



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2M1X / pdb_00002m1x
BMRB ID : 18883
Title : TICAM-1 TIR domain structure
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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

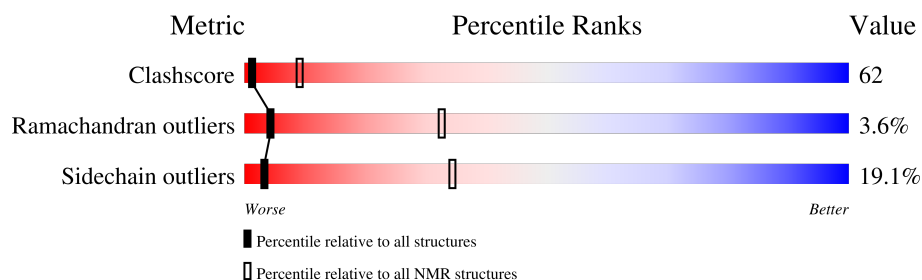
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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	168	

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:395-A:427, A:443-A:533 (124)	0.60	10

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2316 atoms, of which 1051 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	160	Total	C	H	N	O	S	0
			2316	791	1051	229	237	8	

There are 10 discrepancies between the modelled and reference sequences:

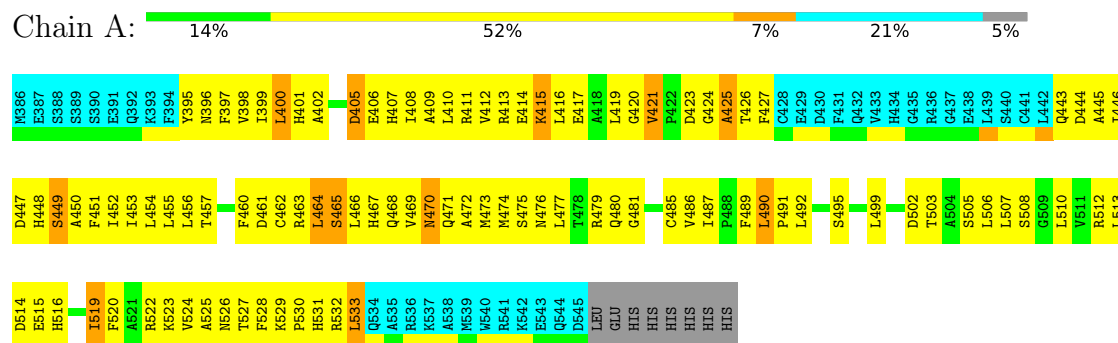
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	expression tag	UNP Q8IUC6
A	434	HIS	PRO	engineered mutation	UNP Q8IUC6
A	546	LEU	-	expression tag	UNP Q8IUC6
A	547	GLU	-	expression tag	UNP Q8IUC6
A	548	HIS	-	expression tag	UNP Q8IUC6
A	549	HIS	-	expression tag	UNP Q8IUC6
A	550	HIS	-	expression tag	UNP Q8IUC6
A	551	HIS	-	expression tag	UNP Q8IUC6
A	552	HIS	-	expression tag	UNP Q8IUC6
A	553	HIS	-	expression tag	UNP Q8IUC6

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.

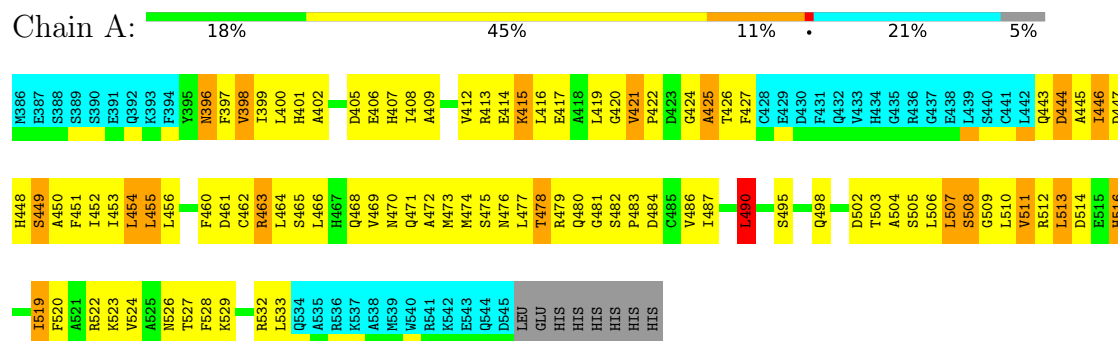
- Molecule 1: TIR domain-containing adapter molecule 1



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

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

- Molecule 1: TIR domain-containing adapter molecule 1



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	2135
Number of shifts mapped to atoms	1848
Number of unparsed shifts	0
Number of shifts with mapping errors	287
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

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	0.82±0.00	0±0/989 (0.0± 0.0%)	1.11±0.01	0±0/1343 (0.0± 0.0%)
All	All	0.82	0/19780 (0.0%)	1.11	10/26860 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	490	LEU	O-C-N	5.47	124.55	121.27	2	10

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	969	829	972	121±8
All	All	19380	16580	19440	2425

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 62.

