wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2MZD
BMRB ID	:	25484
Title	:	Characterization of the p300 Taz2-p53 TAD2 Complex and Comparison with the p300 Taz2-p53 TAD1 Complex
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Deposited on	:	2015-02-11

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:

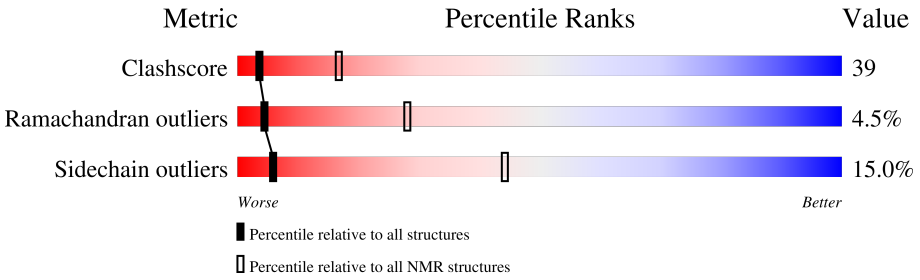
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 82%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	90	24% 48% 14% • 9%
2	B	25	16% 20% 8% 56%

2 Ensemble composition and analysis

This entry contains 15 models. Model 4 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:7-A:88, B:12-B:22 (93)	0.57	4

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1791 atoms, of which 903 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	90	1415	420	726	140	119	10	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	CYS	engineered mutation	UNP Q09472
A	24	ALA	CYS	engineered mutation	UNP Q09472
A	67	ALA	CYS	engineered mutation	UNP Q09472
A	68	ALA	CYS	engineered mutation	UNP Q09472

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	25	376	124	177	28	45	2	0

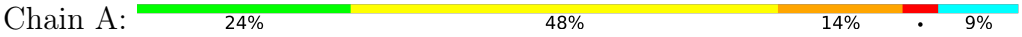
4 Residue-property plots

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: Histone acetyltransferase p300

Chain A:



• Molecule 2: Cellular tumor antigen p53

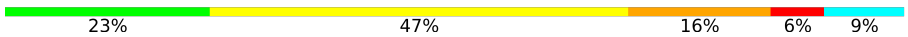
Chain B:

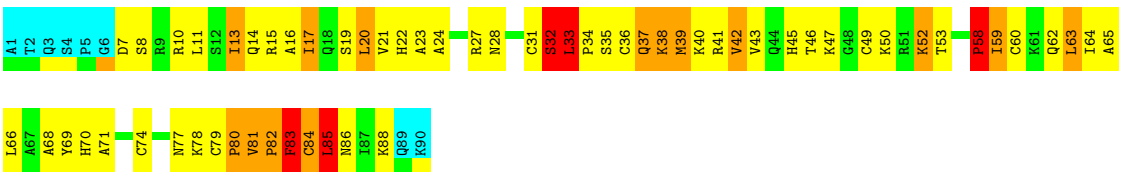
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

• Molecule 1: Histone acetyltransferase p300

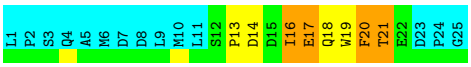
Chain A:





• Molecule 2: Cellular tumor antigen p53

Chain B:


L1
P2
S3
Q4
A5
M6
D7
D8
L9
M10
L11
S12
P13
D14
D15
I16
E17
Q18
W19
F20
T21
E22
D23
P24
G25

5 Refinement protocol and experimental data overview

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

Of the 40000 calculated structures, 15 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
TALOS	structure solution	
CNS	structure solution	
CNS	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	2
Total number of shifts	1270
Number of shifts mapped to atoms	1270
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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	2.04±0.04	17±2/642 (2.6± 0.4%)	1.46±0.03	7±1/861 (0.9± 0.2%)
2	B	1.39±0.13	1±1/100 (0.9± 0.6%)	1.15±0.08	0±0/138 (0.0± 0.2%)
All	All	1.96	268/11130 (2.4%)	1.42	111/14985 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	3.0±0.7
2	B	0.0±0.0	0.1±0.3
All	All	0	47

5 of 42 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	33	LEU	N-CA	-9.80	1.26	1.46	6	15
1	A	59	ILE	N-CA	-8.51	1.29	1.46	15	13
1	A	32	SER	N-CA	-8.50	1.29	1.46	14	15
1	A	53	THR	N-CA	-8.12	1.30	1.46	11	13
2	B	21	THR	N-CA	-7.64	1.31	1.46	5	10

5 of 17 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	58	PRO	N-CA-CB	-10.19	91.07	103.30	2	13
1	A	83	PHE	C-N-CA	9.18	144.65	121.70	9	15
1	A	58	PRO	CA-N-CD	-7.33	101.25	111.50	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	84	CYS	N-CA-C	-7.07	91.90	111.00	9	12
1	A	59	ILE	CB-CA-C	6.74	125.07	111.60	6	9

There are no chirality outliers.

5 of 6 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	32	SER	Peptide	15
1	A	82	PRO	Peptide	14
1	A	58	PRO	Mainchain,Peptide	13
2	B	21	THR	Peptide	2
1	A	10	ARG	Sidechain	1

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	632	668	662	54±5
2	B	96	77	77	9±2
All	All	10920	11175	11088	862

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 39.

5 of 234 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD22	2:B:16:ILE:HG13	0.84	1.49	13	7
1:A:42:VAL:HG13	1:A:59:ILE:HD11	0.81	1.53	14	6
1:A:49:CYS:O	1:A:52:LYS:HG3	0.80	1.77	10	11
1:A:79:CYS:HB2	1:A:84:CYS:SG	0.79	2.18	2	1
1:A:66:LEU:HA	1:A:69:TYR:CE1	0.76	2.15	11	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	82/90 (91%)	71±2 (87±2%)	7±1 (8±2%)	4±1 (5±1%)	4 24
2	B	11/25 (44%)	10±1 (89±8%)	1±1 (11±8%)	0±0 (0±0%)	100 100
All	All	1395/1725 (81%)	1211 (87%)	121 (9%)	63 (5%)	4 28

5 of 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	83	PHE	15
1	A	85	LEU	15
1	A	80	PRO	11
1	A	79	CYS	7
1	A	78	LYS	4

