



wwPDB NMR Structure Validation Summary Report ⓘ

Dec 25, 2024 – 03:49 AM EST

PDB ID : 5KIZ
BMRB ID : 30118
Title : Solution Structure of a repacked version of HIF-2 alpha PAS-B
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Deposited on : 2016-06-17

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

We welcome your comments at validation@mail.wwpdb.org

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<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:

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

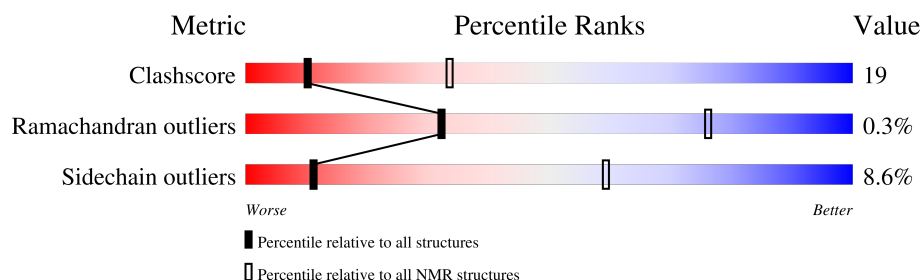
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	114	

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:242-A:294, A:302-A:349 (101)	0.42	8

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	1, 2, 3, 4, 7, 8, 9, 15, 18
2	5, 6, 11, 12, 17, 20
3	10, 13, 16
Single-model clusters	14; 19

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1831 atoms, of which 903 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Endothelial PAS domain-containing protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1831	587	903	156	176	9	

There are 8 discrepancies between the modelled and reference sequences:

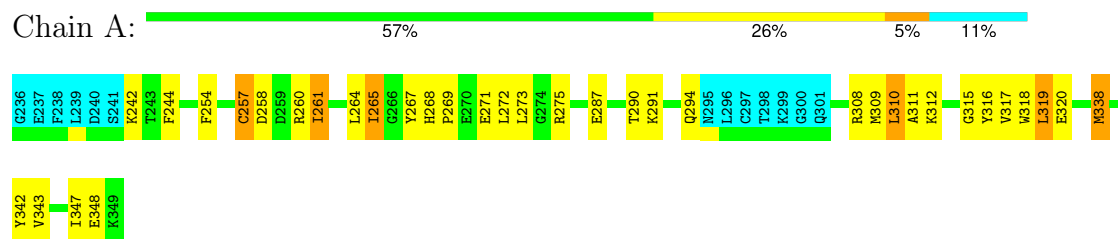
Chain	Residue	Modelled	Actual	Comment	Reference
A	236	GLY	-	expression tag	UNP Q99814
A	237	GLU	-	expression tag	UNP Q99814
A	238	PHE	-	expression tag	UNP Q99814
A	248	PHE	HIS	engineered mutation	UNP Q99814
A	278	SER	TYR	engineered mutation	UNP Q99814
A	281	TRP	TYR	engineered mutation	UNP Q99814
A	323	MET	GLY	engineered mutation	UNP Q99814
A	339	ALA	CYS	engineered mutation	UNP Q99814

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.

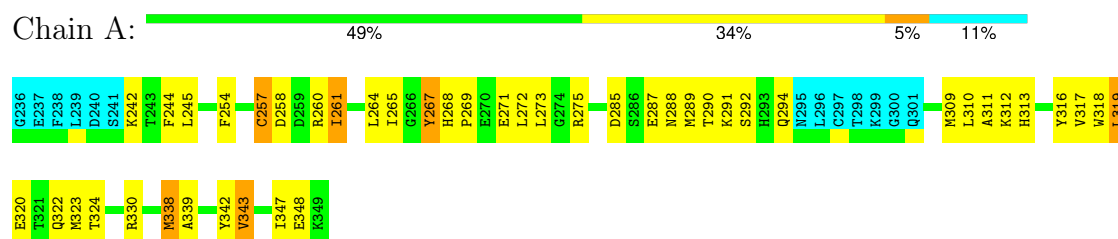
- Molecule 1: Endothelial PAS domain-containing protein 1



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

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: Endothelial PAS domain-containing protein 1



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
ARIA	structure calculation	2.3
ARIA	refinement	2.3

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	1448
Number of shifts mapped to atoms	1448
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	0.48±0.03	0±0/851 (0.0± 0.1%)	0.52±0.01	0±0/1147 (0.0± 0.0%)
All	All	0.49	2/17020 (0.0%)	0.52	0/22940 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	267	TYR	CE2-CZ	5.21	1.45	1.38	8	1
1	A	267	TYR	CE1-CZ	-5.12	1.31	1.38	8	1

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	831	810	806	31±3
All	All	16620	16200	16120	616

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 19.

5 of 107 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:272:LEU:O	1:A:275:ARG:HG2	0.70	1.86	1	20
1:A:267:TYR:CE1	1:A:312:LYS:HA	0.65	2.26	12	19
1:A:287:GLU:O	1:A:291:LYS:HD3	0.65	1.92	1	13
1:A:290:THR:O	1:A:294:GLN:HG3	0.64	1.92	11	10
1:A:260:ARG:HG3	1:A:264:LEU:HD11	0.63	1.68	5	3

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	100/114 (88%)	94±1 (94±1%)	6±1 (6±1%)	0±0 (0±0%)	32	76
All	All	2000/2280 (88%)	1876 (94%)	117 (6%)	7 (0%)	32	76

All 3 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	242	LYS	3
1	A	334	PRO	3
1	A	306	GLN	1

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	92/103 (89%)	84±1 (91±2%)	8±1 (9±2%)	11	59
All	All	1840/2060 (89%)	1682 (91%)	158 (9%)	11	59

5 of 22 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	261	ILE	20
1	A	310	LEU	20
1	A	319	LEU	20
1	A	265	ILE	15
1	A	338	MET	15

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% 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	1448
Number of shifts mapped to atoms	1448
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	112	-0.46 ± 0.28	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	107	-0.09 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}'$	99	-0.09 ± 0.21	None needed (< 0.5 ppm)
^{15}N	108	0.53 ± 0.34	None needed (imprecise)

