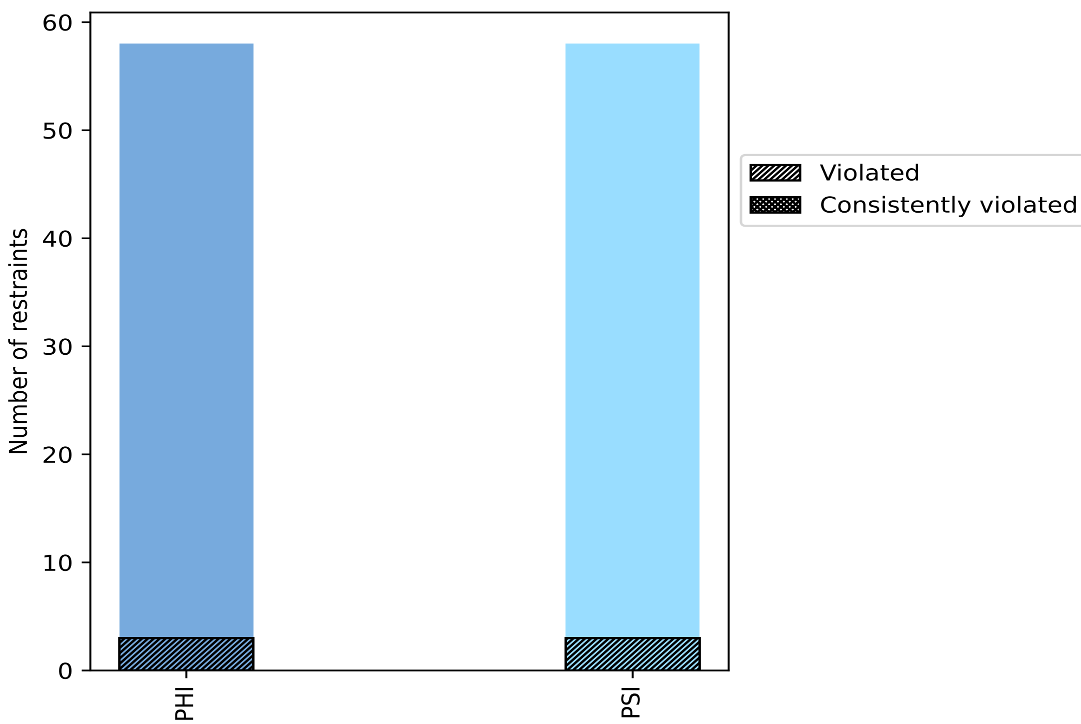
10.1 Summary of dihedral-angle violations (i)

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	58	50.0	3	5.2	2.6	0	0.0	0.0
PSI	58	50.0	3	5.2	2.6	0	0.0	0.0
Total	116	100.0	6	5.2	5.2	0	0.0	0.0

