



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2M1W / pdb_00002m1w
BMRB ID : 18882
Title : TICAM-2 TIR domain
Authors : Enokizono, Y.; Kumeta, H.; Funami, K.; Horiuchi, M.; Sarmiento, J.; Yamashita, K.; Standley, D.M.; Matsumoto, M.; Seya, T.; Inagaki, F.
Deposited on : 2012-12-07

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 ⓘ symbol.

The types of validation reports are described at

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

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

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

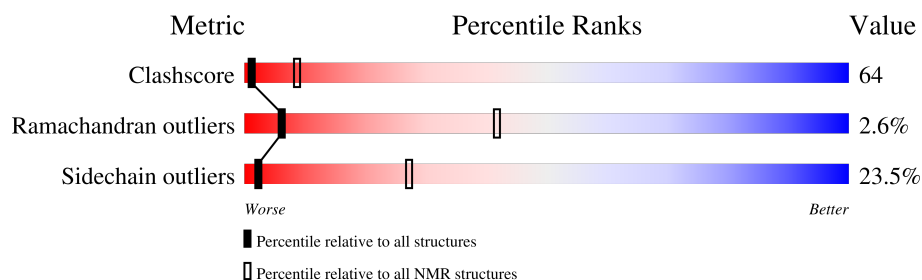
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	166	19% 54% 11% 16%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:77-A:116, A:125-A:224 (140)	0.69	2

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2488 atoms, of which 1122 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TIR domain-containing adapter molecule 2.

Mol	Chain	Residues	Atoms						Trace
1	A	166	Total	C	H	N	O	S	0
			2488	867	1122	240	254	5	

There are 6 discrepancies between the modelled and reference sequences:

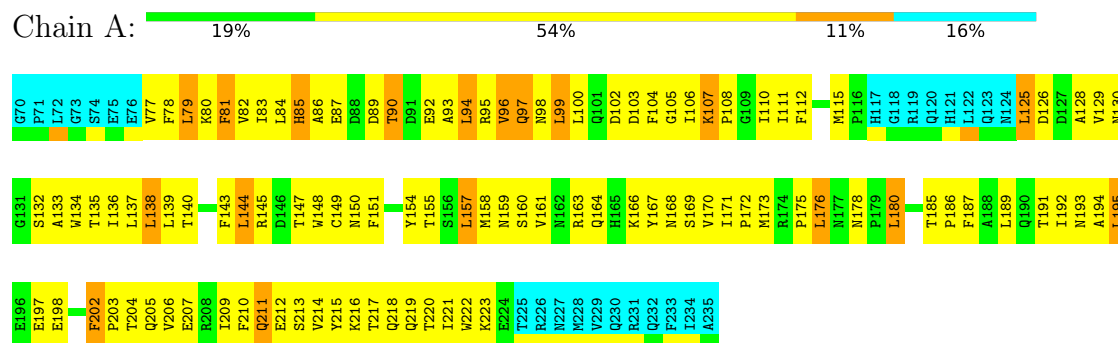
Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLY	-	expression tag	UNP Q86XR7
A	71	PRO	-	expression tag	UNP Q86XR7
A	72	LEU	-	expression tag	UNP Q86XR7
A	73	GLY	-	expression tag	UNP Q86XR7
A	74	SER	-	expression tag	UNP Q86XR7
A	117	HIS	CYS	engineered mutation	UNP Q86XR7

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

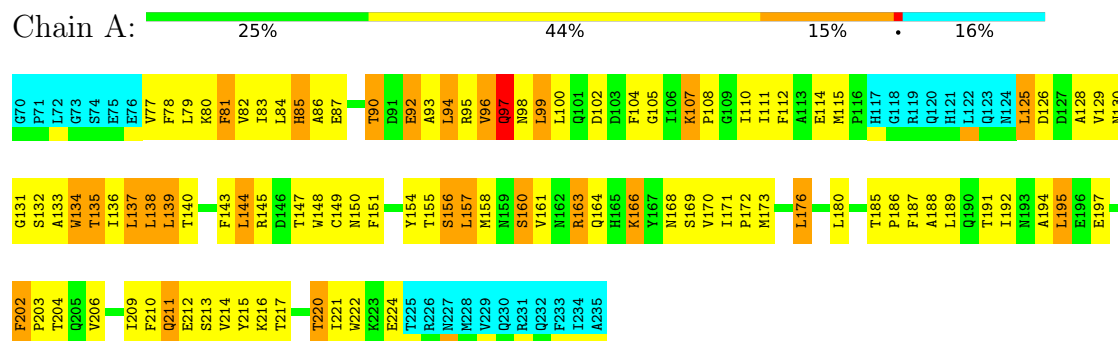
- Molecule 1: TIR domain-containing adapter molecule 2



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

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: TIR domain-containing adapter molecule 2



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Sparky	refinement	3.113
CYANA	structure solution	2.1
CYANA	geometry optimization	2.1
CYANA	refinement	2.1

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	2058
Number of shifts mapped to atoms	1853
Number of unparsed shifts	0
Number of shifts with mapping errors	205
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1156	956	1131	147±11
All	All	23120	19120	22620	2938

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 64.

5 of 871 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:PHE:CE1	1:A:128:ALA:HB2	1.12	1.79	20	8
1:A:81:PHE:CZ	1:A:83:ILE:HD11	1.12	1.79	20	18
1:A:82:VAL:HG11	1:A:128:ALA:HB1	1.08	1.22	4	3
1:A:167:TYR:CD1	1:A:221:ILE:HG22	1.05	1.85	10	1
1:A:93:ALA:HB2	1:A:138:LEU:HD21	1.02	1.25	15	13

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	140/166 (84%)	113±3 (81±2%)	23±3 (17±2%)	4±1 (3±1%)	6	42
All	All	2800/3320 (84%)	2260 (81%)	466 (17%)	74 (3%)	6	42

5 of 15 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	102	ASP	17
1	A	79	LEU	14
1	A	164	GLN	10
1	A	138	LEU	9
1	A	97	GLN	6

6.3.2 Protein sidechains ⓘ

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	129/151 (85%)	99±4 (76±3%)	30±4 (24±3%)	2	27
All	All	2580/3020 (85%)	1973 (76%)	607 (24%)	2	27

5 of 81 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	90	THR	20
1	A	97	GLN	20
1	A	99	LEU	20
1	A	176	LEU	20
1	A	195	LEU	20

6.3.3 RNA ⓘ

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 89% for the well-defined parts and 87% 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	2058
Number of shifts mapped to atoms	1853
Number of unparsed shifts	0
Number of shifts with mapping errors	205
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	11