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	71/77 (92%)	62±2 (87±2%)	9±2 (13±2%)	7 48
2	B	11/23 (48%)	8±1 (73±9%)	3±1 (27±9%)	2 21
All	All	1230/1500 (82%)	1046 (85%)	184 (15%)	6 44

5 of 33 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	27	ARG	15
1	A	39	MET	15

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Mol	Chain	Res	Type	Models (Total)
1	A	85	LEU	15
2	B	16	ILE	15
1	A	58	PRO	14

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	990
Number of shifts mapped to atoms	990
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	87	-0.51 ± 0.18	Should be checked
$^{13}C_{\beta}$	83	0.25 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	74	-0.85 ± 0.10	Should be applied
^{15}N	74	-0.76 ± 0.21	Should be applied

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 72%, i.e. 920 atoms were assigned a chemical shift out of a possible 1274. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	372/458 (81%)	153/184 (83%)	149/186 (80%)	70/88 (80%)
Sidechain	548/743 (74%)	375/479 (78%)	173/224 (77%)	0/40 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/73 (0%)	0/36 (0%)	0/28 (0%)	0/9 (0%)
Overall	920/1274 (72%)	528/699 (76%)	322/438 (74%)	70/137 (51%)

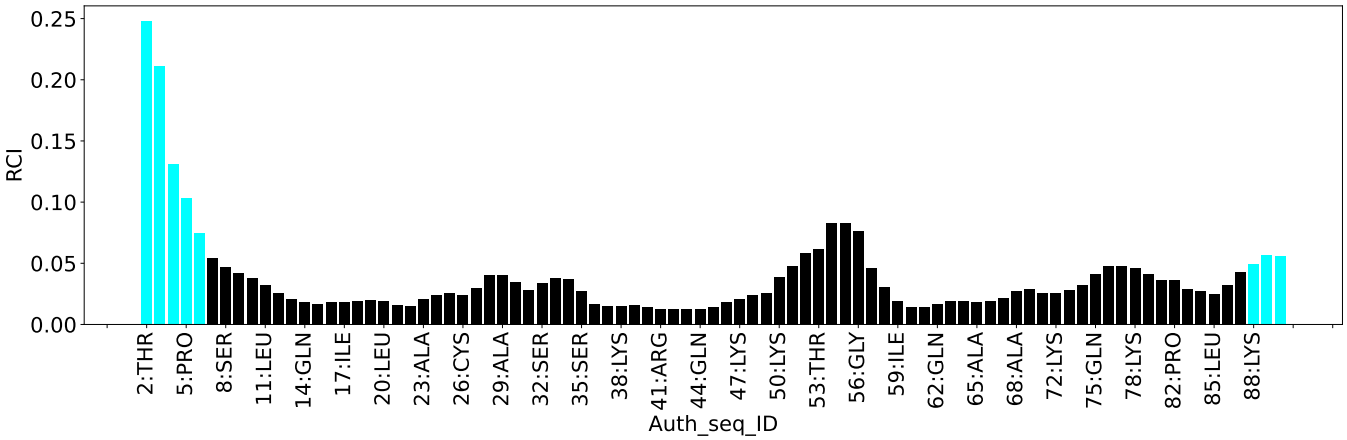
7.1.4 Statistically unusual chemical shifts (i)

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	280
Number of shifts mapped to atoms	280
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

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	25	-0.01 ± 0.38	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	24	—	None (insufficient data)
$^{13}C'$	21	—	None (insufficient data)
^{15}N	22	—	None (insufficient data)

7.2.3 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 10%, i.e. 123 atoms were assigned a chemical shift out of a possible 1274. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	52/458 (11%)	21/184 (11%)	21/186 (11%)	10/88 (11%)
Sidechain	64/743 (9%)	43/479 (9%)	20/224 (9%)	1/40 (2%)
Aromatic	7/73 (10%)	6/36 (17%)	0/28 (0%)	1/9 (11%)
Overall	123/1274 (10%)	70/699 (10%)	41/438 (9%)	12/137 (9%)

7.2.4 Statistically unusual chemical shifts (i)

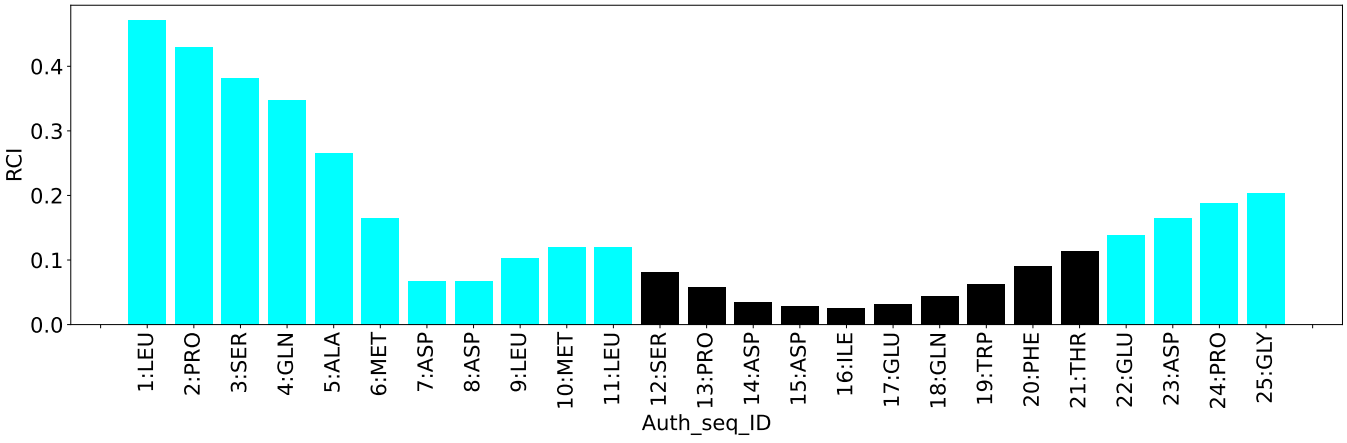
There are no statistically unusual chemical shifts.