5 of 714 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:469:VAL:HG11	1:A:486:VAL:HG22	1.07	1.22	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:397:PHE:CD2	1:A:453:ILE:HD12	0.99	1.92	13	15
1:A:473:MET:HE1	1:A:486:VAL:HG23	0.95	1.37	7	7
1:A:419:LEU:HD13	1:A:524:VAL:HG11	0.95	1.37	19	19
1:A:492:LEU:HD21	1:A:515:GLU:CD	0.95	1.86	16	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	124/168 (74%)	96±3 (77±3%)	24±3 (19±3%)	4±1 (4±1%)	4	32
All	All	2480/3360 (74%)	1914 (77%)	477 (19%)	89 (4%)	4	32

5 of 22 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	425	ALA	20
1	A	450	ALA	8
1	A	463	ARG	8
1	A	420	GLY	6
1	A	417	GLU	5

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	108/148 (73%)	87±3 (81±3%)	21±3 (19±3%)	3	34
All	All	2160/2960 (73%)	1748 (81%)	412 (19%)	3	34

5 of 66 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	415	LYS	20
1	A	421	VAL	20
1	A	519	ILE	20
1	A	495	SER	19
1	A	405	ASP	17

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 94% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *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	2135
Number of shifts mapped to atoms	1848
Number of unparsed shifts	0
Number of shifts with mapping errors	287
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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 287) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	386	MET	HB2	2.169	.	.
1	A	386	MET	HG2	2.604	.	.
1	A	387	GLU	HB2	1.969	.	.
1	A	387	GLU	HG2	2.313	.	.
1	A	388	SER	HB2	3.869	.	.
1	A	389	SER	HB2	3.895	.	.
1	A	390	SER	HB2	3.871	.	.
1	A	391	GLU	HB2	1.953	.	.
1	A	391	GLU	HG2	2.26	.	.
1	A	392	GLN	HB2	1.989	.	.
1	A	392	GLN	HG2	2.277	.	.
1	A	393	LYS	HB2	1.294	.	.
1	A	393	LYS	HD2	1.504	.	.
1	A	393	LYS	HE2	2.775	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	393	LYS	HG2	0.978	.	.
1	A	394	PHE	HB2	1.586	.	.
1	A	395	TYR	HB2	2.839	.	.
1	A	396	ASN	HB2	2.581	.	.
1	A	397	PHE	HB2	2.687	.	.
1	A	399	ILE	HG12	0.751	.	.
1	A	400	LEU	HB2	1.791	.	.
1	A	401	HIS	HB2	2.715	.	.
1	A	403	ARG	HB2	1.877	.	.
1	A	403	ARG	HD2	3.075	.	.
1	A	403	ARG	HG2	1.629	.	.
1	A	405	ASP	HB2	2.773	.	.
1	A	406	GLU	HB2	2.146	.	.
1	A	406	GLU	HG2	2.056	.	.
1	A	407	HIS	HB2	3.234	.	.
1	A	408	ILE	HG12	0.751	.	.
1	A	410	LEU	HB2	1.503	.	.
1	A	411	ARG	HB2	1.72	.	.
1	A	411	ARG	HD2	2.892	.	.
1	A	411	ARG	HG2	1.568	.	.
1	A	413	ARG	HB2	1.813	.	.
1	A	413	ARG	HD2	2.861	.	.
1	A	413	ARG	HG2	1.502	.	.
1	A	414	GLU	HB2	2.068	.	.
1	A	414	GLU	HG2	2.273	.	.
1	A	415	LYS	HB2	1.88	.	.
1	A	415	LYS	HD2	1.777	.	.
1	A	415	LYS	HE2	2.932	.	.
1	A	415	LYS	HG2	1.543	.	.
1	A	416	LEU	HB2	0.696	.	.
1	A	417	GLU	HB2	2.031	.	.
1	A	417	GLU	HG2	2.787	.	.
1	A	419	LEU	HB2	1.776	.	.
1	A	422	PRO	HB2	1.887	.	.
1	A	422	PRO	HD2	3.516	.	.
1	A	422	PRO	HG2	1.731	.	.
1	A	423	ASP	HB2	2.794	.	.
1	A	427	PHE	HB2	2.477	.	.
1	A	428	CYS	HB2	2.149	.	.
1	A	429	GLU	HB2	1.9	.	.
1	A	429	GLU	HG2	2.272	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	430	ASP	HB2	2.624	.	.
1	A	431	PHE	HB2	2.946	.	.
1	A	432	GLN	HB2	1.889	.	.
1	A	432	GLN	HG2	2.273	.	.
1	A	434	HIS	HB2	3.159	.	.
1	A	436	ARG	HB2	1.787	.	.
1	A	436	ARG	HD2	3.206	.	.
1	A	436	ARG	HG2	1.678	.	.
1	A	438	GLU	HB2	1.994	.	.
1	A	438	GLU	HG2	2.271	.	.
1	A	439	LEU	HB2	1.2	.	.
1	A	440	SER	HB2	3.929	.	.
1	A	442	LEU	HB2	1.56	.	.
1	A	443	GLN	HB2	1.991	.	.
1	A	443	GLN	HG2	2.325	.	.