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 205) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	PRO	HB2	1.942	.	.
1	A	71	PRO	HD2	3.555	.	.
1	A	71	PRO	HG2	2.006	.	.
1	A	72	LEU	HB2	1.613	.	.
1	A	74	SER	HB2	3.85	.	.
1	A	75	GLU	HB2	1.974	.	.
1	A	75	GLU	HG2	2.301	.	.
1	A	76	GLU	HB2	2.061	.	.
1	A	76	GLU	HG2	2.335	.	.
1	A	78	PHE	HB2	2.128	.	.
1	A	79	LEU	HB2	1.172	.	.
1	A	80	LYS	HB2	1.554	.	.
1	A	80	LYS	HD2	1.411	.	.
1	A	80	LYS	HE2	2.139	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	LYS	HG2	0.994	.	.
1	A	81	PHE	HB2	2.904	.	.
1	A	83	ILE	HG12	1.952	.	.
1	A	84	LEU	HB2	1.082	.	.
1	A	85	HIS	HB2	2.932	.	.
1	A	87	GLU	HB2	2.11	.	.
1	A	87	GLU	HG2	2.383	.	.
1	A	88	ASP	HB2	2.318	.	.
1	A	89	ASP	HB2	2.891	.	.
1	A	91	ASP	HB2	2.613	.	.
1	A	92	GLU	HB2	1.839	.	.
1	A	92	GLU	HG2	2.252	.	.
1	A	94	LEU	HB2	1.527	.	.
1	A	95	ARG	HB2	1.503	.	.
1	A	95	ARG	HD2	3.462	.	.
1	A	95	ARG	HG2	1.004	.	.
1	A	97	GLN	HB2	1.958	.	.
1	A	97	GLN	HG2	2.097	.	.
1	A	98	ASN	HB2	2.827	.	.
1	A	99	LEU	HB2	1.722	.	.
1	A	100	LEU	HB2	0.775	.	.
1	A	101	GLN	HB2	1.931	.	.
1	A	101	GLN	HG2	2.908	.	.
1	A	102	ASP	HB2	2.615	.	.
1	A	103	ASP	HB2	2.088	.	.
1	A	104	PHE	HB2	3.175	.	.
1	A	106	ILE	HG12	0.932	.	.
1	A	107	LYS	HB2	1.635	.	.
1	A	107	LYS	HD2	1.564	.	.
1	A	107	LYS	HE2	2.878	.	.
1	A	107	LYS	HG2	1.235	.	.
1	A	108	PRO	HB2	1.63	.	.
1	A	108	PRO	HD2	3.528	.	.
1	A	108	PRO	HG2	1.256	.	.
1	A	110	ILE	HG12	1.338	.	.
1	A	111	ILE	HG12	1.417	.	.
1	A	112	PHE	HB2	2.999	.	.
1	A	114	GLU	HB2	2.304	.	.
1	A	114	GLU	HG2	2.194	.	.
1	A	115	MET	HB2	1.686	.	.
1	A	115	MET	HG2	2.373	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	PRO	HB2	1.79	.	.
1	A	116	PRO	HD2	3.546	.	.
1	A	116	PRO	HG2	1.97	.	.
1	A	117	HIS	HB2	3.107	.	.
1	A	120	GLN	HB2	1.889	.	.
1	A	120	GLN	HG2	2.202	.	.
1	A	121	HIS	HB2	3.096	.	.
1	A	122	LEU	HB2	1.527	.	.
1	A	123	GLN	HB2	1.921	.	.
1	A	123	GLN	HG2	2.069	.	.
1	A	125	LEU	HB2	0.448	.	.
1	A	126	ASP	HB2	2.572	.	.
1	A	127	ASP	HB2	2.842	.	.
1	A	130	ASN	HB2	3.368	.	.
1	A	132	SER	HB2	3.294	.	.
1	A	134	TRP	HB2	2.979	.	.
1	A	136	ILE	HG12	0.995	.	.
1	A	137	LEU	HB2	1.046	.	.
1	A	138	LEU	HB2	0.992	.	.
1	A	139	LEU	HB2	1.046	.	.
1	A	141	GLU	HB2	1.946	.	.
1	A	141	GLU	HG2	2.246	.	.
1	A	142	ASN	HB2	2.73	.	.
1	A	143	PHE	HB2	3.644	.	.
1	A	144	LEU	HB2	1.661	.	.
1	A	145	ARG	HB2	1.924	.	.
1	A	145	ARG	HD2	3.213	.	.
1	A	145	ARG	HG2	1.767	.	.
1	A	146	ASP	HB2	2.784	.	.
1	A	148	TRP	HB2	2.821	.	.
1	A	149	CYS	HB2	2.939	.	.
1	A	150	ASN	HB2	3.314	.	.
1	A	151	PHE	HB2	2.626	.	.
1	A	152	GLN	HB2	1.513	.	.
1	A	152	GLN	HG2	0.906	.	.
1	A	153	PHE	HB2	2.428	.	.
1	A	154	TYR	HB2	2.549	.	.
1	A	156	SER	HB2	3.902	.	.
1	A	157	LEU	HB2	1.097	.	.
1	A	158	MET	HG2	2.594	.	.
1	A	159	ASN	HB2	2.367	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	160	SER	HB2	3.693	.	.
1	A	162	ASN	HB2	2.808	.	.
1	A	163	ARG	HB2	1.743	.	.
1	A	163	ARG	HD2	3.339	.	.
1	A	163	ARG	HG2	2.186	.	.
1	A	164	GLN	HB2	1.722	.	.
1	A	164	GLN	HG2	2.314	.	.
1	A	165	HIS	HB2	3.59	.	.
1	A	166	LYS	HB2	1.662	.	.
1	A	166	LYS	HD2	1.659	.	.
1	A	166	LYS	HE2	2.97	.	.
1	A	166	LYS	HG2	1.462	.	.
1	A	167	TYR	HB2	2.705	.	.
1	A	168	ASN	HB2	2.544	.	.
1	A	169	SER	HB2	3.7	.	.
1	A	171	ILE	HG12	1.195	.	.
1	A	172	PRO	HB2	1.724	.	.
1	A	172	PRO	HD2	3.766	.	.
1	A	172	PRO	HG2	1.76	.	.
1	A	173	MET	HB2	1.57	.	.
1	A	173	MET	HG2	1.913	.	.
1	A	174	ARG	HB2	1.628	.	.
1	A	174	ARG	HD2	2.859	.	.
1	A	175	PRO	HB2	1.28	.	.
1	A	175	PRO	HD2	3.598	.	.
1	A	175	PRO	HG2	0.777	.	.
1	A	176	LEU	HB2	1.176	.	.
1	A	177	ASN	HB2	2.288	.	.
1	A	178	ASN	HB2	2.812	.	.
1	A	179	PRO	HD2	3.214	.	.
1	A	180	LEU	HB2	0.674	.	.
1	A	181	PRO	HB2	1.606	.	.
1	A	181	PRO	HD2	3.451	.	.
1	A	181	PRO	HG2	2.048	.	.
1	A	182	ARG	HB2	1.727	.	.
1	A	182	ARG	HD2	3.179	.	.
1	A	182	ARG	HG2	1.503	.	.
1	A	183	GLU	HB2	2.039	.	.
1	A	183	GLU	HG2	2.264	.	.
1	A	184	ARG	HB2	1.311	.	.
1	A	184	ARG	HD2	2.988	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	184	ARG	HG2	1.529	.	.
1	A	186	PRO	HB2	2.133	.	.
1	A	186	PRO	HD2	2.864	.	.
1	A	186	PRO	HG2	1.627	.	.
1	A	187	PHE	HB2	3.066	.	.
1	A	189	LEU	HB2	1.295	.	.
1	A	190	GLN	HB2	1.919	.	.
1	A	190	GLN	HG2	2.176	.	.
1	A	192	ILE	HG12	1.049	.	.
1	A	193	ASN	HB2	2.704	.	.
1	A	195	LEU	HB2	1.475	.	.
1	A	196	GLU	HB2	2.035	.	.
1	A	196	GLU	HG2	1.99	.	.
1	A	197	GLU	HB2	1.291	.	.
1	A	197	GLU	HG2	0.98	.	.
1	A	198	GLU	HB2	0.682	.	.
1	A	198	GLU	HG2	2.051	.	.
1	A	199	SER	HB2	4.021	.	.
1	A	200	ARG	HB2	1.935	.	.
1	A	200	ARG	HD2	3.281	.	.
1	A	200	ARG	HG2	1.797	.	.
1	A	202	PHE	HB2	3.22	.	.
1	A	203	PRO	HB2	2.028	.	.
1	A	203	PRO	HD2	3.915	.	.
1	A	203	PRO	HG2	2.25	.	.
1	A	205	GLN	HB2	1.843	.	.
1	A	205	GLN	HG2	2.285	.	.
1	A	207	GLU	HB2	2.068	.	.
1	A	207	GLU	HG2	2.22	.	.
1	A	208	ARG	HB2	1.803	.	.
1	A	208	ARG	HD2	3.113	.	.
1	A	208	ARG	HG2	1.621	.	.
1	A	209	ILE	HG12	0.716	.	.
1	A	210	PHE	HB2	2.48	.	.
1	A	211	GLN	HB2	1.971	.	.
1	A	211	GLN	HG2	2.503	.	.
1	A	212	GLU	HB2	2.146	.	.
1	A	212	GLU	HG2	2.473	.	.
1	A	213	SER	HB2	4.012	.	.
1	A	215	TYR	HB2	3.505	.	.
1	A	216	LYS	HB2	1.946	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	216	LYS	HD2	1.792	.	.
1	A	216	LYS	HE2	3.103	.	.
1	A	216	LYS	HG2	1.648	.	.
1	A	218	GLN	HG2	2.702	.	.
1	A	219	GLN	HB2	1.334	.	.
1	A	219	GLN	HG2	1.924	.	.
1	A	221	ILE	HG12	1.083	.	.
1	A	222	TRP	HB2	1.316	.	.
1	A	223	LYS	HB2	1.781	.	.
1	A	223	LYS	HD2	1.606	.	.
1	A	223	LYS	HE2	2.89	.	.
1	A	223	LYS	HG2	1.329	.	.
1	A	224	GLU	HB2	2.095	.	.
1	A	224	GLU	HG2	2.229	.	.
1	A	226	ARG	HB2	1.328	.	.
1	A	226	ARG	HD2	2.251	.	.
1	A	226	ARG	HG2	0.952	.	.
1	A	227	ASN	HB2	2.687	.	.
1	A	228	MET	HB2	1.978	.	.
1	A	228	MET	HG2	2.5	.	.
1	A	230	GLN	HB2	1.999	.	.
1	A	230	GLN	HG2	2.354	.	.
1	A	231	ARG	HD2	3.213	.	.
1	A	232	GLN	HB2	2.009	.	.
1	A	232	GLN	HG2	2.3	.	.
1	A	233	PHE	HB2	3.0	.	.
1	A	234	ILE	HG12	1.105	.	.