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 92%, i.e. 1304 atoms were assigned a chemical shift out of a possible 1418. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	490/504 (97%)	202/204 (99%)	190/202 (94%)	98/98 (100%)
Sidechain	688/764 (90%)	468/497 (94%)	210/238 (88%)	10/29 (34%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	126/150 (84%)	63/72 (88%)	61/68 (90%)	2/10 (20%)
Overall	1304/1418 (92%)	733/773 (95%)	461/508 (91%)	110/137 (80%)

7.1.4 Statistically unusual chemical shifts ⓘ

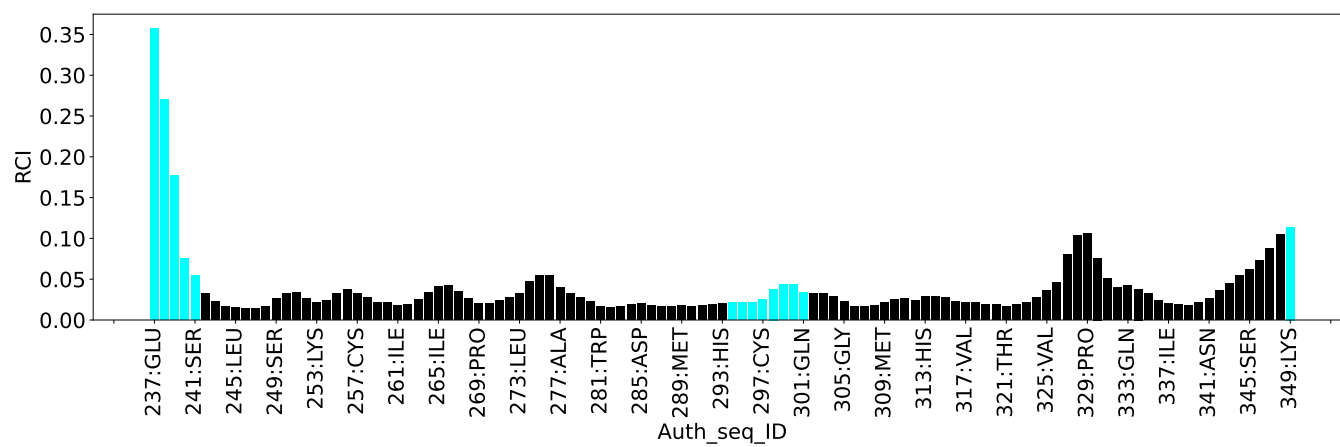
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	321	THR	HG1	6.13	0.08 – 2.19	23.7
1	A	324	THR	HG1	5.78	0.08 – 2.19	22.0
1	A	290	THR	HG1	5.52	0.08 – 2.19	20.8
1	A	308	ARG	HG2	-0.96	0.26 – 2.87	-9.7
1	A	308	ARG	HD3	1.17	1.81 – 4.39	-7.5
1	A	312	LYS	HB3	0.03	0.46 – 3.04	-6.7
1	A	289	MET	HB3	-0.17	0.33 – 3.66	-6.5
1	A	308	ARG	HG3	-0.25	0.15 – 2.94	-6.4
1	A	272	LEU	HD21	-0.93	-0.65 – 2.13	-6.0
1	A	272	LEU	HD22	-0.93	-0.65 – 2.13	-6.0
1	A	272	LEU	HD23	-0.93	-0.65 – 2.13	-6.0
1	A	308	ARG	HD2	1.80	1.97 – 4.26	-5.8
1	A	289	MET	HG2	0.52	0.65 – 4.19	-5.4
1	A	284	LEU	H	11.41	5.09 – 11.34	5.1

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:



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	2243
Intra-residue ($ i-j =0$)	773
Sequential ($ i-j =1$)	463
Medium range ($ i-j >1$ and $ i-j <5$)	297
Long range ($ i-j \geq 5$)	682
Inter-chain	0
Hydrogen bond restraints	28
Disulfide bond restraints	0
Total dihedral-angle restraints	186
Number of unmapped restraints	0
Number of restraints per residue	21.3
Number of long range restraints per residue ¹	6.1

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)	110.8	0.2
0.2-0.5 (Medium)	228.8	0.5
>0.5 (Large)	187.2	3.45

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)	11.9	4.98
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