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

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



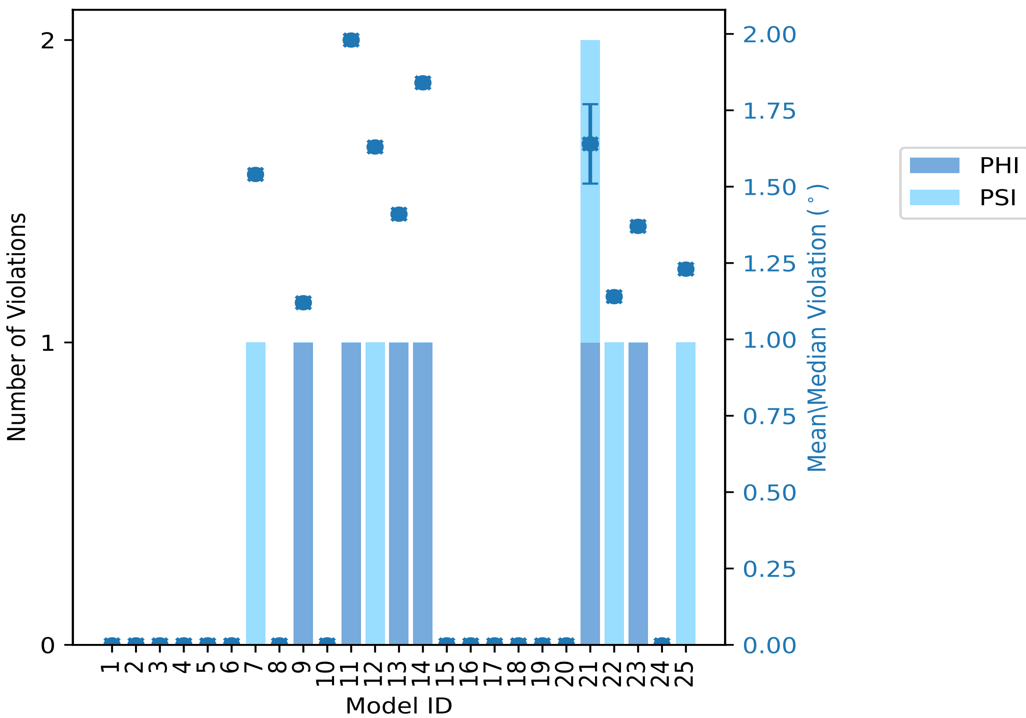
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	1	1	1.54	1.54	0.0	1.54
8	0	0	0	0.0	0.0	0.0	0.0
9	1	0	1	1.12	1.12	0.0	1.12
10	0	0	0	0.0	0.0	0.0	0.0
11	1	0	1	1.98	1.98	0.0	1.98
12	0	1	1	1.63	1.63	0.0	1.63
13	1	0	1	1.41	1.41	0.0	1.41
14	1	0	1	1.84	1.84	0.0	1.84
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0
21	1	1	2	1.64	1.77	0.13	1.64
22	0	1	1	1.14	1.14	0.0	1.14
23	1	0	1	1.37	1.37	0.0	1.37
24	0	0	0	0.0	0.0	0.0	0.0
25	0	1	1	1.23	1.23	0.0	1.23

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
1	1	2	1	4.0
1	2	3	2	8.0
1	0	1	3	12.0
0	0	0	4	16.0
0	0	0	5	20.0
0	0	0	6	24.0
0	0	0	7	28.0
0	0	0	8	32.0
0	0	0	9	36.0
0	0	0	10	40.0
0	0	0	11	44.0

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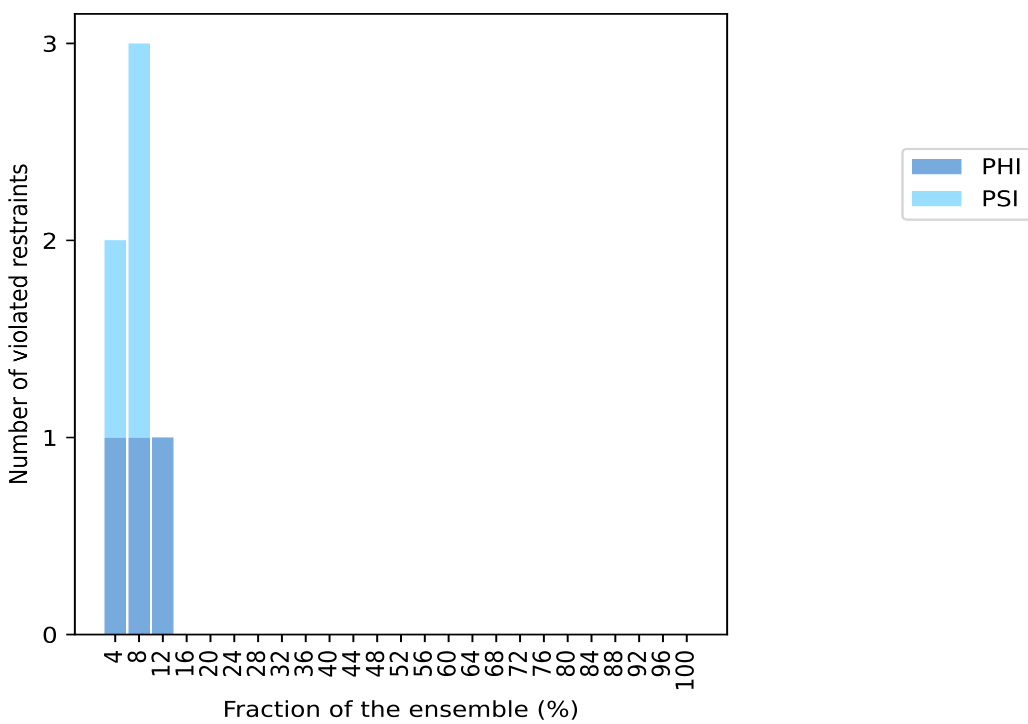
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	48.0
0	0	0	13	52.0
0	0	0	14	56.0
0	0	0	15	60.0
0	0	0	16	64.0
0	0	0	17	68.0
0	0	0	18	72.0
0	0	0	19	76.0
0	0	0	20	80.0
0	0	0	21	84.0
0	0	0	22	88.0
0	0	0	23	92.0
0	0	0	24	96.0
0	0	0	25	100.0