7.2.5 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 B:



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	2081
Intra-residue (|i-j|=0)	535
Sequential (|i-j|=1)	546
Medium range (|i-j|>1 and |i-j|<5)	595
Long range (|i-j|≥5)	277
Inter-chain	40
Hydrogen bond restraints	88
Disulfide bond restraints	0
Total dihedral-angle restraints	180
Number of unmapped restraints	0
Number of restraints per residue	19.7
Number of long range restraints per residue[1]	2.4

[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

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)	120.5	0.2
0.2-0.5 (Medium)	142.4	0.5
>0.5 (Large)	32.1	4.51

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)	28.1	10.0
10.0-20.0 (Medium)	3.7	19.7
>20.0 (Large)	3.5	136.5

9 Distance violation analysis (i)

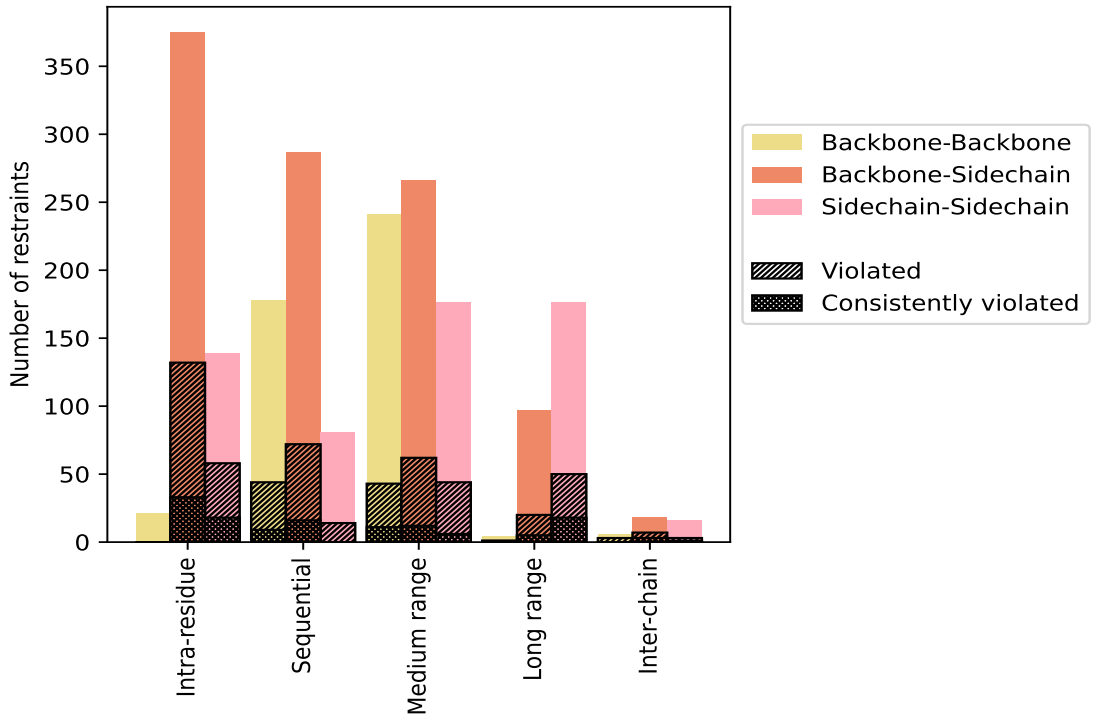
9.1 Summary of distance violations (i)

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)	535	25.7	190	35.5	9.1	51	9.5	2.5
Backbone-Backbone	21	1.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	375	18.0	132	35.2	6.3	33	8.8	1.6
Sidechain-Sidechain	139	6.7	58	41.7	2.8	18	12.9	0.9
Sequential (|i-j|=1)	546	26.2	130	23.8	6.2	25	4.6	1.2
Backbone-Backbone	178	8.6	44	24.7	2.1	9	5.1	0.4
Backbone-Sidechain	287	13.8	72	25.1	3.5	16	5.6	0.8
Sidechain-Sidechain	81	3.9	14	17.3	0.7	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	595	28.6	135	22.7	6.5	25	4.2	1.2
Backbone-Backbone	153	7.4	29	19.0	1.4	7	4.6	0.3
Backbone-Sidechain	266	12.8	62	23.3	3.0	12	4.5	0.6
Sidechain-Sidechain	176	8.5	44	25.0	2.1	6	3.4	0.3
Long range (|i-j|≥5)	277	13.3	71	25.6	3.4	24	8.7	1.2
Backbone-Backbone	4	0.2	1	25.0	0.0	1	25.0	0.0
Backbone-Sidechain	97	4.7	20	20.6	1.0	5	5.2	0.2
Sidechain-Sidechain	176	8.5	50	28.4	2.4	18	10.2	0.9
Inter-chain	40	1.9	13	32.5	0.6	4	10.0	0.2
Backbone-Backbone	6	0.3	3	50.0	0.1	0	0.0	0.0
Backbone-Sidechain	18	0.9	7	38.9	0.3	3	16.7	0.1
Sidechain-Sidechain	16	0.8	3	18.8	0.1	1	6.2	0.0
Hydrogen bond	88	4.2	14	15.9	0.7	4	4.5	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2081	100.0	553	26.6	26.6	133	6.4	6.4
Backbone-Backbone	450	21.6	91	20.2	4.4	21	4.7	1.0
Backbone-Sidechain	1043	50.1	293	28.1	14.1	69	6.6	3.3
Sidechain-Sidechain	588	28.3	169	28.7	8.1	43	7.3	2.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	114	63	72	39	8	296	0.31	3.49	0.35	0.22
2	97	64	71	41	8	281	0.34	4.25	0.4	0.25
3	103	64	73	44	6	290	0.33	2.94	0.32	0.25
4	103	65	78	43	8	297	0.33	4.51	0.43	0.24
5	101	67	78	36	7	289	0.32	3.35	0.37	0.23
6	106	70	74	36	7	293	0.31	3.46	0.35	0.23
7	105	68	83	47	8	311	0.32	2.91	0.34	0.23
8	104	67	75	40	8	294	0.33	3.82	0.39	0.23
9	106	64	73	39	7	289	0.36	4.35	0.46	0.24
10	102	70	74	36	7	289	0.32	3.24	0.37	0.23
11	104	68	91	41	6	310	0.39	4.27	0.57	0.24