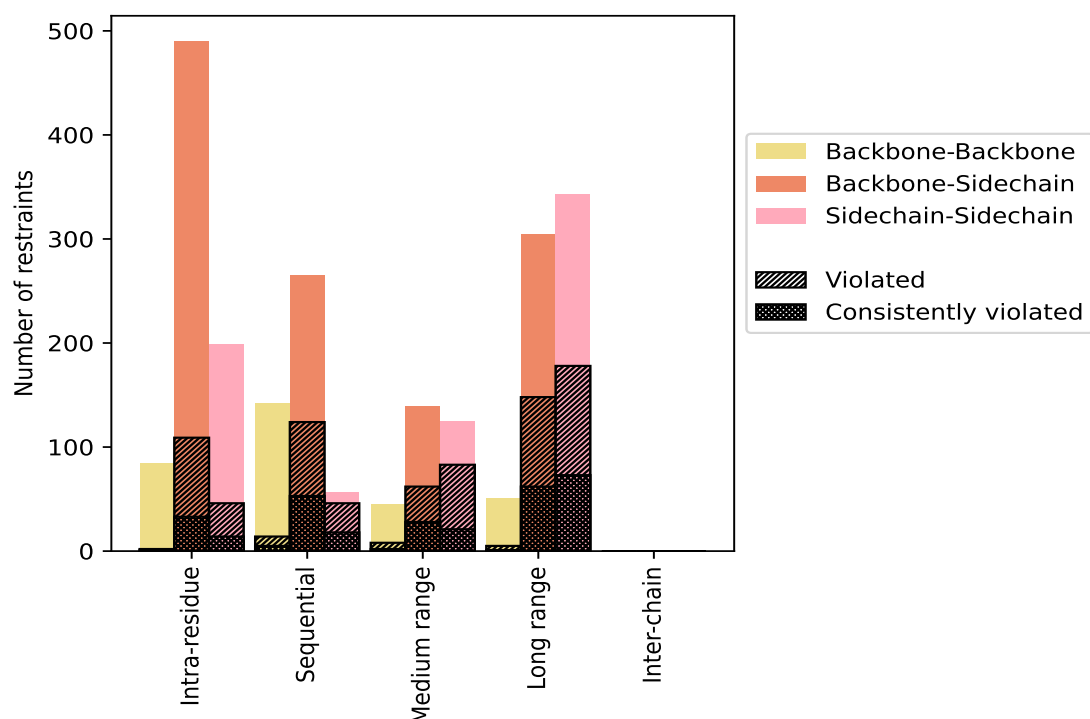
9.1 Summary of distance violations ⓘ

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)	773	34.5	157	20.3	7.0	48	6.2	2.1
Backbone-Backbone	84	3.7	2	2.4	0.1	1	1.2	0.0
Backbone-Sidechain	490	21.8	109	22.2	4.9	33	6.7	1.5
Sidechain-Sidechain	199	8.9	46	23.1	2.1	14	7.0	0.6
Sequential (i-j =1)	463	20.6	184	39.7	8.2	76	16.4	3.4
Backbone-Backbone	142	6.3	14	9.9	0.6	5	3.5	0.2
Backbone-Sidechain	265	11.8	124	46.8	5.5	53	20.0	2.4
Sidechain-Sidechain	56	2.5	46	82.1	2.1	18	32.1	0.8
Medium range (i-j >1 & i-j <5)	297	13.2	151	50.8	6.7	51	17.2	2.3
Backbone-Backbone	45	2.0	8	17.8	0.4	2	4.4	0.1
Backbone-Sidechain	127	5.7	60	47.2	2.7	28	22.0	1.2
Sidechain-Sidechain	125	5.6	83	66.4	3.7	21	16.8	0.9
Long range (i-j ≥5)	682	30.4	326	47.8	14.5	136	19.9	6.1
Backbone-Backbone	51	2.3	5	9.8	0.2	1	2.0	0.0
Backbone-Sidechain	288	12.8	143	49.7	6.4	62	21.5	2.8
Sidechain-Sidechain	343	15.3	178	51.9	7.9	73	21.3	3.3
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	28	1.2	7	25.0	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2243	100.0	825	36.8	36.8	311	13.9	13.9
Backbone-Backbone	322	14.4	29	9.0	1.3	9	2.8	0.4
Backbone-Sidechain	1198	53.4	443	37.0	19.8	176	14.7	7.8
Sidechain-Sidechain	723	32.2	353	48.8	15.7	126	17.4	5.6

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	95	125	83	224	0	527	0.47	2.33	0.34	0.39
2	99	118	88	221	0	526	0.48	2.31	0.34	0.4
3	98	125	89	230	0	542	0.47	2.36	0.34	0.38
4	95	116	91	234	0	536	0.49	2.33	0.36	0.38
5	107	126	88	231	0	552	0.47	2.41	0.35	0.38
6	100	134	87	230	0	551	0.46	2.31	0.33	0.37
7	96	127	87	216	0	526	0.47	2.34	0.33	0.39
8	97	127	100	222	0	546	0.45	2.3	0.33	0.37
9	98	121	91	218	0	528	0.48	2.33	0.34	0.39
10	96	128	83	227	0	534	0.47	2.45	0.34	0.39

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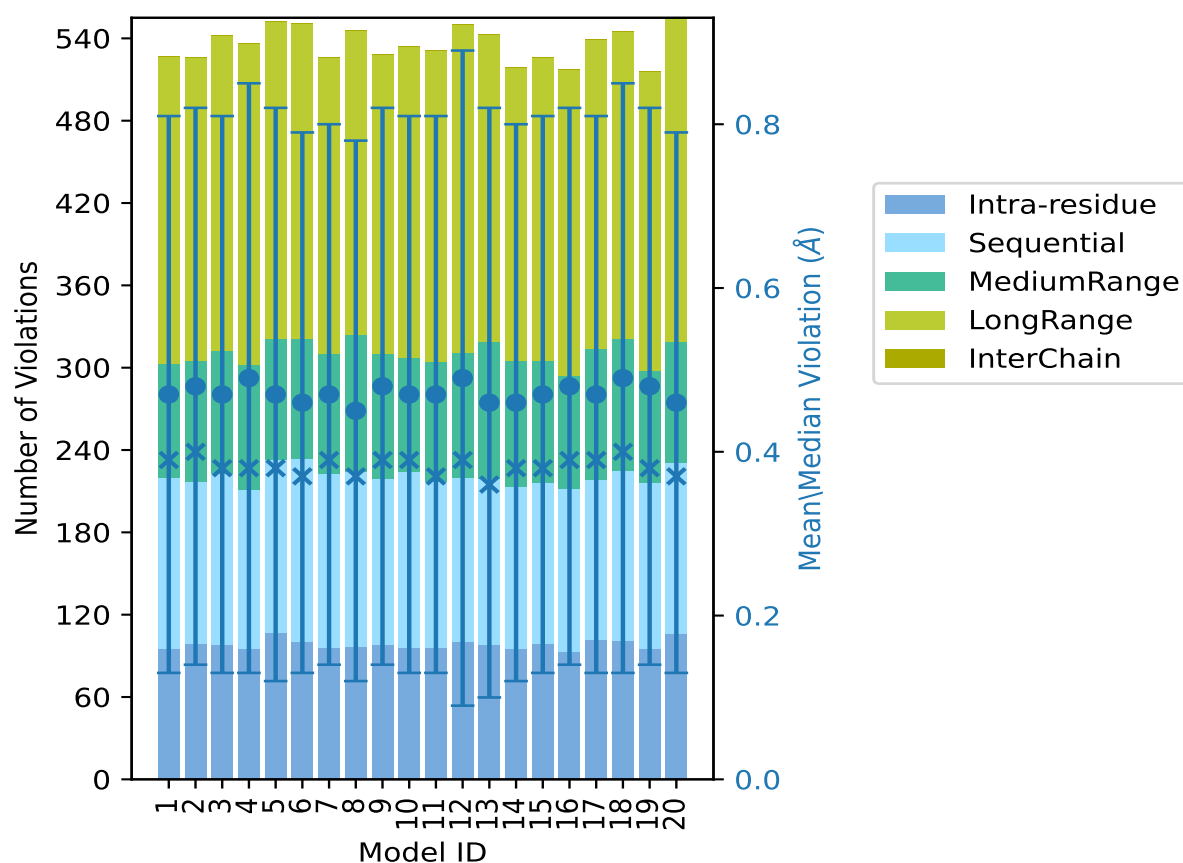
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	96	121	87	227	0	531	0.47	2.31	0.34	0.37
12	100	120	91	239	0	550	0.49	3.45	0.4	0.39
13	98	121	100	224	0	543	0.46	2.48	0.36	0.36
14	95	118	92	214	0	519	0.46	2.39	0.34	0.38
15	99	117	89	221	0	526	0.47	2.39	0.34	0.38
16	93	119	82	223	0	517	0.48	2.31	0.34	0.39
17	102	116	96	225	0	539	0.47	2.36	0.34	0.39
18	101	124	96	224	0	545	0.49	2.58	0.36	0.4
19	95	121	82	218	0	516	0.48	2.35	0.34	0.38
20	106	125	88	236	0	555	0.46	2.41	0.33	0.37