[1] Number of models with violations

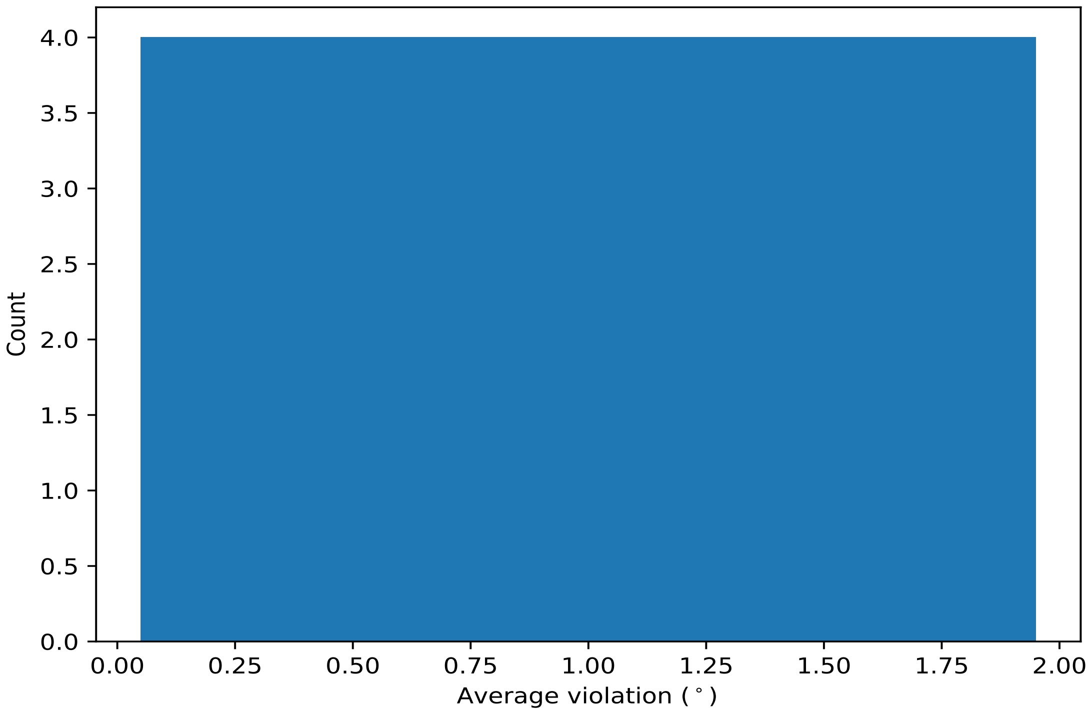
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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.