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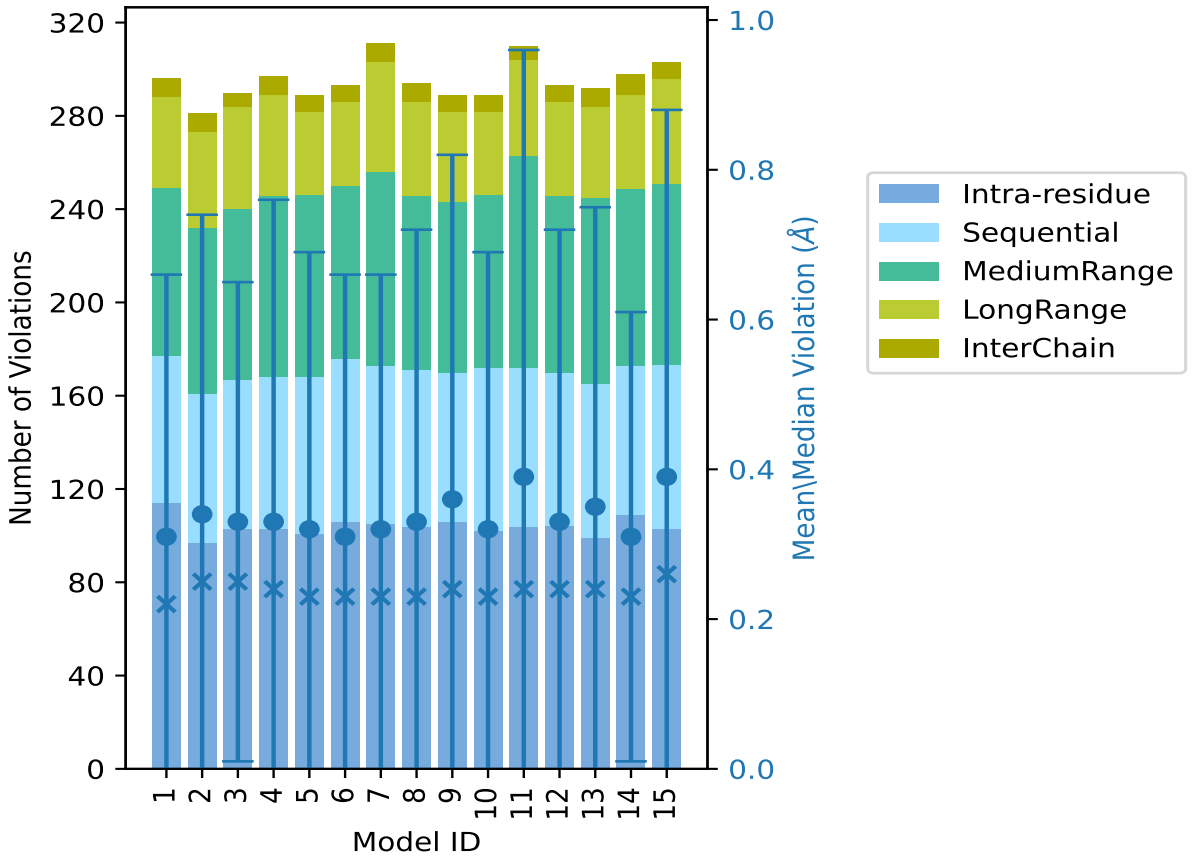
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	104	66	76	40	7	293	0.33	4.28	0.39	0.24
13	99	66	80	39	8	292	0.35	3.37	0.4	0.24
14	109	64	76	40	9	298	0.31	2.53	0.3	0.23
15	103	70	78	45	7	303	0.39	4.06	0.49	0.26

[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



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

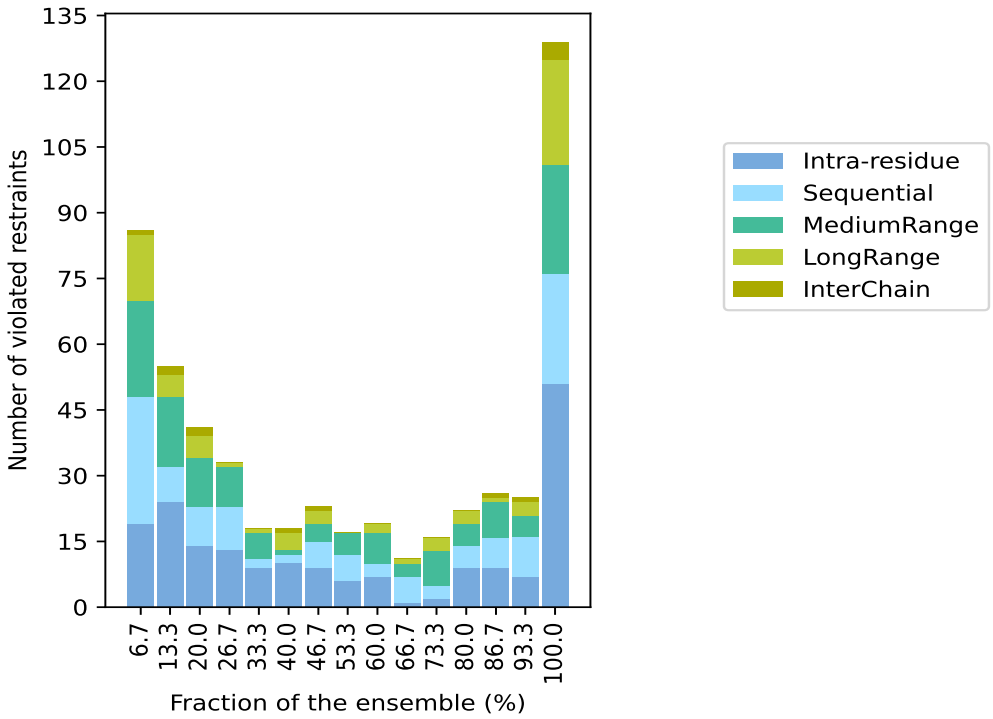
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for

a given fraction of the ensemble. In total, 1454(IR:345, SQ:416, MR:460, LR:206, IC:27) 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]	%
19	29	22	15	1	86	1	6.7
24	8	16	5	2	55	2	13.3
14	9	11	5	2	41	3	20.0
13	10	9	1	0	33	4	26.7
9	2	6	1	0	18	5	33.3
10	2	1	4	1	18	6	40.0
9	6	4	3	1	23	7	46.7
6	6	5	0	0	17	8	53.3
7	3	7	2	0	19	9	60.0
1	6	3	1	0	11	10	66.7
2	3	8	3	0	16	11	73.3
9	5	5	3	0	22	12	80.0
9	7	8	1	1	26	13	86.7
7	9	5	3	1	25	14	93.3
51	25	25	24	4	129	15	100.0