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 ⓘ



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

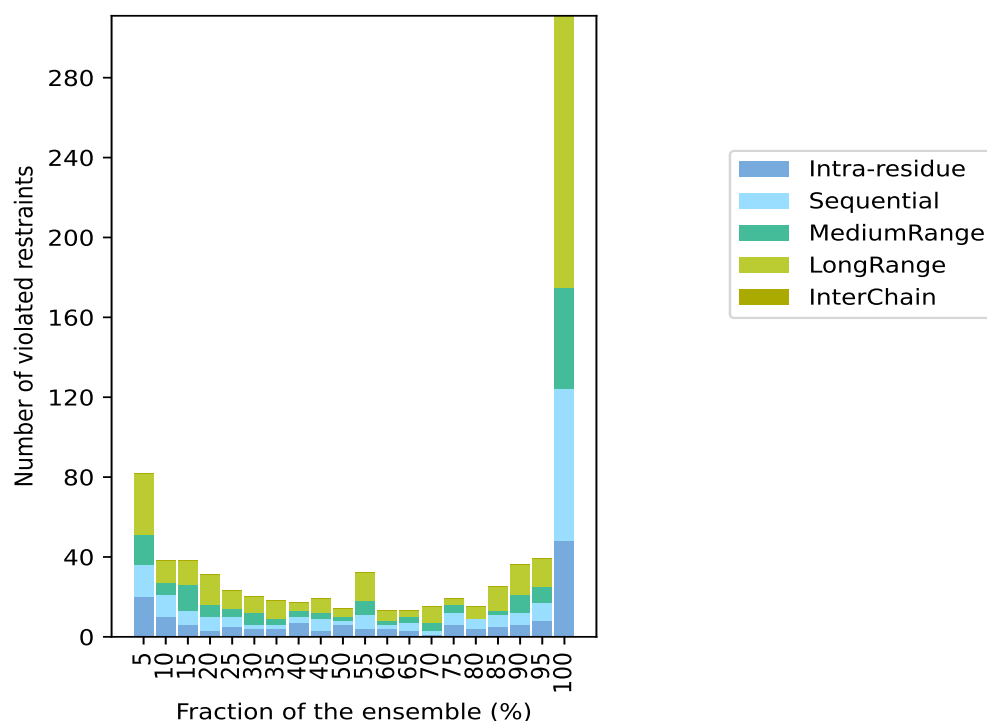
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1397(IR:616, SQ:279, MR:146, LR:356, IC:0) restraints are 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	%
20	16	15	31	0	82	1	5.0
10	11	6	11	0	38	2	10.0
6	7	13	12	0	38	3	15.0
3	7	6	15	0	31	4	20.0
5	5	4	9	0	23	5	25.0
4	2	6	8	0	20	6	30.0
4	2	3	9	0	18	7	35.0
7	3	3	4	0	17	8	40.0
3	6	3	7	0	19	9	45.0
6	2	2	4	0	14	10	50.0
4	7	7	14	0	32	11	55.0
4	2	2	5	0	13	12	60.0
3	4	3	3	0	13	13	65.0
1	2	4	8	0	15	14	70.0
6	6	4	3	0	19	15	75.0
4	5	0	6	0	15	16	80.0
5	6	2	12	0	25	17	85.0
6	6	9	15	0	36	18	90.0
8	9	8	14	0	39	19	95.0
48	76	51	136	0	311	20	100.0