1	A	444	ASP	HB2	2.711	.	.
1	A	446	ILE	HG12	1.227	.	.
1	A	447	ASP	HB2	2.49	.	.
1	A	448	HIS	HB2	2.822	.	.
1	A	449	SER	HB2	3.347	.	.
1	A	451	PHE	HB2	2.957	.	.
1	A	452	ILE	HG12	1.258	.	.
1	A	453	ILE	HG12	1.201	.	.
1	A	454	LEU	HB2	1.528	.	.
1	A	455	LEU	HB2	0.807	.	.
1	A	456	LEU	HB2	1.329	.	.
1	A	458	SER	HB2	3.983	.	.
1	A	459	ASN	HB2	2.753	.	.
1	A	460	PHE	HB2	3.377	.	.
1	A	461	ASP	HB2	2.352	.	.
1	A	462	CYS	HB2	2.983	.	.
1	A	463	ARG	HB2	1.872	.	.
1	A	463	ARG	HD2	3.173	.	.
1	A	463	ARG	HG2	1.445	.	.
1	A	464	LEU	HB2	1.39	.	.
1	A	465	SER	HB2	3.619	.	.
1	A	466	LEU	HB2	1.713	.	.
1	A	467	HIS	HB2	3.408	.	.
1	A	468	GLN	HB2	1.964	.	.
1	A	468	GLN	HG2	2.428	.	.
1	A	470	ASN	HB2	2.729	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	471	GLN	HB2	2.028	.	.
1	A	471	GLN	HG2	2.211	.	.
1	A	473	MET	HB2	2.084	.	.
1	A	473	MET	HG2	2.457	.	.
1	A	474	MET	HB2	2.145	.	.
1	A	474	MET	HG2	2.636	.	.
1	A	475	SER	HB2	3.945	.	.
1	A	476	ASN	HB2	2.795	.	.
1	A	477	LEU	HB2	1.64	.	.
1	A	479	ARG	HB2	1.805	.	.
1	A	479	ARG	HD2	3.201	.	.
1	A	479	ARG	HG2	1.615	.	.
1	A	480	GLN	HB2	2.035	.	.
1	A	480	GLN	HG2	2.4	.	.
1	A	482	SER	HB2	3.897	.	.
1	A	483	PRO	HB2	2.043	.	.
1	A	483	PRO	HD2	3.785	.	.
1	A	483	PRO	HG2	2.045	.	.
1	A	484	ASP	HB2	2.749	.	.
1	A	485	CYS	HB2	2.89	.	.
1	A	487	ILE	HG12	1.298	.	.
1	A	488	PRO	HB2	1.99	.	.
1	A	488	PRO	HD2	3.973	.	.
1	A	488	PRO	HG2	1.792	.	.
1	A	489	PHE	HB2	2.611	.	.
1	A	490	LEU	HB2	1.237	.	.
1	A	491	PRO	HB2	1.872	.	.
1	A	491	PRO	HD2	4.229	.	.
1	A	491	PRO	HG2	1.688	.	.
1	A	492	LEU	HB2	1.17	.	.
1	A	493	GLU	HB2	1.817	.	.
1	A	493	GLU	HG2	2.276	.	.
1	A	494	SER	HB2	3.82	.	.
1	A	495	SER	HB2	3.785	.	.
1	A	496	PRO	HB2	1.925	.	.
1	A	496	PRO	HD2	3.576	.	.
1	A	496	PRO	HG2	1.717	.	.
1	A	498	GLN	HB2	2.158	.	.
1	A	498	GLN	HG2	2.383	.	.
1	A	499	LEU	HB2	1.577	.	.
1	A	500	SER	HB2	4.079	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	501	SER	HB2	4.007	.	.
1	A	502	ASP	HB2	2.681	.	.
1	A	505	SER	HB2	3.999	.	.
1	A	506	LEU	HB2	1.554	.	.
1	A	507	LEU	HB2	1.7	.	.
1	A	508	SER	HB2	4.007	.	.
1	A	510	LEU	HB2	1.558	.	.
1	A	512	ARG	HB2	1.678	.	.
1	A	512	ARG	HD2	3.101	.	.
1	A	512	ARG	HG2	1.392	.	.
1	A	513	LEU	HB2	1.171	.	.
1	A	514	ASP	HB2	2.363	.	.
1	A	515	GLU	HB2	1.388	.	.
1	A	515	GLU	HG2	1.08	.	.
1	A	516	HIS	HB2	3.168	.	.
1	A	517	SER	HB2	3.815	.	.
1	A	518	GLN	HB2	2.163	.	.
1	A	518	GLN	HG2	2.562	.	.
1	A	519	ILE	HG12	1.095	.	.
1	A	520	PHE	HB2	2.926	.	.
1	A	522	ARG	HB2	1.947	.	.
1	A	522	ARG	HD2	3.198	.	.
1	A	522	ARG	HG2	1.707	.	.
1	A	523	LYS	HB2	1.652	.	.
1	A	523	LYS	HD2	1.643	.	.
1	A	523	LYS	HE2	2.888	.	.
1	A	523	LYS	HG2	1.365	.	.
1	A	526	ASN	HB2	2.787	.	.
1	A	528	PHE	HB2	2.68	.	.
1	A	529	LYS	HB2	1.677	.	.
1	A	529	LYS	HD2	1.793	.	.
1	A	529	LYS	HE2	3.168	.	.
1	A	529	LYS	HG2	1.592	.	.
1	A	530	PRO	HB2	2.082	.	.
1	A	530	PRO	HD2	3.931	.	.
1	A	530	PRO	HG2	2.201	.	.
1	A	531	HIS	HB2	3.203	.	.
1	A	532	ARG	HB2	2.11	.	.
1	A	532	ARG	HD2	3.339	.	.
1	A	532	ARG	HG2	1.633	.	.
1	A	533	LEU	HB2	1.756	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	534	GLN	HB2	2.131	.	.
1	A	534	GLN	HG2	2.475	.	.
1	A	536	ARG	HB2	2.025	.	.
1	A	536	ARG	HD2	3.233	.	.
1	A	536	ARG	HG2	1.829	.	.
1	A	537	LYS	HB2	1.605	.	.
1	A	537	LYS	HD2	1.607	.	.
1	A	537	LYS	HE2	2.882	.	.
1	A	537	LYS	HG2	0.853	.	.
1	A	539	MET	HB2	2.186	.	.
1	A	539	MET	HG2	2.637	.	.
1	A	540	TRP	HB2	3.155	.	.