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	161	-0.23 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	154	0.21 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	149	0.13 ± 0.08	None needed (< 0.5 ppm)
^{15}N	141	0.12 ± 0.34	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 89%, i.e. 1777 atoms were assigned a chemical shift out of a possible 2000. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	663/688 (96%)	271/276 (98%)	270/280 (96%)	122/132 (92%)
Sidechain	1012/1135 (89%)	686/734 (93%)	307/353 (87%)	19/48 (40%)
Aromatic	102/177 (58%)	71/88 (81%)	28/84 (33%)	3/5 (60%)
Overall	1777/2000 (89%)	1028/1098 (94%)	605/717 (84%)	144/185 (78%)

7.1.4 Statistically unusual chemical shifts [i](#)

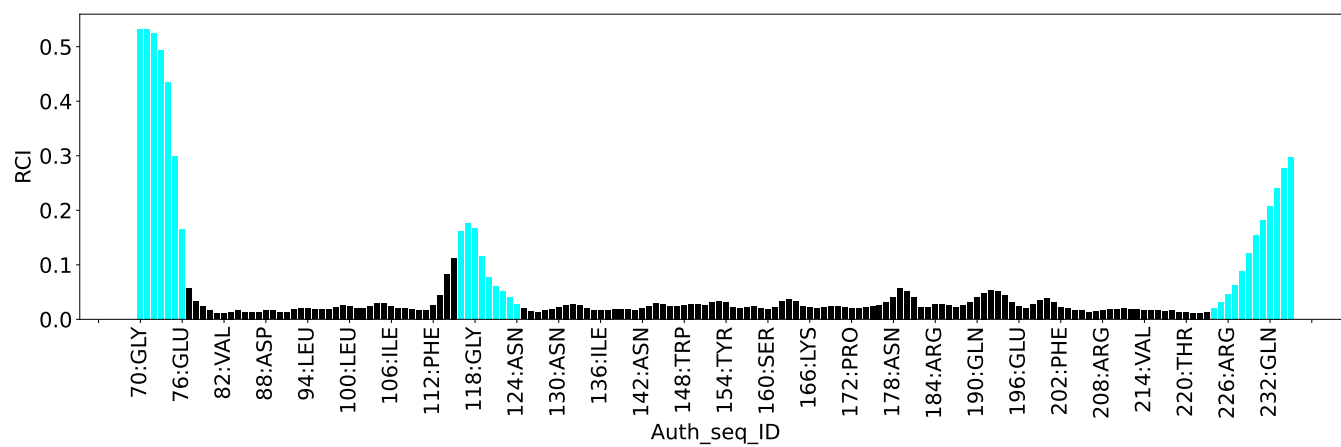
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	90	THR	HG1	6.53	0.08 – 2.19	25.5
1	A	185	THR	HG1	5.12	0.08 – 2.19	18.9
1	A	109	GLY	HA3	1.32	2.08 – 5.71	-7.1
1	A	198	GLU	HB2	0.68	1.00 – 3.05	-6.5
1	A	197	GLU	HG2	0.98	1.24 – 3.30	-6.2
1	A	222	TRP	HB2	1.32	1.51 – 4.87	-5.6
1	A	174	ARG	CD	38.16	38.57 – 47.75	-5.4
1	A	152	GLN	HG2	0.91	1.01 – 3.62	-5.4
1	A	209	ILE	HG21	-0.60	-0.56 – 2.11	-5.2
1	A	209	ILE	HG22	-0.60	-0.56 – 2.11	-5.2
1	A	209	ILE	HG23	-0.60	-0.56 – 2.11	-5.2

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2421
Intra-residue ($ i-j =0$)	727
Sequential ($ i-j =1$)	568
Medium range ($ i-j >1$ and $ i-j <5$)	482
Long range ($ i-j \geq 5$)	644
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	248
Number of unmapped restraints	0
Number of restraints per residue	16.1
Number of long range restraints per residue ¹	3.9

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.6	0.2
0.2-0.5 (Medium)	1.1	0.45
>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)	3.6	4.88
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