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

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

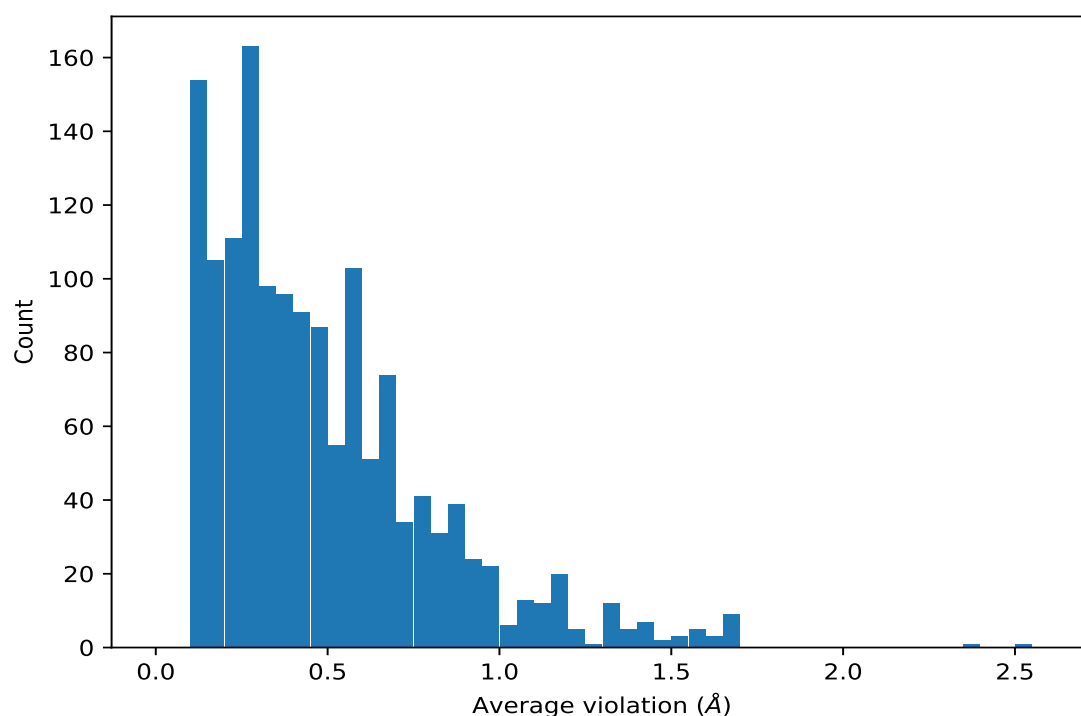
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 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)
(1,421)	1:310:A:LEU:HD12	1:280:A:PHE:HB2	20	2.35	0.04	2.34
(2,433)	1:341:A:ASN:HD22	1:245:A:LEU:HD11	20	1.7	0.13	1.74
(2,433)	1:341:A:ASN:HD22	1:319:A:LEU:HD22	20	1.7	0.13	1.74
(2,433)	1:341:A:ASN:HD22	1:277:A:ALA:HB2	20	1.7	0.13	1.74
(1,674)	1:265:A:ILE:HG21	1:267:A:TYR:HB3	20	1.67	0.04	1.66
(1,674)	1:265:A:ILE:HG22	1:267:A:TYR:HB3	20	1.67	0.04	1.66
(1,674)	1:265:A:ILE:HG23	1:267:A:TYR:HB3	20	1.67	0.04	1.66
(2,197)	1:261:A:ILE:HG23	1:268:A:HIS:HB2	20	1.67	0.05	1.67
(2,197)	1:261:A:ILE:HG22	1:268:A:HIS:HB2	20	1.67	0.05	1.67
(2,197)	1:261:A:ILE:HG21	1:268:A:HIS:HB2	20	1.67	0.05	1.67
(2,382)	1:271:A:GLU:H	1:272:A:LEU:HB3	20	1.65	0.02	1.66
(2,382)	1:271:A:GLU:H	1:273:A:LEU:HD11	20	1.65	0.02	1.66
(1,321)	1:265:A:ILE:HG12	1:261:A:ILE:HG12	20	1.63	0.03	1.63
(1,275)	1:265:A:ILE:HG13	1:267:A:TYR:HB3	20	1.57	0.07	1.54
(2,134)	1:317:A:VAL:HG11	1:267:A:TYR:HD2	20	1.54	0.08	1.52
(2,134)	1:317:A:VAL:HG13	1:267:A:TYR:HD2	20	1.54	0.08	1.52

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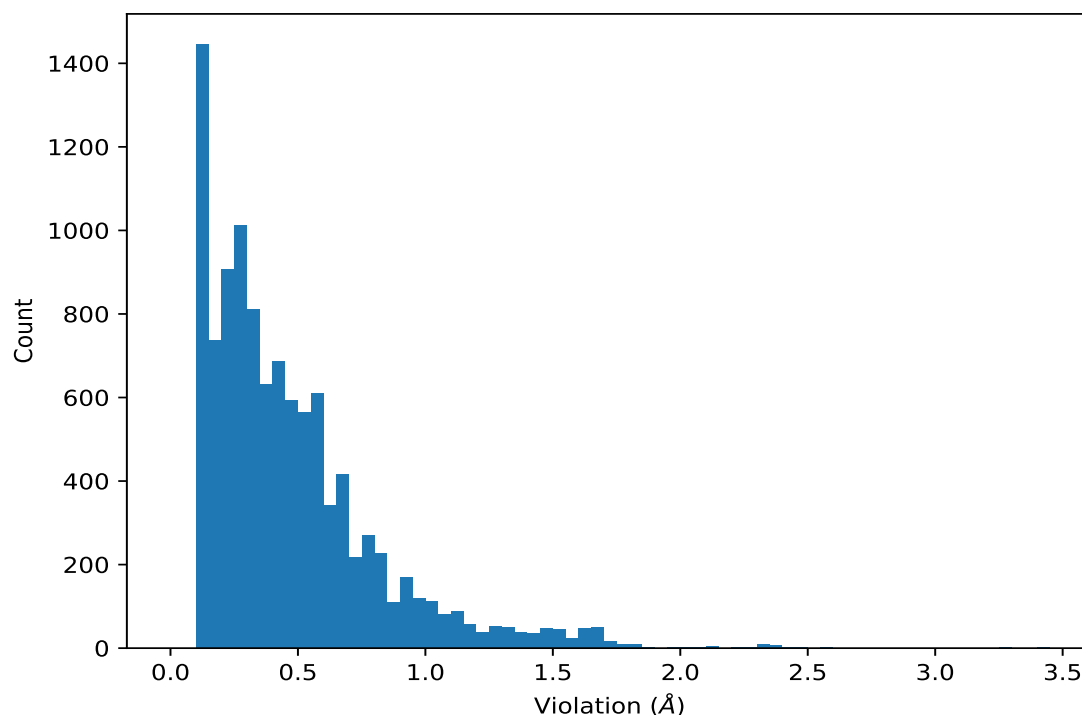
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,134)	1:317:A:VAL:HG12	1:267:A:TYR:HD2	20	1.54	0.08	1.52
(1,659)	1:258:A:ASP:HB2	1:244:A:PHE:HD2	20	1.49	0.07	1.52
(1,1684)	1:266:A:GLY:H	1:264:A:LEU:HB3	20	1.47	0.02	1.47