1	A	541	ARG	HB2	1.819	.	.
1	A	541	ARG	HD2	3.099	.	.
1	A	541	ARG	HG2	1.604	.	.
1	A	542	LYS	HB2	1.887	.	.
1	A	542	LYS	HD2	1.698	.	.
1	A	542	LYS	HE2	2.975	.	.
1	A	542	LYS	HG2	1.409	.	.
1	A	543	GLU	HB2	2.051	.	.
1	A	543	GLU	HG2	2.288	.	.
1	A	544	GLN	HB2	1.664	.	.
1	A	544	GLN	HG2	1.504	.	.
1	A	545	ASP	HB2	2.682	.	.
1	A	546	LEU	H	7.882	.	1
1	A	546	LEU	HA	4.101	.	1
1	A	546	LEU	HB2	1.527	.	.
1	A	546	LEU	HB3	1.7	.	.
1	A	546	LEU	HD11	0.824	.	.
1	A	546	LEU	HD12	0.824	.	.
1	A	546	LEU	HD13	0.824	.	.
1	A	546	LEU	HD21	0.846	.	.
1	A	546	LEU	HD22	0.846	.	.
1	A	546	LEU	HD23	0.846	.	.
1	A	546	LEU	HG	1.52	.	1
1	A	546	LEU	C	178.697	.	1
1	A	546	LEU	CA	56.611	.	1
1	A	546	LEU	CB	42.028	.	1
1	A	546	LEU	CD1	23.317	.	.
1	A	546	LEU	CD2	26.04	.	.
1	A	546	LEU	CG	26.977	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	546	LEU	N	120.836	.	1
1	A	547	GLU	H	8.027	.	1
1	A	547	GLU	HA	4.055	.	1
1	A	547	GLU	HB2	1.875	.	.
1	A	547	GLU	HB3	1.875	.	.
1	A	547	GLU	HG2	2.15	.	.
1	A	547	GLU	HG3	2.238	.	.
1	A	547	GLU	C	177.245	.	1
1	A	547	GLU	CA	57.473	.	1
1	A	547	GLU	CB	29.478	.	1
1	A	547	GLU	CG	35.739	.	1
1	A	547	GLU	N	118.309	.	1
1	A	548	HIS	H	8.042	.	1
1	A	548	HIS	HA	4.539	.	1
1	A	548	HIS	HB2	3.084	.	.
1	A	548	HIS	HB3	3.19	.	.
1	A	548	HIS	HD2	7.178	.	1
1	A	548	HIS	C	174.796	.	1
1	A	548	HIS	CA	55.94	.	1
1	A	548	HIS	CB	28.547	.	1
1	A	548	HIS	CD2	120.197	.	1
1	A	548	HIS	N	116.181	.	1
1	A	549	HIS	H	8.205	.	1
1	A	549	HIS	HA	4.592	.	1
1	A	549	HIS	HB2	3.1	.	.
1	A	549	HIS	HB3	3.195	.	.
1	A	549	HIS	HD2	7.204	.	1
1	A	549	HIS	C	174.413	.	1
1	A	549	HIS	CA	55.881	.	1
1	A	549	HIS	CB	28.677	.	1
1	A	549	HIS	CD2	119.958	.	1
1	A	549	HIS	N	117.324	.	1
1	A	550	HIS	H	8.385	.	1
1	A	550	HIS	HA	4.654	.	1
1	A	550	HIS	HB2	3.102	.	.
1	A	550	HIS	HB3	3.192	.	.
1	A	550	HIS	HD2	7.205	.	1
1	A	550	HIS	C	174.278	.	1
1	A	550	HIS	CA	55.422	.	1
1	A	550	HIS	CB	29.128	.	1
1	A	550	HIS	CD2	119.588	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	550	HIS	N	118.46	.	1
1	A	551	HIS	H	8.492	.	1
1	A	551	HIS	HA	4.648	.	1
1	A	551	HIS	HB2	3.1	.	.
1	A	551	HIS	HB3	3.192	.	.
1	A	551	HIS	C	174.07	.	1
1	A	551	HIS	CA	55.524	.	1
1	A	551	HIS	CB	29.322	.	1
1	A	551	HIS	N	119.21	.	1
1	A	552	HIS	H	8.529	.	1
1	A	552	HIS	HA	4.648	.	1
1	A	552	HIS	HB2	3.193	.	.
1	A	552	HIS	HB3	3.193	.	.
1	A	552	HIS	HD2	7.208	.	1
1	A	552	HIS	C	173.536	.	1
1	A	552	HIS	CA	55.562	.	1
1	A	552	HIS	CB	29.484	.	1
1	A	552	HIS	CD2	119.65	.	1
1	A	552	HIS	N	120.145	.	1
1	A	553	HIS	H	8.329	.	1
1	A	553	HIS	HA	4.454	.	1
1	A	553	HIS	HB2	3.117	.	.
1	A	553	HIS	HB3	3.239	.	.
1	A	553	HIS	C	178.843	.	1
1	A	553	HIS	CA	57.106	.	1
1	A	553	HIS	CB	29.761	.	1
1	A	553	HIS	N	125.197	.	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	168	-0.07 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	161	0.40 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	163	0.08 ± 0.06	None needed (< 0.5 ppm)
^{15}N	158	0.37 ± 0.16	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 94%, i.e. 1602 atoms were assigned a chemical shift out of a possible 1710. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	606/612 (99%)	245/246 (100%)	244/248 (98%)	117/118 (99%)
Sidechain	919/976 (94%)	616/640 (96%)	284/298 (95%)	19/38 (50%)
Aromatic	77/122 (63%)	46/63 (73%)	30/52 (58%)	1/7 (14%)
Overall	1602/1710 (94%)	907/949 (96%)	558/598 (93%)	137/163 (84%)