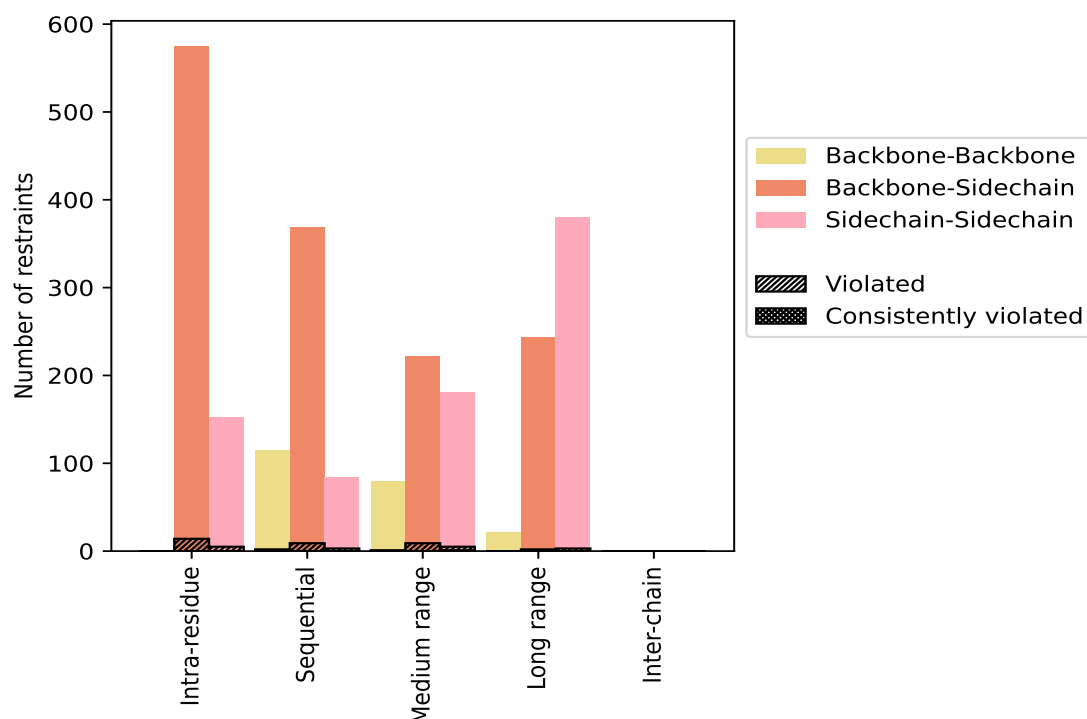
9.1 Summary of distance violations

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)	727	30.0	19	2.6	0.8	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	575	23.8	14	2.4	0.6	0	0.0	0.0
Sidechain-Sidechain	152	6.3	5	3.3	0.2	0	0.0	0.0
Sequential (i-j =1)	568	23.5	14	2.5	0.6	0	0.0	0.0
Backbone-Backbone	115	4.8	2	1.7	0.1	0	0.0	0.0
Backbone-Sidechain	369	15.2	9	2.4	0.4	0	0.0	0.0
Sidechain-Sidechain	84	3.5	3	3.6	0.1	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	482	19.9	15	3.1	0.6	1	0.2	0.0
Backbone-Backbone	79	3.3	1	1.3	0.0	0	0.0	0.0
Backbone-Sidechain	222	9.2	9	4.1	0.4	0	0.0	0.0
Sidechain-Sidechain	181	7.5	5	2.8	0.2	1	0.6	0.0
Long range (i-j ≥5)	644	26.6	5	0.8	0.2	0	0.0	0.0
Backbone-Backbone	21	0.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	243	10.0	2	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	380	15.7	3	0.8	0.1	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2421	100.0	53	2.2	2.2	1	0.0	0.0
Backbone-Backbone	215	8.9	3	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	1409	58.2	34	2.4	1.4	0	0.0	0.0
Sidechain-Sidechain	797	32.9	16	2.0	0.7	1	0.1	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	3	1	1	0	0	5	0.14	0.17	0.02	0.13
2	1	1	1	0	0	3	0.14	0.2	0.04	0.12
3	5	1	1	0	0	7	0.14	0.23	0.04	0.13
4	4	2	2	0	0	8	0.15	0.17	0.02	0.16
5	2	1	2	0	0	5	0.16	0.21	0.03	0.15
6	3	2	1	0	0	6	0.15	0.19	0.03	0.15
7	2	2	1	1	0	6	0.17	0.28	0.07	0.16
8	3	1	1	0	0	5	0.16	0.2	0.03	0.15
9	4	0	1	0	0	5	0.2	0.45	0.13	0.14
10	2	0	3	0	0	5	0.18	0.29	0.06	0.16

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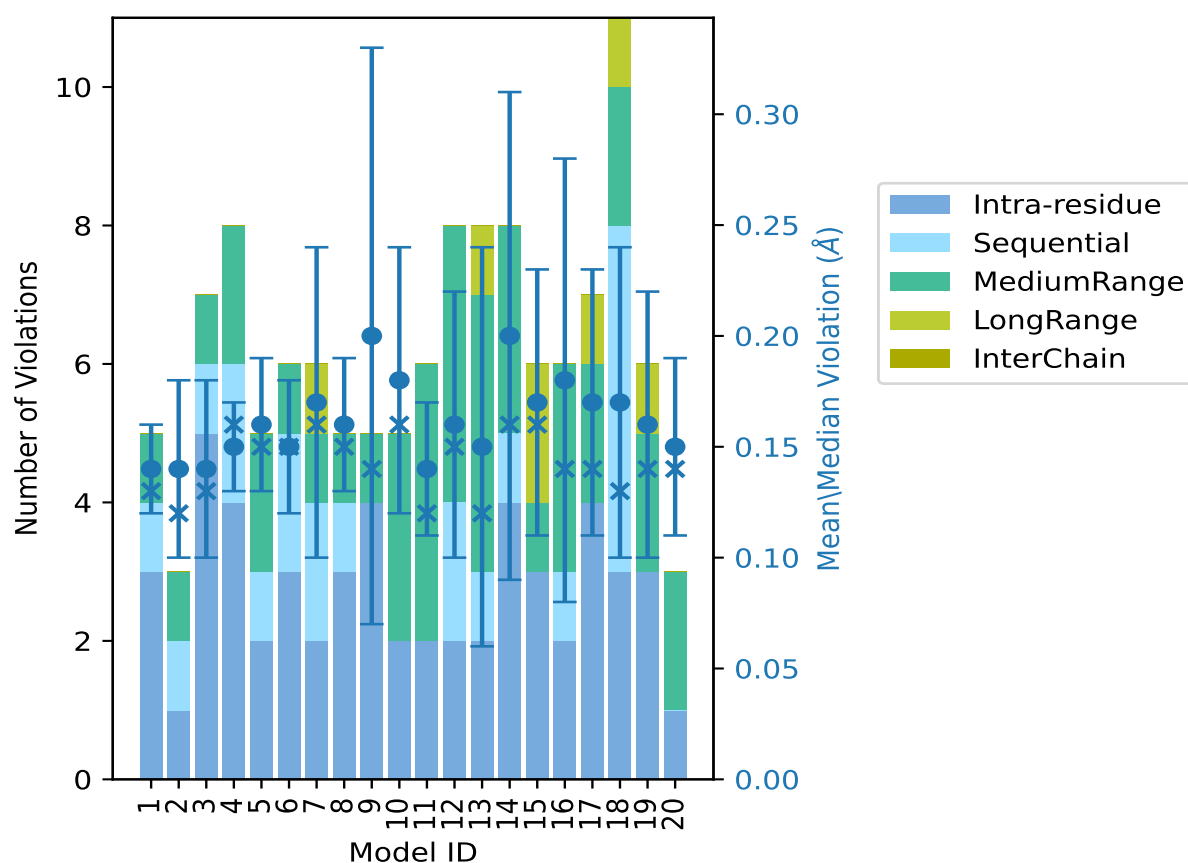
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2	0	4	0	0	6	0.14	0.21	0.03	0.12
12	2	2	4	0	0	8	0.16	0.3	0.06	0.15
13	2	1	4	1	0	8	0.15	0.39	0.09	0.12
14	4	1	3	0	0	8	0.2	0.45	0.11	0.16
15	3	0	1	2	0	6	0.17	0.27	0.06	0.16
16	2	1	3	0	0	6	0.18	0.4	0.1	0.14
17	4	0	2	1	0	7	0.17	0.3	0.06	0.14
18	3	5	2	1	0	11	0.17	0.31	0.07	0.13
19	3	0	2	1	0	6	0.16	0.28	0.06	0.14
20	1	0	2	0	0	3	0.15	0.21	0.04	0.14