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

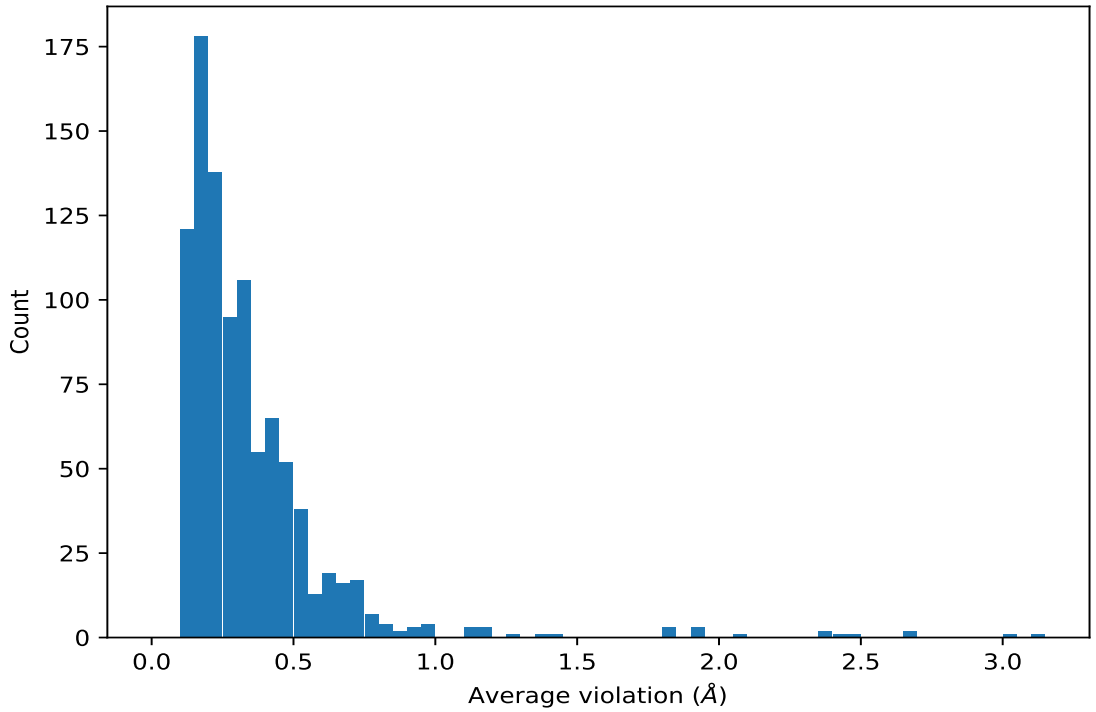
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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.

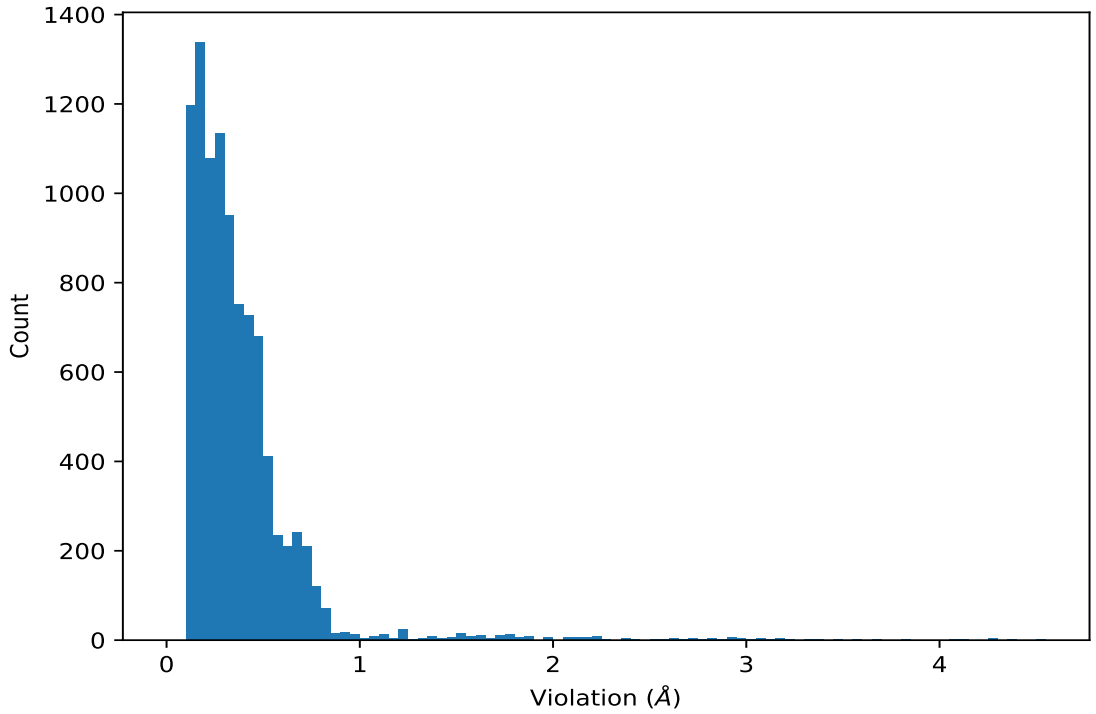
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1647)	1:A:50:LYS:HG2	1:A:53:THR:HA	15	3.1	1.22	3.24
(1,992)	1:A:5:PRO:HA	1:A:8:SER:HA	15	3.03	0.32	2.97
(1,786)	1:A:86:ASN:H	1:A:90:LYS:H	15	2.45	1.34	2.84
(1,3)	1:A:39:MET:HE1	2:B:19:TRP:HZ2	15	1.81	0.18	1.79
(1,3)	1:A:39:MET:HE2	2:B:19:TRP:HZ2	15	1.81	0.18	1.79
(1,3)	1:A:39:MET:HE3	2:B:19:TRP:HZ2	15	1.81	0.18	1.79
(1,42)	2:B:21:THR:H	1:A:39:MET:HB3	15	1.38	0.16	1.41
(1,1828)	1:A:66:LEU:HD11	1:A:68:ALA:HA	15	1.19	0.25	1.2
(1,1828)	1:A:66:LEU:HD12	1:A:68:ALA:HA	15	1.19	0.25	1.2
(1,1828)	1:A:66:LEU:HD13	1:A:68:ALA:HA	15	1.19	0.25	1.2
(2,81)	1:A:81:VAL:O	1:A:85:LEU:H	15	0.89	0.79	0.4
(1,1245)	1:A:23:ALA:HB1	1:A:39:MET:HB2	15	0.8	0.02	0.8
(1,1245)	1:A:23:ALA:HB2	1:A:39:MET:HB2	15	0.8	0.02	0.8
(1,1245)	1:A:23:ALA:HB3	1:A:39:MET:HB2	15	0.8	0.02	0.8
(1,974)	1:A:4:SER:HA	1:A:5:PRO:HD2	15	0.79	0.39	1.03
(1,28)	2:B:16:ILE:H	1:A:20:LEU:HD21	15	0.77	0.15	0.78