7.1.4 Statistically unusual chemical shifts [i](#)

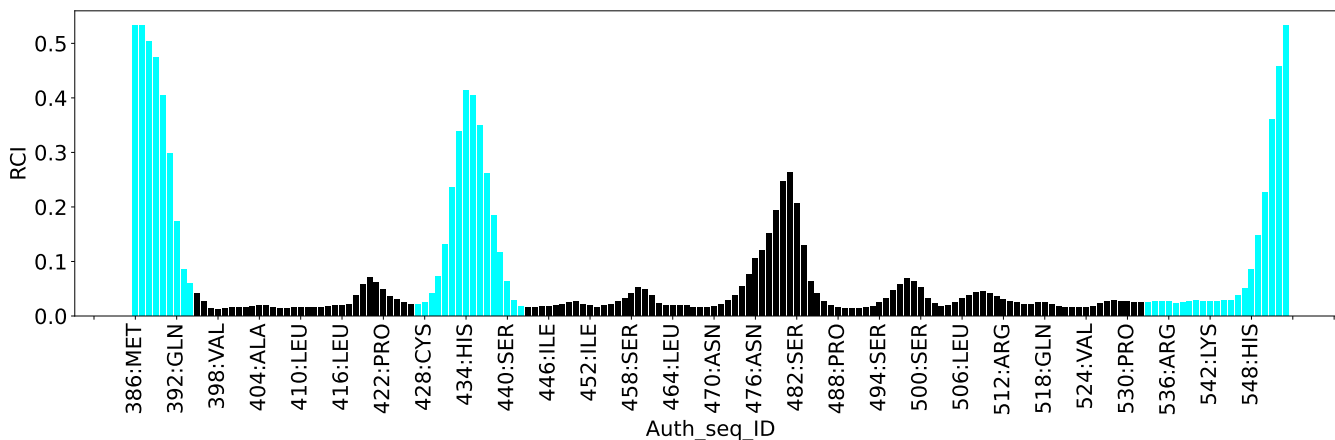
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	515	GLU	HG2	1.08	1.24 – 3.30	-5.8

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	2867
Intra-residue ($ i-j =0$)	831
Sequential ($ i-j =1$)	845
Medium range ($ i-j >1$ and $ i-j <5$)	575
Long range ($ i-j \geq 5$)	616
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	203
Number of unmapped restraints	60
Number of restraints per residue	18.3
Number of long range restraints per residue ¹	3.7

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)	1.9	0.18
0.2-0.5 (Medium)	1.6	0.5
>0.5 (Large)	2.7	2.47

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.8	2.44
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