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

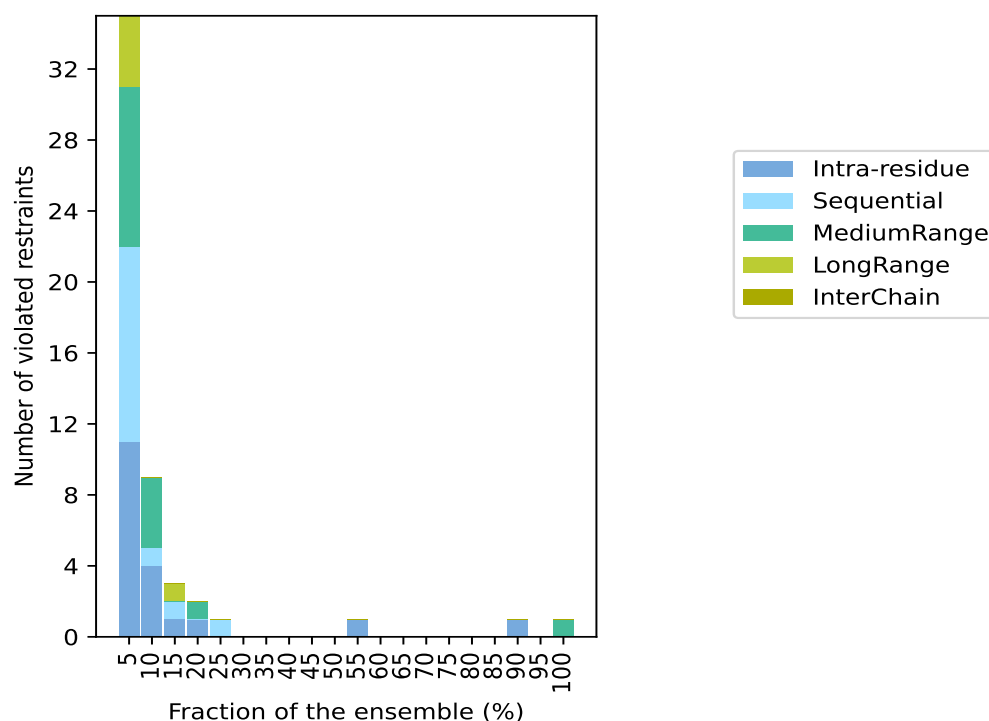
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2368(IR:708, SQ:554, MR:467, LR:639, IC:0) restraints are 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	%
11	11	9	4	0	35	1	5.0
4	1	4	0	0	9	2	10.0
1	1	0	1	0	3	3	15.0
1	0	1	0	0	2	4	20.0
0	1	0	0	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
1	0	0	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
1	0	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	0	1	0	0	1	20	100.0

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

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

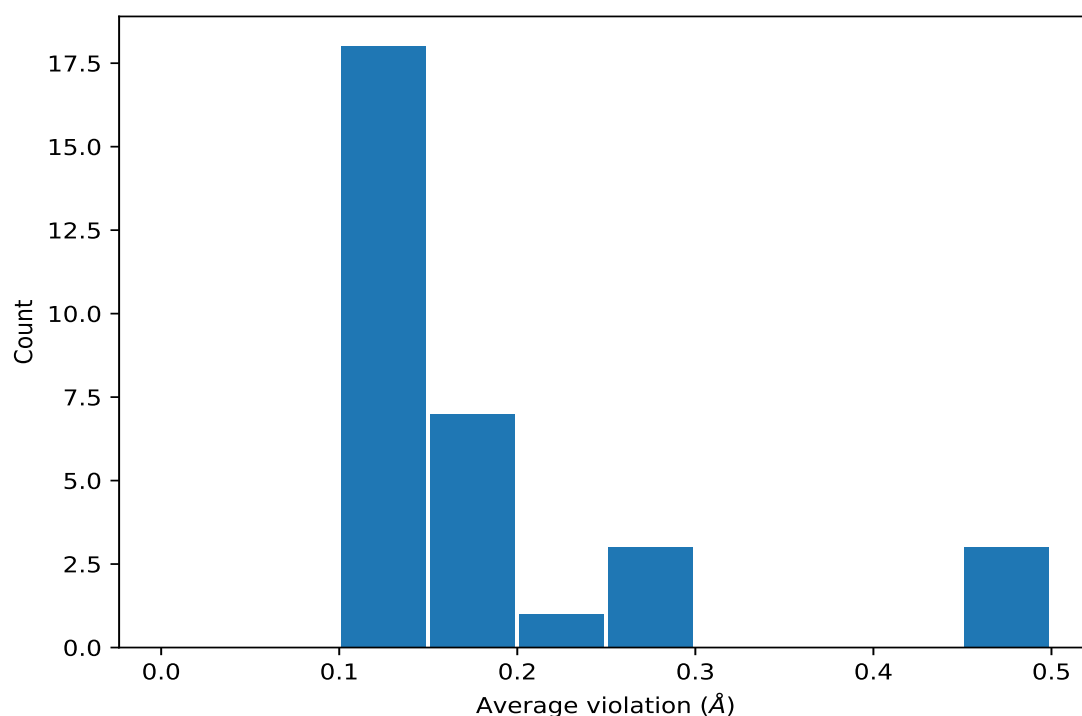
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,952)	1:211:A:GLN:HB3	1:214:A:VAL:HG11	20	0.15	0.08	0.12
(1,952)	1:211:A:GLN:HB3	1:214:A:VAL:HG12	20	0.15	0.08	0.12
(1,952)	1:211:A:GLN:HB3	1:214:A:VAL:HG13	20	0.15	0.08	0.12
(1,448)	1:214:A:VAL:H	1:214:A:VAL:HG11	18	0.19	0.02	0.19
(1,448)	1:214:A:VAL:H	1:214:A:VAL:HG12	18	0.19	0.02	0.19
(1,448)	1:214:A:VAL:H	1:214:A:VAL:HG13	18	0.19	0.02	0.19
(1,821)	1:173:A:MET:H	1:173:A:MET:HE1	11	0.13	0.02	0.12
(1,821)	1:173:A:MET:H	1:173:A:MET:HE2	11	0.13	0.02	0.12
(1,821)	1:173:A:MET:H	1:173:A:MET:HE3	11	0.13	0.02	0.12
(1,1268)	1:210:A:PHE:HA	1:211:A:GLN:HG3	5	0.13	0.02	0.12
(1,1587)	1:203:A:PRO:HA	1:206:A:VAL:HB	4	0.3	0.01	0.3
(1,1392)	1:107:A:LYS:HA	1:107:A:LYS:HE3	3	0.28	0.01	0.28
(1,1329)	1:101:A:GLN:HA	1:107:A:LYS:HE3	3	0.21	0.01	0.21
(1,1372)	1:163:A:ARG:HD3	1:164:A:GLN:H	3	0.17	0.02	0.16
(1,673)	1:115:A:MET:HA	1:115:A:MET:HE1	2	0.45	0.0	0.45
(1,673)	1:115:A:MET:HA	1:115:A:MET:HE2	2	0.45	0.0	0.45