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 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)
(1,1283)	1:323:A:MET:H	1:302:A:VAL:HG11	12	3.45
(1,540)	1:323:A:MET:H	1:302:A:VAL:HG11	12	3.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:284:A:LEU:HD11	1:282:A:HIS:HE1	18	2.58
(1,371)	1:284:A:LEU:HD11	1:282:A:HIS:HE1	13	2.48
(1,421)	1:310:A:LEU:HD12	1:280:A:PHE:HB2	10	2.45
(1,421)	1:310:A:LEU:HD12	1:280:A:PHE:HB2	5	2.41
(1,421)	1:310:A:LEU:HD12	1:280:A:PHE:HB2	20	2.41
(1,421)	1:310:A:LEU:HD12	1:280:A:PHE:HB2	12	2.4
(1,421)	1:310:A:LEU:HD12	1:280:A:PHE:HB2	14	2.39
(1,421)	1:310:A:LEU:HD12	1:280:A:PHE:HB2	15	2.39

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

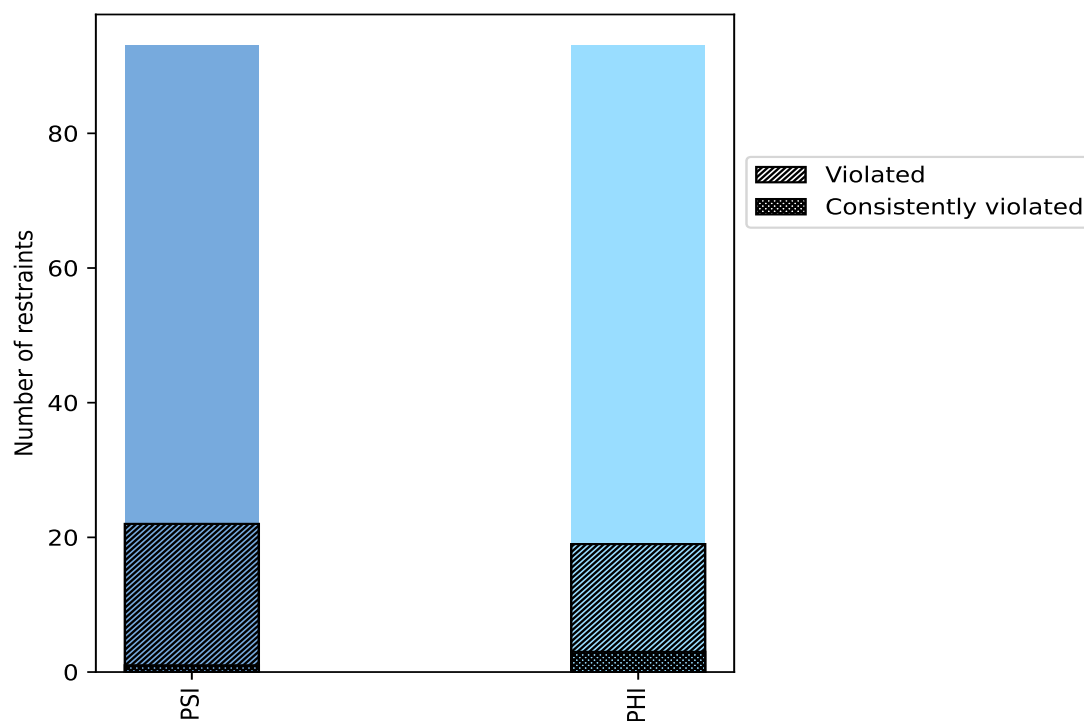
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	93	50.0	22	23.7	11.8	1	1.1	0.5
PHI	93	50.0	19	20.4	10.2	3	3.2	1.6
Total	186	100.0	41	22.0	22.0	4	2.2	2.2

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](#)



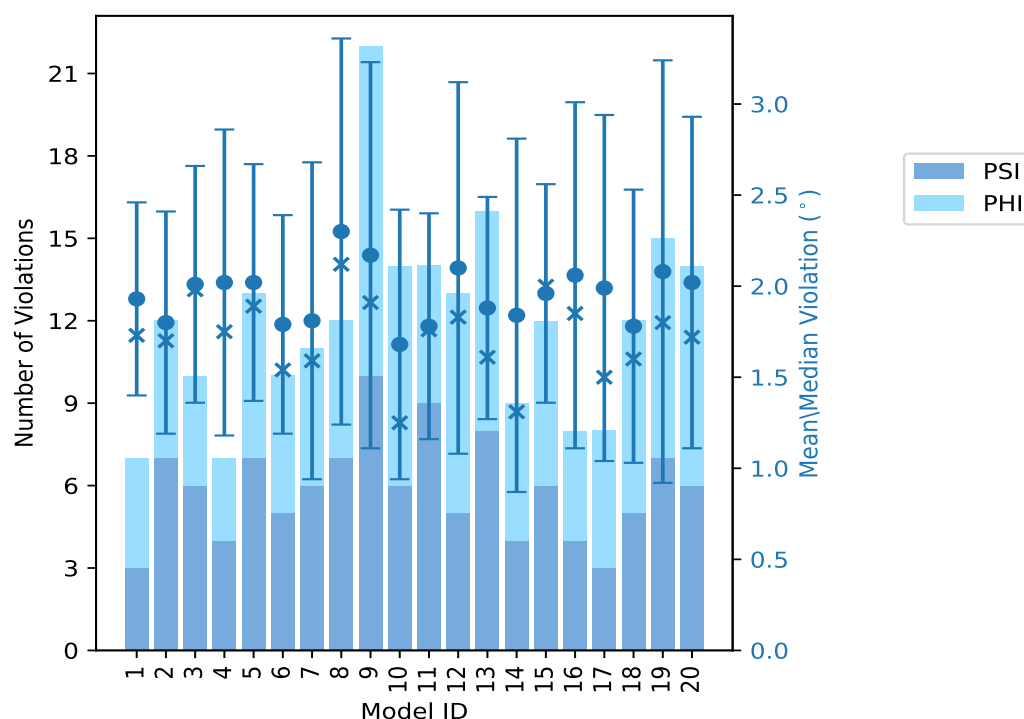
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	3	4	7	1.93	3.01	0.53	1.73
2	7	5	12	1.8	3.44	0.61	1.7
3	6	4	10	2.01	3.32	0.65	1.98
4	4	3	7	2.02	3.75	0.84	1.75
5	7	6	13	2.02	3.12	0.65	1.89
6	5	5	10	1.79	3.05	0.6	1.54
7	6	5	11	1.81	4.42	0.87	1.59
8	7	5	12	2.3	4.62	1.06	2.12
9	10	12	22	2.17	4.98	1.06	1.91
10	6	8	14	1.68	3.38	0.74	1.25
11	9	5	14	1.78	3.66	0.62	1.76
12	5	8	13	2.1	4.51	1.02	1.83
13	8	8	16	1.88	3.62	0.61	1.61
14	4	5	9	1.84	4.21	0.97	1.31
15	6	6	12	1.96	3.13	0.6	2.0
16	4	4	8	2.06	3.74	0.95	1.85
17	3	5	8	1.99	4.19	0.95	1.5
18	5	7	12	1.78	3.47	0.75	1.6
19	7	8	15	2.08	4.69	1.16	1.8
20	6	8	14	2.02	4.1	0.91	1.72