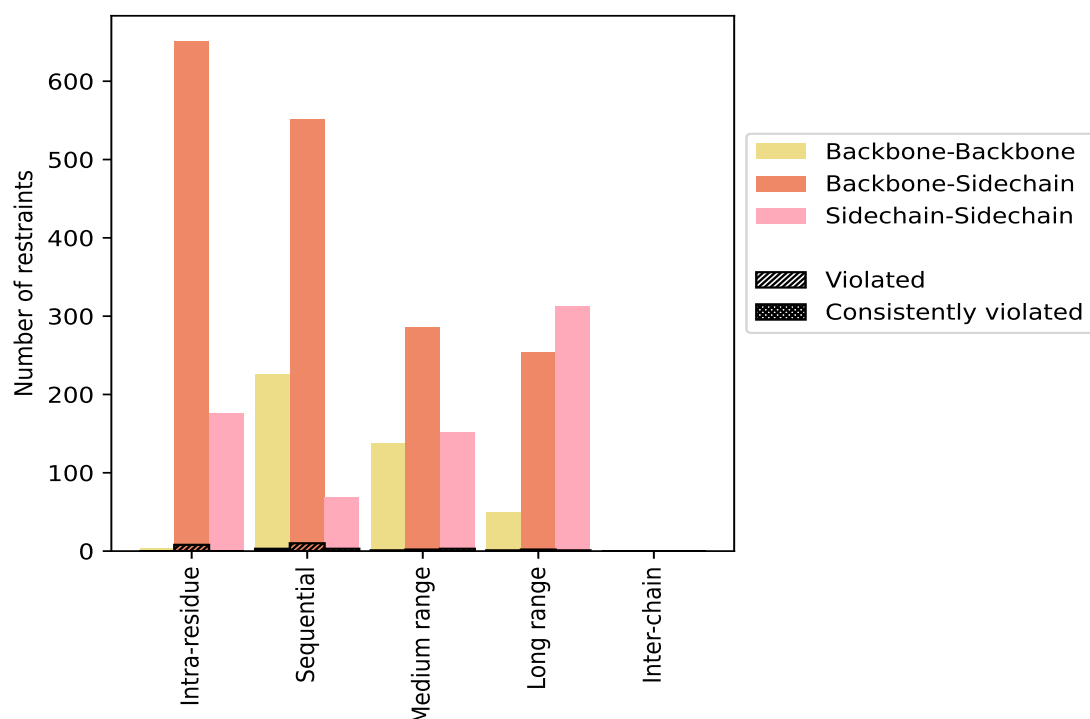
9.1 Summary of distance violations

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 ($i-j =0$)	831	29.0	8	1.0	0.3	0	0.0	0.0
Backbone-Backbone	4	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	651	22.7	8	1.2	0.3	0	0.0	0.0
Sidechain-Sidechain	176	6.1	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	845	29.5	16	1.9	0.6	2	0.2	0.1
Backbone-Backbone	226	7.9	3	1.3	0.1	2	0.9	0.1
Backbone-Sidechain	551	19.2	10	1.8	0.3	0	0.0	0.0
Sidechain-Sidechain	68	2.4	3	4.4	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	575	20.1	6	1.0	0.2	0	0.0	0.0
Backbone-Backbone	137	4.8	1	0.7	0.0	0	0.0	0.0
Backbone-Sidechain	286	10.0	2	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	152	5.3	3	2.0	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	616	21.5	4	0.6	0.1	0	0.0	0.0
Backbone-Backbone	49	1.7	1	2.0	0.0	0	0.0	0.0
Backbone-Sidechain	254	8.9	2	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	313	10.9	1	0.3	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	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	2867	100.0	34	1.2	1.2	2	0.1	0.1
Backbone-Backbone	416	14.5	5	1.2	0.2	2	0.5	0.1
Backbone-Sidechain	1742	60.8	22	1.3	0.8	0	0.0	0.0
Sidechain-Sidechain	709	24.7	7	1.0	0.2	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	3	0	0	0	4	0.91	2.47	0.92	0.52
2	0	4	0	1	0	5	0.81	2.43	0.82	0.54
3	0	4	0	1	0	5	0.78	2.45	0.85	0.54
4	0	7	0	0	0	7	0.58	2.31	0.73	0.24
5	0	3	1	0	0	4	0.34	0.54	0.2	0.36
6	1	4	2	2	0	9	0.52	2.46	0.71	0.24
7	0	3	0	2	0	5	0.58	1.66	0.57	0.44
8	2	3	0	1	0	6	0.27	0.54	0.18	0.18
9	0	5	0	1	0	6	0.53	1.37	0.4	0.44
10	1	6	1	2	0	10	0.27	0.64	0.21	0.14

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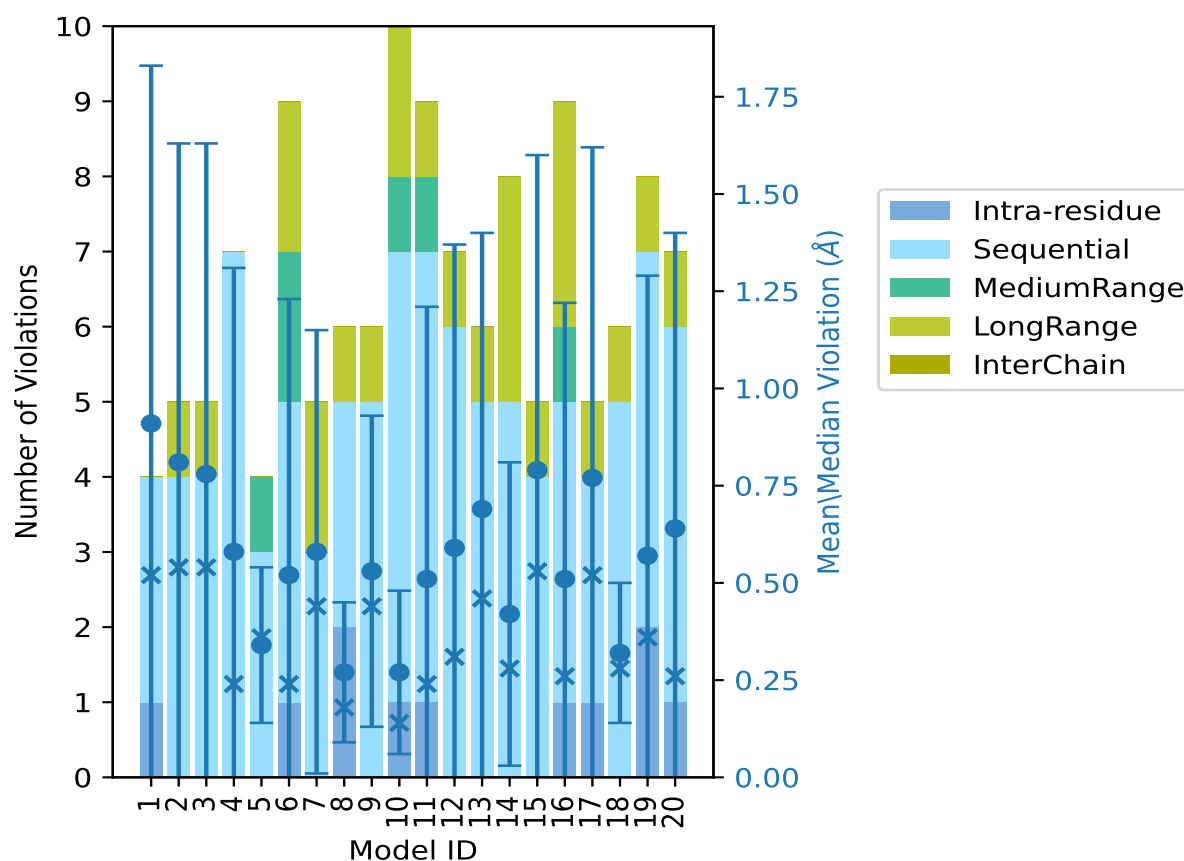
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	6	1	1	0	9	0.51	2.45	0.7	0.24
12	0	6	0	1	0	7	0.59	2.44	0.78	0.31
13	0	5	0	1	0	6	0.69	2.26	0.71	0.46
14	0	5	0	3	0	8	0.42	1.34	0.39	0.28
15	0	4	0	1	0	5	0.79	2.38	0.81	0.53
16	1	4	1	3	0	9	0.51	2.46	0.71	0.26
17	1	3	0	1	0	5	0.77	2.44	0.85	0.52
18	0	5	0	1	0	6	0.32	0.55	0.18	0.28
19	2	5	0	1	0	8	0.57	2.42	0.72	0.36
20	1	5	0	1	0	7	0.64	2.47	0.76	0.26