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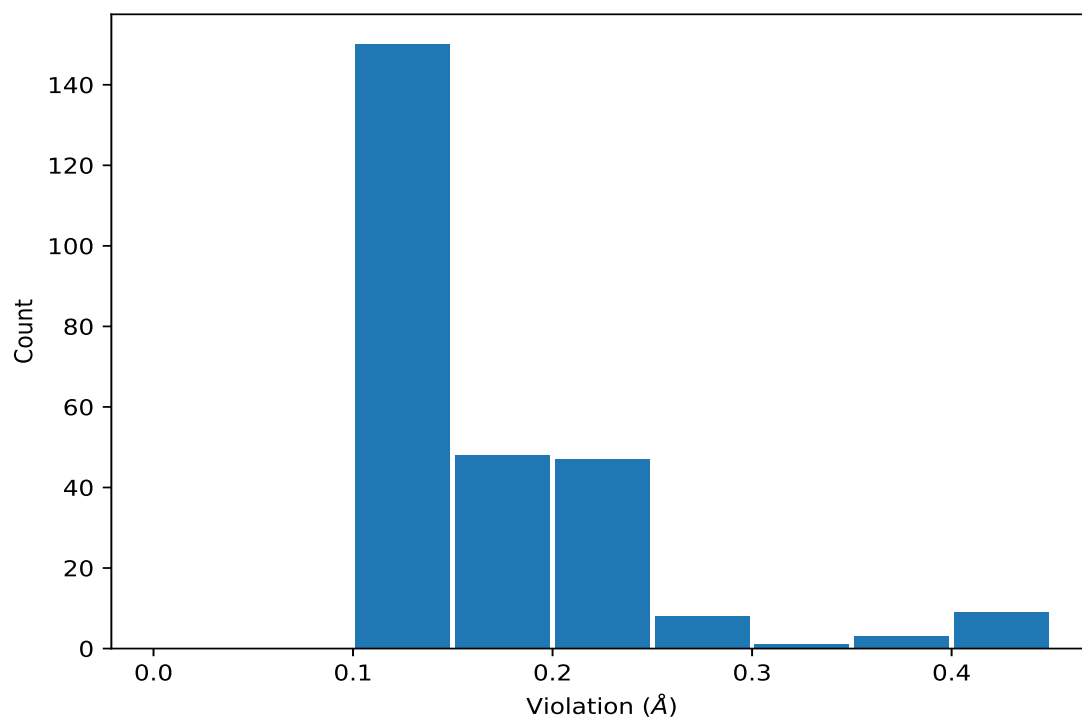
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,673)	1:115:A:MET:HA	1:115:A:MET:HE3	2	0.45	0.0	0.45
(1,1475)	1:74:A:SER:HA	1:75:A:GLU:H	2	0.28	0.0	0.28

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)
(1,673)	1:115:A:MET:HA	1:115:A:MET:HE1	9	0.45
(1,673)	1:115:A:MET:HA	1:115:A:MET:HE2	9	0.45
(1,673)	1:115:A:MET:HA	1:115:A:MET:HE3	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:115:A:MET:HA	1:115:A:MET:HE1	14	0.45
(1,673)	1:115:A:MET:HA	1:115:A:MET:HE2	14	0.45
(1,673)	1:115:A:MET:HA	1:115:A:MET:HE3	14	0.45
(1,952)	1:211:A:GLN:HB3	1:214:A:VAL:HG11	16	0.4
(1,952)	1:211:A:GLN:HB3	1:214:A:VAL:HG12	16	0.4
(1,952)	1:211:A:GLN:HB3	1:214:A:VAL:HG13	16	0.4
(1,952)	1:211:A:GLN:HB3	1:214:A:VAL:HG11	13	0.39
(1,952)	1:211:A:GLN:HB3	1:214:A:VAL:HG12	13	0.39
(1,952)	1:211:A:GLN:HB3	1:214:A:VAL:HG13	13	0.39
(1,1587)	1:203:A:PRO:HA	1:206:A:VAL:HB	18	0.31
(1,1587)	1:203:A:PRO:HA	1:206:A:VAL:HB	12	0.3
(1,1392)	1:107:A:LYS:HA	1:107:A:LYS:HE3	17	0.3
(1,1587)	1:203:A:PRO:HA	1:206:A:VAL:HB	10	0.29
(1,1587)	1:203:A:PRO:HA	1:206:A:VAL:HB	14	0.28
(1,1475)	1:74:A:SER:HA	1:75:A:GLU:H	7	0.28

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

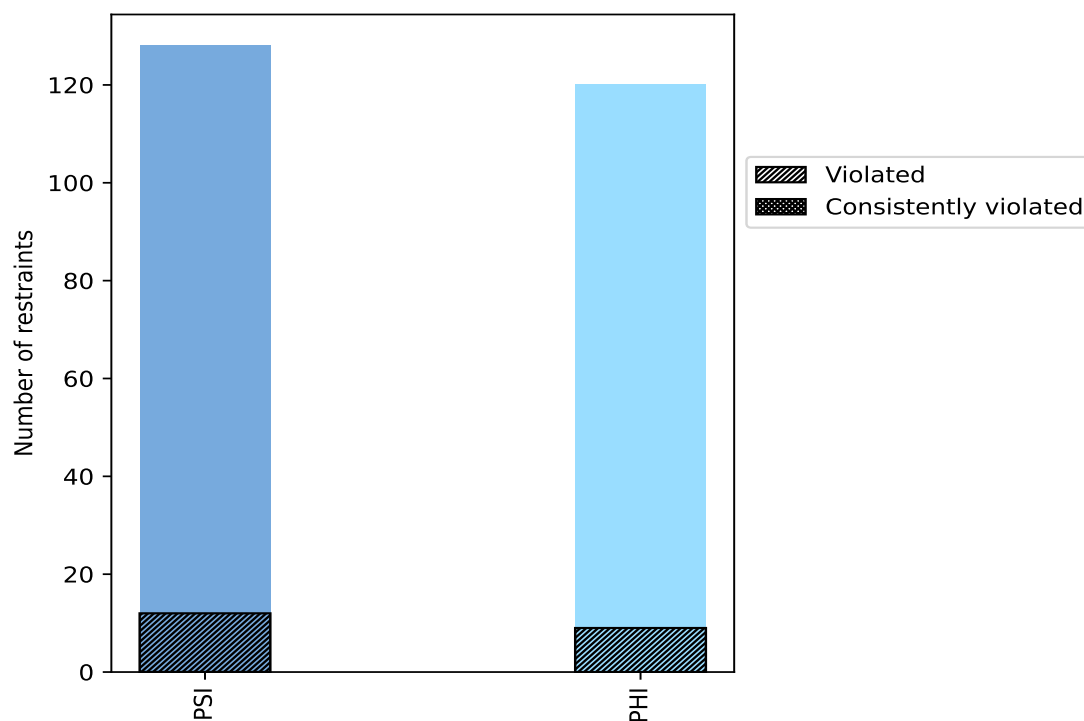
10.1 Summary of dihedral-angle violations [i](#)