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	
PSI	PHI	Total	Count ¹	%
7	5	12	1	5.0
2	4	6	2	10.0
1	1	2	3	15.0
4	0	4	4	20.0
1	3	4	5	25.0
0	0	0	6	30.0
1	1	2	7	35.0
0	1	1	8	40.0
1	0	1	9	45.0
1	0	1	10	50.0
0	0	0	11	55.0

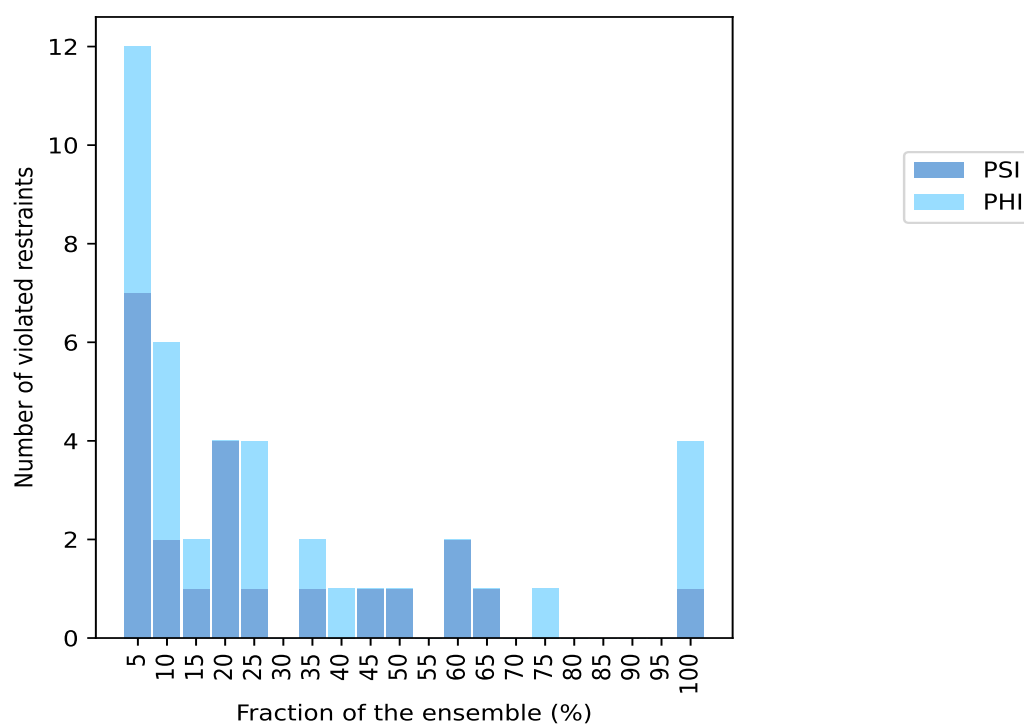
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
2	0	2	12	60.0
1	0	1	13	65.0
0	0	0	14	70.0
0	1	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
1	3	4	20	100.0

¹ Number of models with violations

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

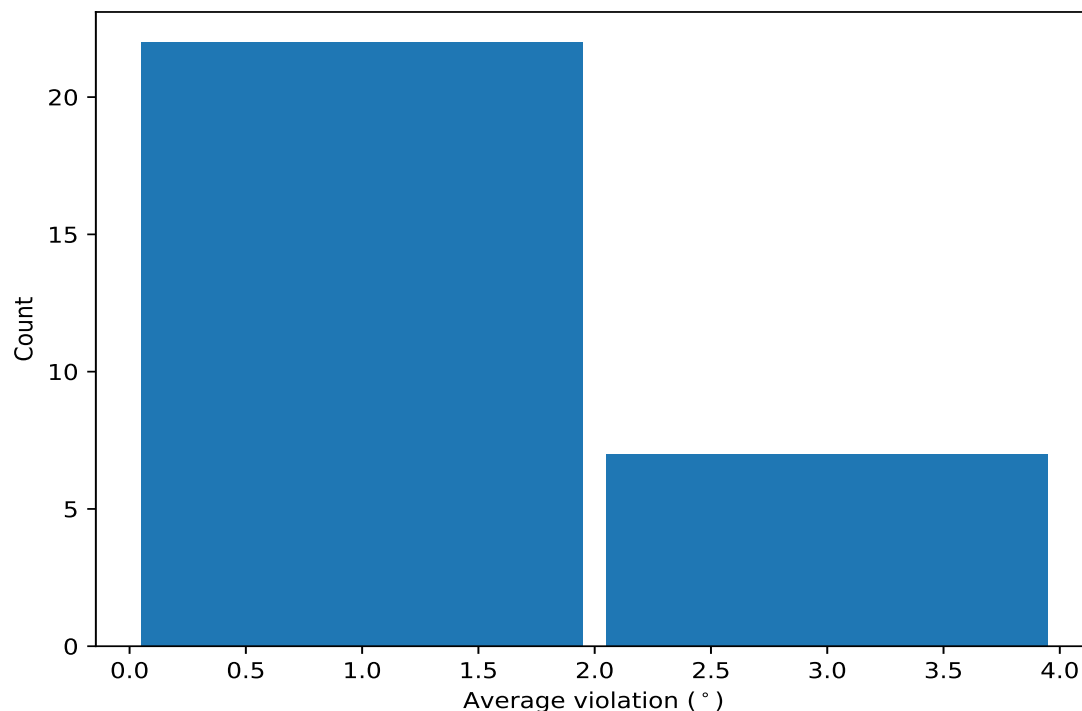


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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.