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 ⓘ

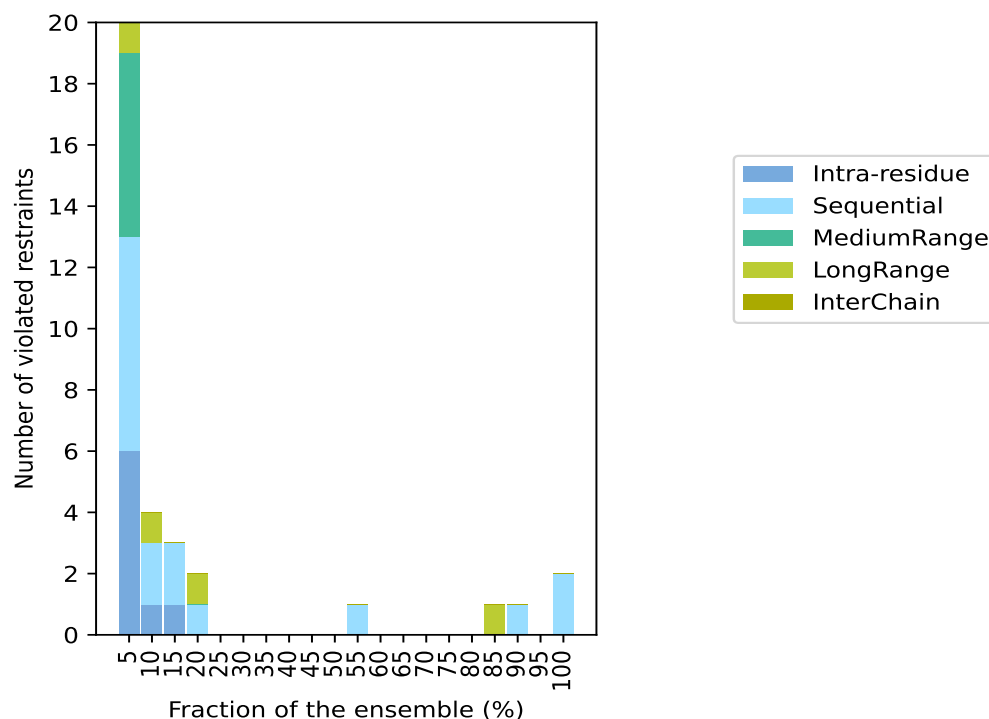
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2833(IR:823, SQ:829, MR:569, LR:612, IC:0) restraints are 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	%
6	7	6	1	0	20	1	5.0
1	2	0	1	0	4	2	10.0
1	2	0	0	0	3	3	15.0
0	1	0	1	0	2	4	20.0
0	0	0	0	0	0	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
0	1	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	1	0	1	17	85.0
0	1	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	2	0	0	0	2	20	100.0

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

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

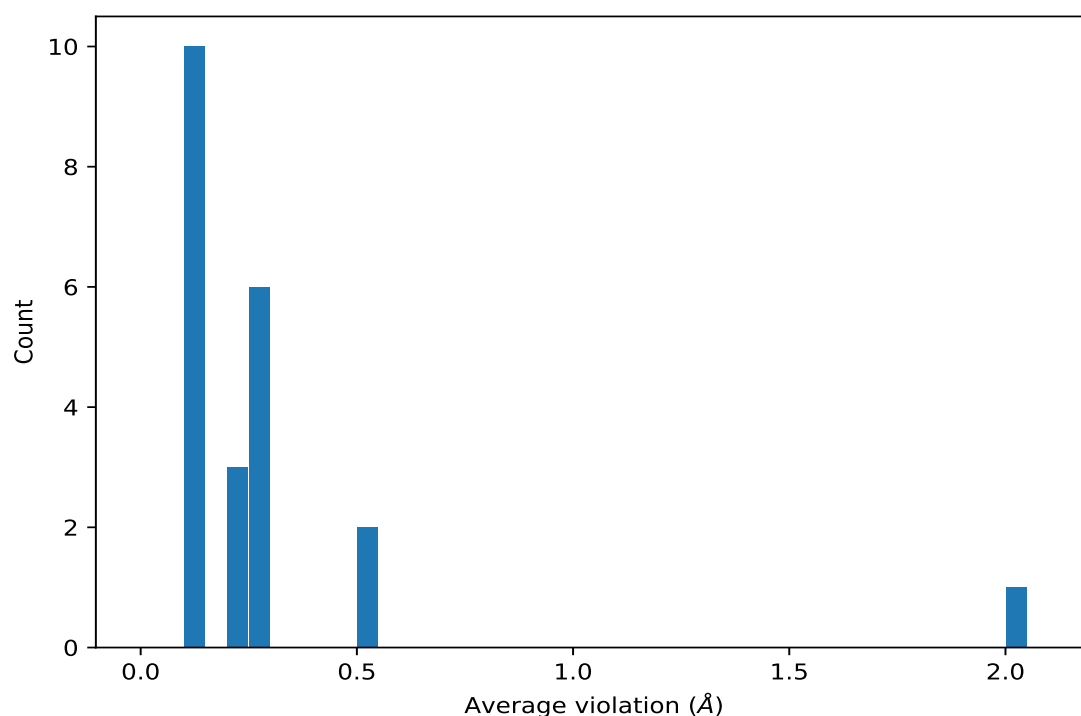
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