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	128	51.6	12	9.4	4.8	0	0.0	0.0
PHI	120	48.4	9	7.5	3.6	0	0.0	0.0
Total	248	100.0	21	8.5	8.5	0	0.0	0.0

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

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



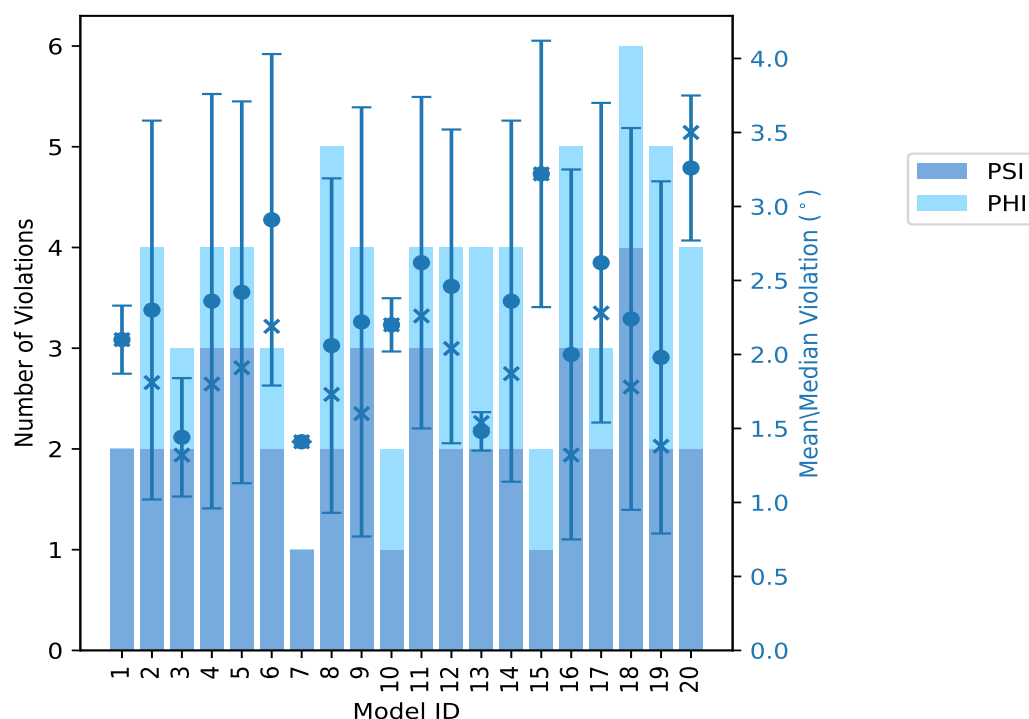
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	2	0	2	2.1	2.34	0.23	2.1
2	2	2	4	2.3	4.4	1.28	1.81
3	2	1	3	1.44	1.98	0.4	1.32
4	3	1	4	2.36	4.71	1.4	1.8
5	3	1	4	2.42	4.58	1.29	1.91
6	2	1	3	2.91	4.5	1.12	2.19
7	1	0	1	1.41	1.41	0.0	1.41
8	2	3	5	2.06	4.23	1.13	1.73
9	3	1	4	2.22	4.61	1.45	1.6
10	1	1	2	2.2	2.38	0.18	2.2
11	3	1	4	2.62	4.47	1.12	2.26
12	2	2	4	2.46	4.24	1.06	2.04
13	2	2	4	1.48	1.61	0.13	1.54
14	2	2	4	2.36	4.41	1.22	1.87
15	1	1	2	3.22	4.12	0.9	3.22
16	3	2	5	2.0	4.41	1.25	1.32
17	2	1	3	2.62	4.08	1.08	2.28
18	4	2	6	2.24	4.88	1.29	1.78
19	2	3	5	1.98	4.3	1.19	1.38
20	2	2	4	3.26	3.6	0.49	3.5

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	4	11	1	5.0
1	1	2	2	10.0
2	2	4	3	15.0
0	0	0	4	20.0
0	1	1	5	25.0
0	0	0	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

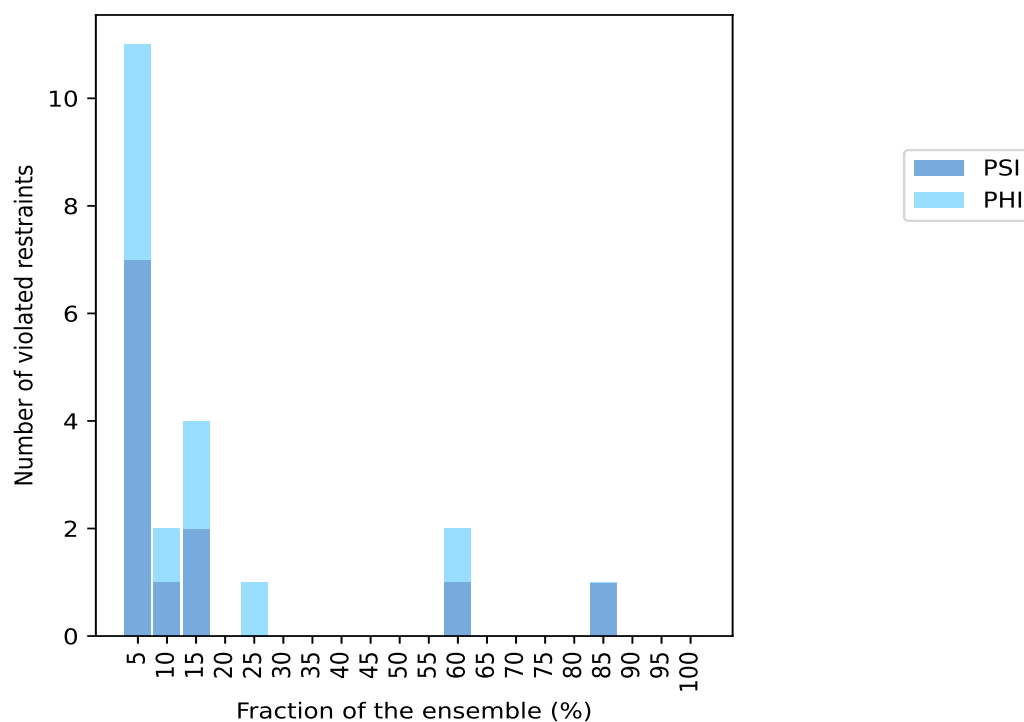
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
1	1	2	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