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

The following table provides 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. 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)
(1,1647)	1:A:50:LYS:HG2	1:A:53:THR:HA	4	4.51
(1,1647)	1:A:50:LYS:HG2	1:A:53:THR:HA	9	4.35
(1,1647)	1:A:50:LYS:HG2	1:A:53:THR:HA	12	4.28
(1,786)	1:A:86:ASN:H	1:A:90:LYS:H	11	4.27
(1,18)	2:B:5:ALA:H	1:A:17:ILE:H	2	4.25
(1,1647)	1:A:50:LYS:HG2	1:A:53:THR:HA	11	4.13
(1,786)	1:A:86:ASN:H	1:A:90:LYS:H	4	4.09
(1,1647)	1:A:50:LYS:HG2	1:A:53:THR:HA	15	4.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,786)	1:A:86:ASN:H	1:A:90:LYS:H	8	3.82
(1,992)	1:A:5:PRO:HA	1:A:8:SER:HA	11	3.69

10 Dihedral-angle violation analysis

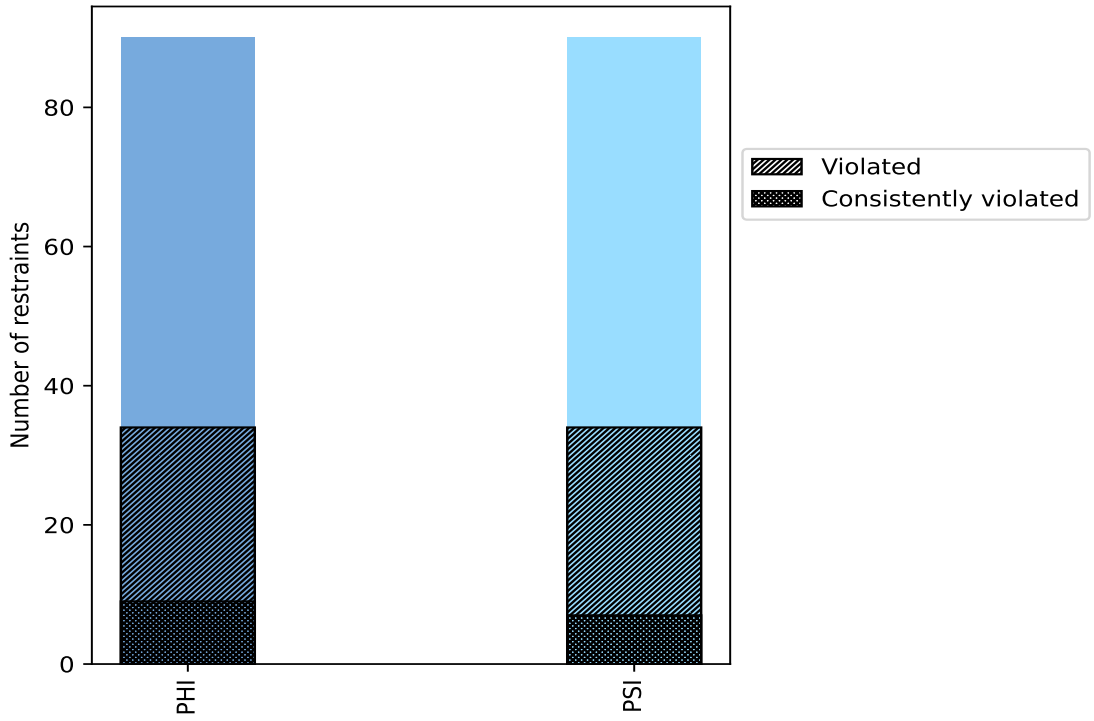
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	90	50.0	34	37.8	18.9	9	10.0	5.0
PSI	90	50.0	34	37.8	18.9	7	7.8	3.9
Total	180	100.0	68	37.8	37.8	16	8.9	8.9