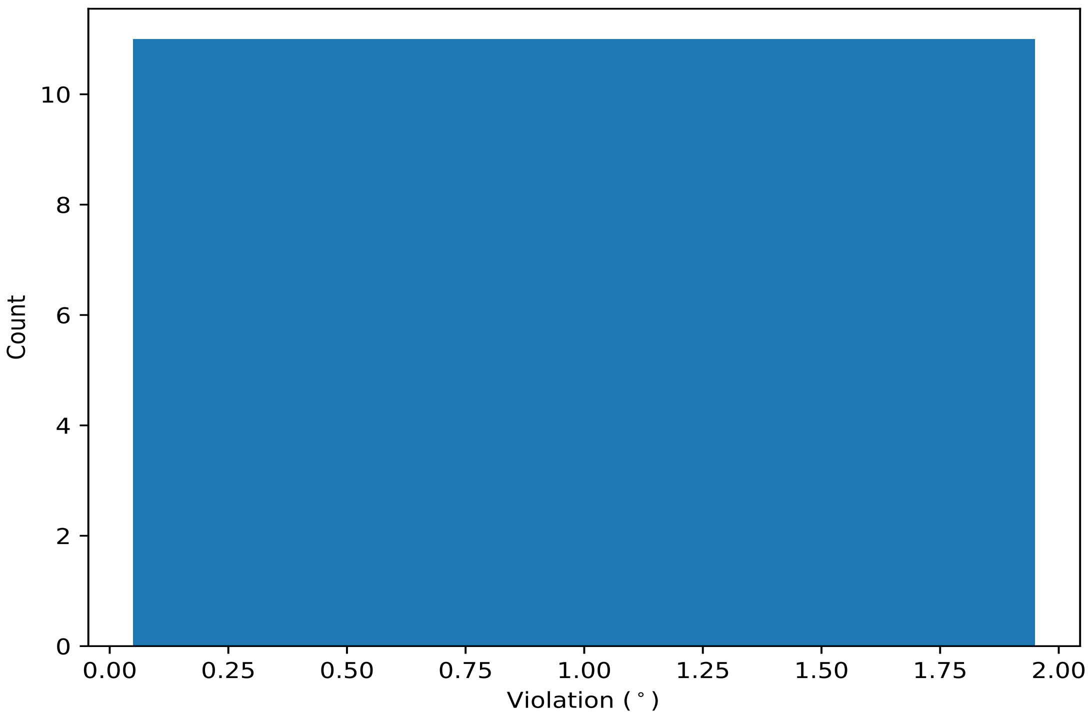
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,79)	1:123:B:SER:C	1:124:B:ARG:N	1:124:B:ARG:CA	1:124:B:ARG:C	3	1.33	0.16	1.37
(1,21)	1:23:A:SER:C	1:24:A:ARG:N	1:24:A:ARG:CA	1:24:A:ARG:C	2	1.69	0.29	1.69
(1,58)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:GLU:N	2	1.58	0.04	1.58
(1,22)	1:24:A:ARG:N	1:24:A:ARG:CA	1:24:A:ARG:C	1:25:A:LEU:N	2	1.18	0.05	1.18

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



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

The following table provides the list of violations for the 10 worst performing restraints, sorted by the violation 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 (°)
(1,21)	1:23:A:SER:C	1:24:A:ARG:N	1:24:A:ARG:CA	1:24:A:ARG:C	11	1.98
(1,73)	1:120:B:SER:C	1:121:B:ARG:N	1:121:B:ARG:CA	1:121:B:ARG:C	14	1.84
(1,116)	1:142:B:LEU:N	1:142:B:LEU:CA	1:142:B:LEU:C	1:143:B:GLU:N	21	1.77
(1,58)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:GLU:N	12	1.63
(1,58)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:GLU:N	7	1.54
(1,79)	1:123:B:SER:C	1:124:B:ARG:N	1:124:B:ARG:CA	1:124:B:ARG:C	21	1.51
(1,21)	1:23:A:SER:C	1:24:A:ARG:N	1:24:A:ARG:CA	1:24:A:ARG:C	13	1.41
(1,79)	1:123:B:SER:C	1:124:B:ARG:N	1:124:B:ARG:CA	1:124:B:ARG:C	23	1.37
(1,22)	1:24:A:ARG:N	1:24:A:ARG:CA	1:24:A:ARG:C	1:25:A:LEU:N	25	1.23
(1,22)	1:24:A:ARG:N	1:24:A:ARG:CA	1:24:A:ARG:C	1:25:A:LEU:N	22	1.14