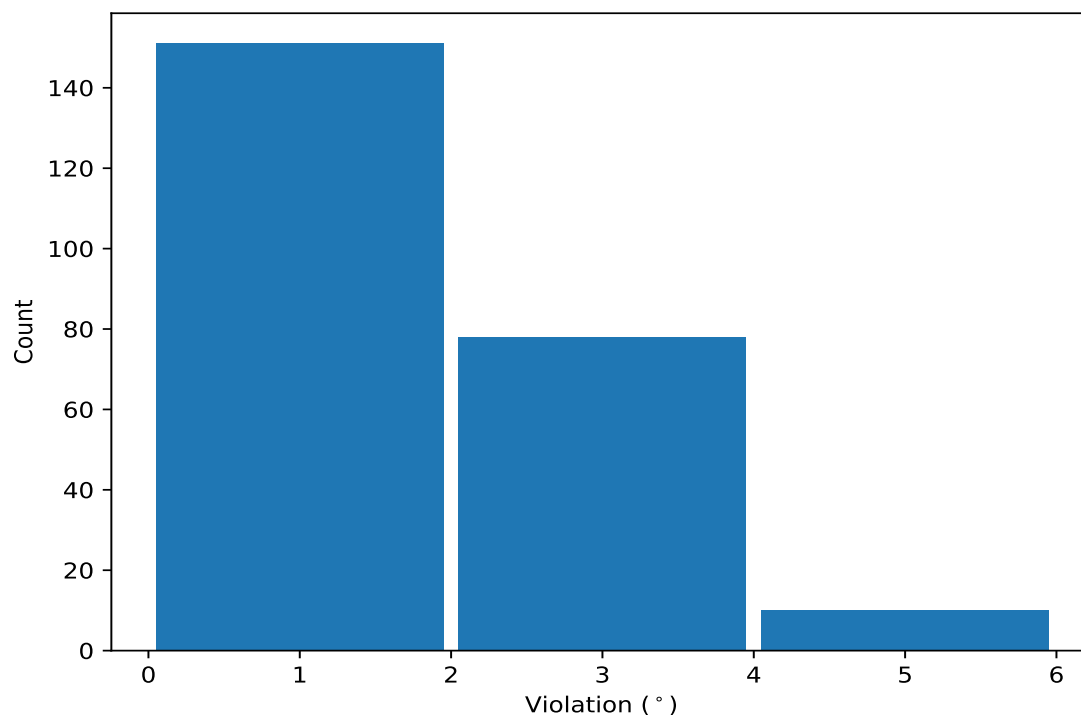
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,23)	1:265:A:ILE:C	1:266:A:GLY:N	1:266:A:GLY:CA	1:266:A:GLY:C	20	3.59	0.46	3.54
(1,96)	1:243:A:THR:N	1:243:A:THR:CA	1:243:A:THR:C	1:244:A:PHE:N	20	2.11	0.46	2.17
(1,18)	1:260:A:ARG:C	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	20	1.96	0.35	1.92
(1,19)	1:261:A:ILE:C	1:262:A:THR:N	1:262:A:THR:CA	1:262:A:THR:C	20	1.58	0.34	1.57
(1,64)	1:316:A:TYR:C	1:317:A:VAL:N	1:317:A:VAL:CA	1:317:A:VAL:C	15	1.65	0.46	1.77
(1,134)	1:287:A:GLU:N	1:287:A:GLU:CA	1:287:A:GLU:C	1:288:A:ASN:N	13	2.12	0.51	2.04
(1,138)	1:291:A:LYS:N	1:291:A:LYS:CA	1:291:A:LYS:C	1:292:A:SER:N	12	2.01	0.64	1.96
(1,112)	1:262:A:THR:N	1:262:A:THR:CA	1:262:A:THR:C	1:263:A:GLU:N	12	1.51	0.23	1.49
(1,177)	1:338:A:MET:N	1:338:A:MET:CA	1:338:A:MET:C	1:339:A:ALA:N	10	1.41	0.37	1.24
(1,179)	1:340:A:VAL:N	1:340:A:VAL:CA	1:340:A:VAL:C	1:341:A:ASN:N	9	1.51	0.46	1.42

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 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 (°)
(1,2)	1:240:A:ASP:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	9	4.98
(1,94)	1:240:A:ASP:N	1:240:A:ASP:CA	1:240:A:ASP:C	1:241:A:SER:N	9	4.95
(1,145)	1:300:A:GLY:N	1:300:A:GLY:CA	1:300:A:GLY:C	1:301:A:GLN:N	19	4.69
(1,23)	1:265:A:ILE:C	1:266:A:GLY:N	1:266:A:GLY:CA	1:266:A:GLY:C	8	4.62
(1,145)	1:300:A:GLY:N	1:300:A:GLY:CA	1:300:A:GLY:C	1:301:A:GLN:N	12	4.51
(1,23)	1:265:A:ILE:C	1:266:A:GLY:N	1:266:A:GLY:CA	1:266:A:GLY:C	7	4.42
(1,53)	1:300:A:GLY:C	1:301:A:GLN:N	1:301:A:GLN:CA	1:301:A:GLN:C	19	4.31
(1,23)	1:265:A:ILE:C	1:266:A:GLY:N	1:266:A:GLY:CA	1:266:A:GLY:C	14	4.21
(1,23)	1:265:A:ILE:C	1:266:A:GLY:N	1:266:A:GLY:CA	1:266:A:GLY:C	17	4.19
(1,145)	1:300:A:GLY:N	1:300:A:GLY:CA	1:300:A:GLY:C	1:301:A:GLN:N	20	4.1