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



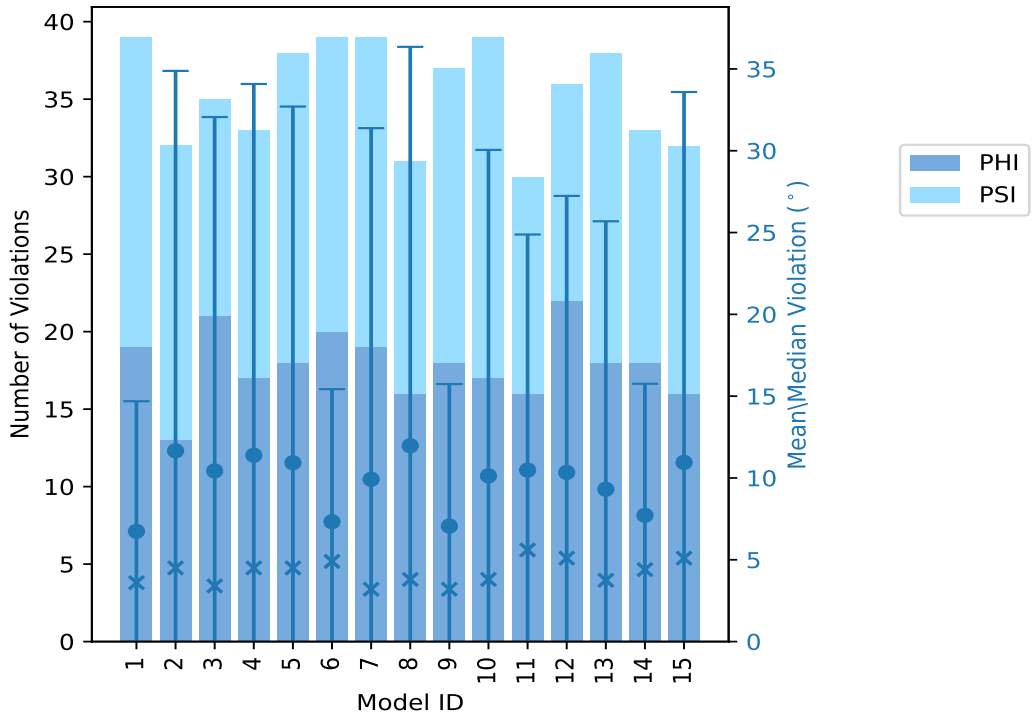
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	19	20	39	6.74	40.6	7.95	3.6
2	13	19	32	11.66	131.3	23.22	4.5
3	21	14	35	10.43	126.5	21.63	3.4
4	17	16	33	11.39	129.7	22.69	4.5
5	18	20	38	10.93	133.7	21.77	4.5
6	20	19	39	7.33	42.5	8.1	4.9
7	19	20	39	9.92	131.0	21.46	3.2
8	16	15	31	11.97	136.5	24.38	3.8
9	18	19	37	7.06	41.5	8.68	3.2
10	17	22	39	10.13	121.8	19.92	3.8
11	16	14	30	10.48	73.8	14.4	5.6
12	22	14	36	10.34	97.2	16.9	5.1
13	18	20	38	9.31	96.0	16.38	3.75
14	18	15	33	7.72	39.4	8.04	4.4
15	16	16	32	10.95	130.5	22.64	5.1

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

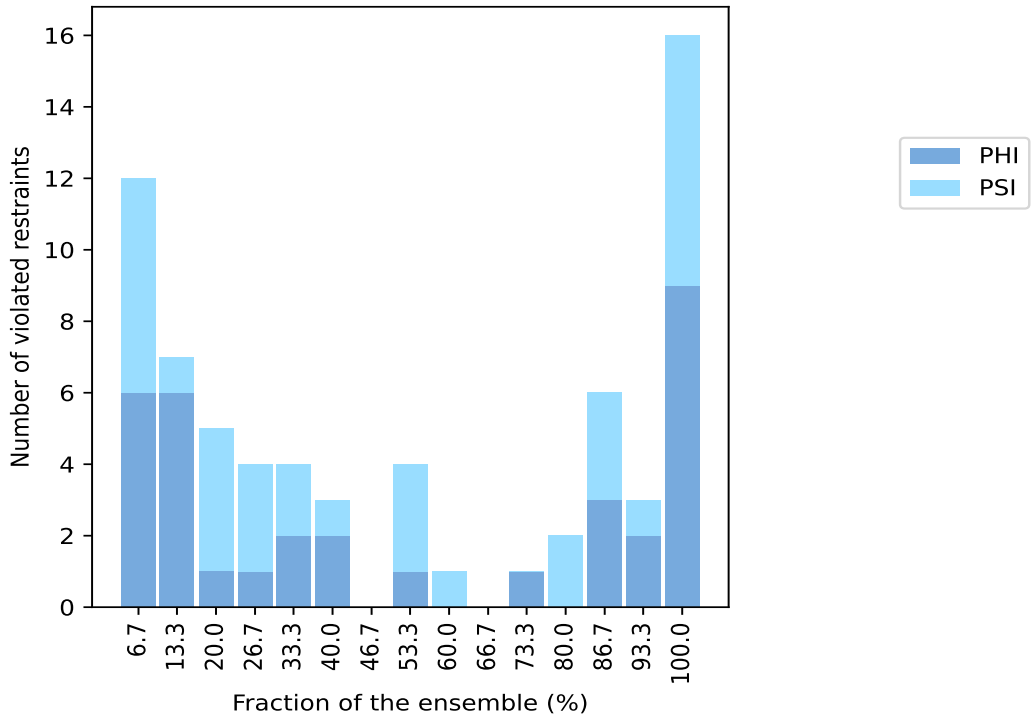
10.3 Dihedral-angle violation statistics for the ensemble (i)

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]	%
6	6	12	1	6.7
6	1	7	2	13.3
1	4	5	3	20.0
1	3	4	4	26.7
2	2	4	5	33.3
2	1	3	6	40.0
0	0	0	7	46.7
1	3	4	8	53.3
0	1	1	9	60.0
0	0	0	10	66.7
1	0	1	11	73.3
0	2	2	12	80.0
3	3	6	13	86.7
2	1	3	14	93.3
9	7	16	15	100.0