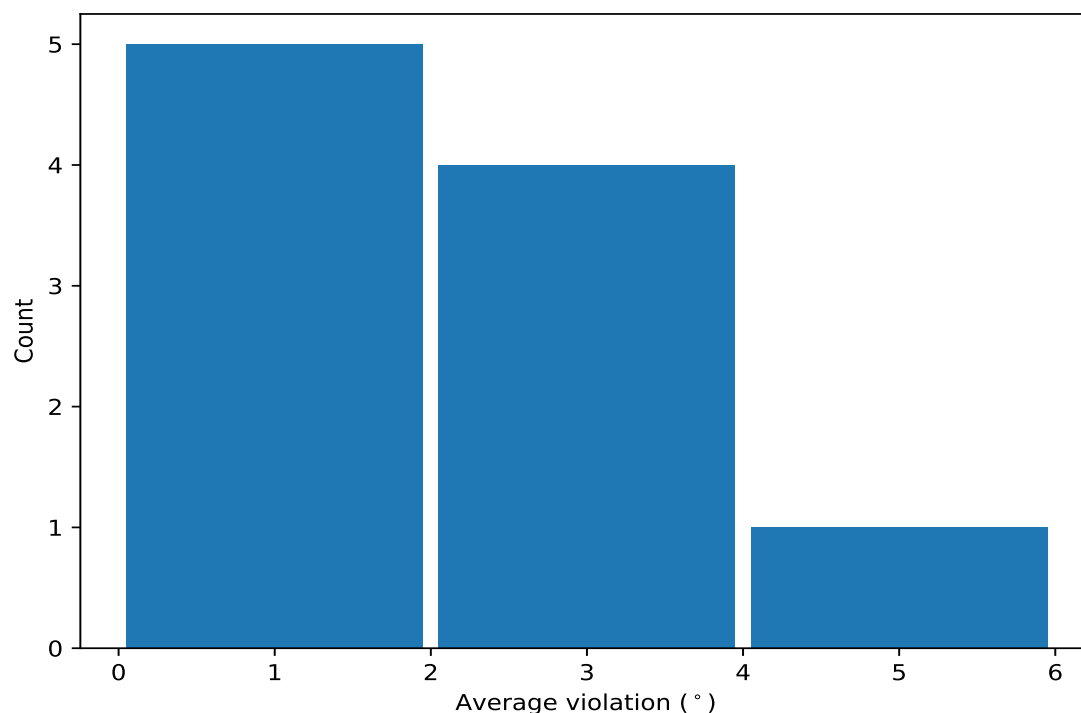


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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.

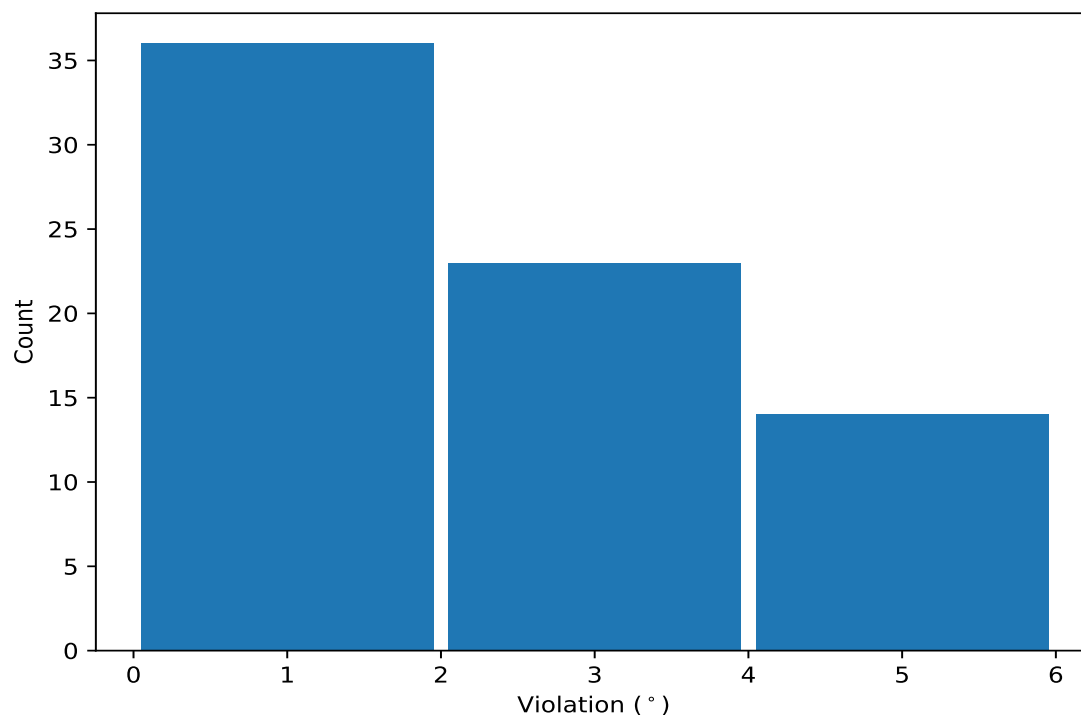
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,40)	1:99:A:LEU:N	1:99:A:LEU:CA	1:99:A:LEU:C	1:100:A:LEU:N	17	1.95	1.0	1.51
(1,173)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:ALA:N	12	4.46	0.2	4.44
(1,176)	1:188:A:ALA:C	1:189:A:LEU:N	1:189:A:LEU:CA	1:189:A:LEU:C	12	2.16	0.09	2.13
(1,155)	1:176:A:LEU:C	1:177:A:ASN:N	1:177:A:ASN:CA	1:177:A:ASN:C	5	1.44	0.29	1.26
(1,45)	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	1:104:A:PHE:N	3	2.36	0.83	2.28
(1,136)	1:161:A:VAL:N	1:161:A:VAL:CA	1:161:A:VAL:C	1:162:A:ASN:N	3	2.07	0.57	2.34
(1,44)	1:102:A:ASP:C	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	3	2.07	1.09	1.49
(1,203)	1:205:A:GLN:C	1:206:A:VAL:N	1:206:A:VAL:CA	1:206:A:VAL:C	3	1.82	0.4	1.62
(1,39)	1:98:A:ASN:C	1:99:A:LEU:N	1:99:A:LEU:CA	1:99:A:LEU:C	2	1.82	0.6	1.82
(1,64)	1:113:A:ALA:N	1:113:A:ALA:CA	1:113:A:ALA:C	1:114:A:GLU:N	2	1.16	0.12	1.16

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 (°)
(1,173)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:ALA:N	18	4.88
(1,173)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:ALA:N	4	4.71
(1,173)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:ALA:N	9	4.61
(1,173)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:ALA:N	5	4.58
(1,173)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:ALA:N	6	4.5
(1,173)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:ALA:N	11	4.47
(1,173)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:ALA:N	14	4.41
(1,173)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:ALA:N	16	4.41
(1,173)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:ALA:N	2	4.4
(1,40)	1:99:A:LEU:N	1:99:A:LEU:CA	1:99:A:LEU:C	1:100:A:LEU:N	19	4.3