[1] Number of models with violations

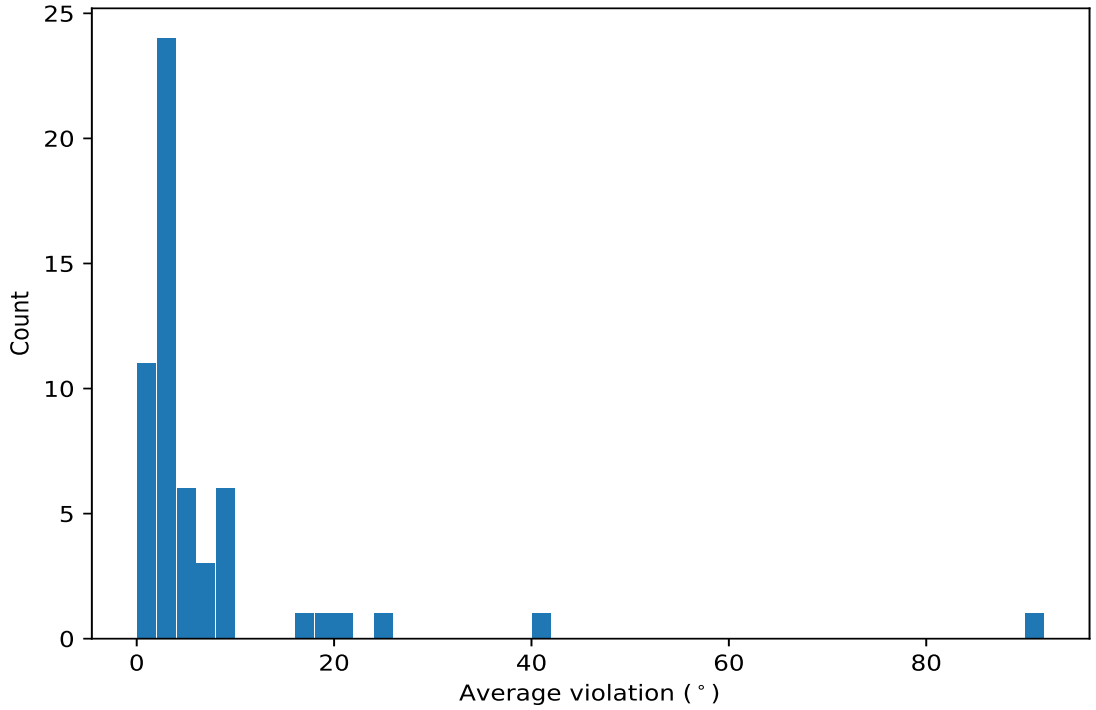
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



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

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

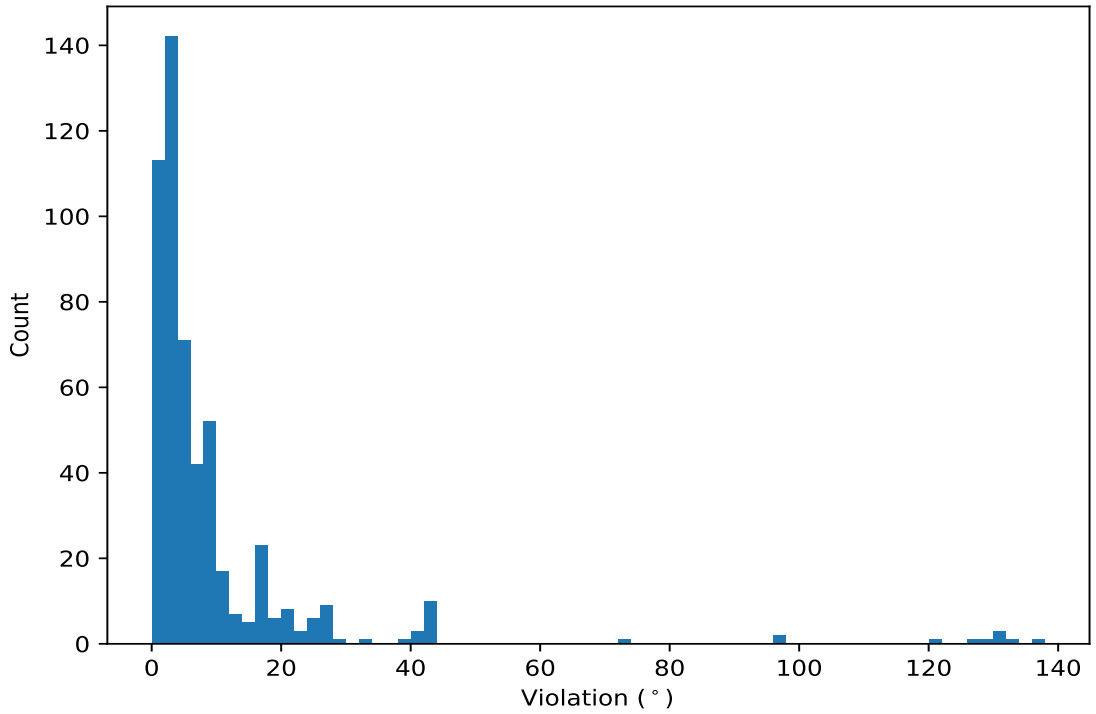
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	15	90.53	49.97	121.8
(1,102)	1:A:58:PRO:N	1:A:58:PRO:CA	1:A:58:PRO:C	1:A:59:ILE:N	15	41.74	2.38	42.5
(1,56)	1:A:32:SER:N	1:A:32:SER:CA	1:A:32:SER:C	1:A:33:LEU:N	15	25.34	1.84	26.0
(1,146)	1:A:84:CYS:N	1:A:84:CYS:CA	1:A:84:CYS:C	1:A:85:LEU:N	15	20.08	2.53	20.2
(1,103)	1:A:58:PRO:C	1:A:59:ILE:N	1:A:59:ILE:CA	1:A:59:ILE:C	15	18.67	4.6	17.4
(1,57)	1:A:32:SER:C	1:A:33:LEU:N	1:A:33:LEU:CA	1:A:33:LEU:C	15	16.61	1.15	16.9
(1,144)	1:A:83:PHE:N	1:A:83:PHE:CA	1:A:83:PHE:C	1:A:84:CYS:N	15	9.72	2.95	10.6
(1,97)	1:A:52:LYS:C	1:A:53:THR:N	1:A:53:THR:CA	1:A:53:THR:C	15	9.63	0.77	9.7
(1,46)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:ASN:N	15	8.96	0.72	9.1
(1,96)	1:A:52:LYS:N	1:A:52:LYS:CA	1:A:52:LYS:C	1:A:53:THR:N	15	8.67	1.05	8.7

[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

The following table provides the list of violationsfor 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 (°)
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	8	136.5
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	5	133.7
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	2	131.3
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	7	131.0
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	15	130.5
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	4	129.7
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	3	126.5
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	10	121.8
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	12	97.2
(1,3)	1:A:5:PRO:C	1:A:6:GLY:N	1:A:6:GLY:CA	1:A:6:GLY:C	13	96.0