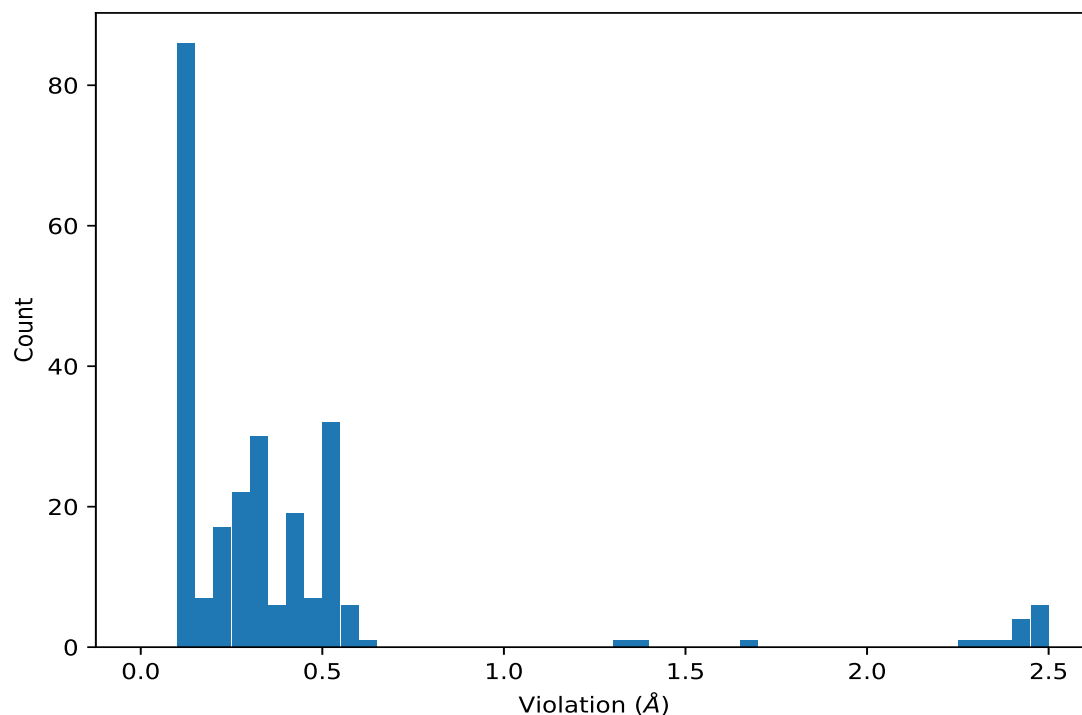
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,895)	1:420:A:GLY:HA2	1:421:A:VAL:H	20	0.54	0.01	0.54
(1,266)	1:481:A:GLY:HA3	1:482:A:SER:H	20	0.53	0.02	0.54
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	18	2.03	0.69	2.42
(1,2316)	1:420:A:GLY:HA2	1:524:A:VAL:HG11	17	0.3	0.1	0.31
(1,2316)	1:420:A:GLY:HA2	1:524:A:VAL:HG12	17	0.3	0.1	0.31
(1,2316)	1:420:A:GLY:HA2	1:524:A:VAL:HG13	17	0.3	0.1	0.31
(1,2316)	1:420:A:GLY:HA2	1:524:A:VAL:HG21	17	0.3	0.1	0.31
(1,2316)	1:420:A:GLY:HA2	1:524:A:VAL:HG22	17	0.3	0.1	0.31
(1,2316)	1:420:A:GLY:HA2	1:524:A:VAL:HG23	17	0.3	0.1	0.31
(1,484)	1:419:A:LEU:H	1:420:A:GLY:HA3	11	0.23	0.03	0.23
(1,238)	1:492:A:LEU:HG	1:493:A:GLU:H	4	0.12	0.02	0.11
(1,1869)	1:491:A:PRO:HA	1:515:A:GLU:HA	4	0.11	0.01	0.12
(1,786)	1:471:A:GLN:HB3	1:472:A:ALA:H	3	0.14	0.02	0.15
(1,1655)	1:432:A:GLN:HA	1:432:A:GLN:HG3	3	0.13	0.0	0.13
(1,1203)	1:471:A:GLN:HB3	1:472:A:ALA:HB1	3	0.12	0.02	0.13

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)
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	1	2.47
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	20	2.47
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	6	2.46
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	16	2.46
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	3	2.45
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	11	2.45
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	12	2.44
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	17	2.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	2	2.43
(1,2557)	1:479:A:ARG:HH22	1:480:A:GLN:H	19	2.42

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

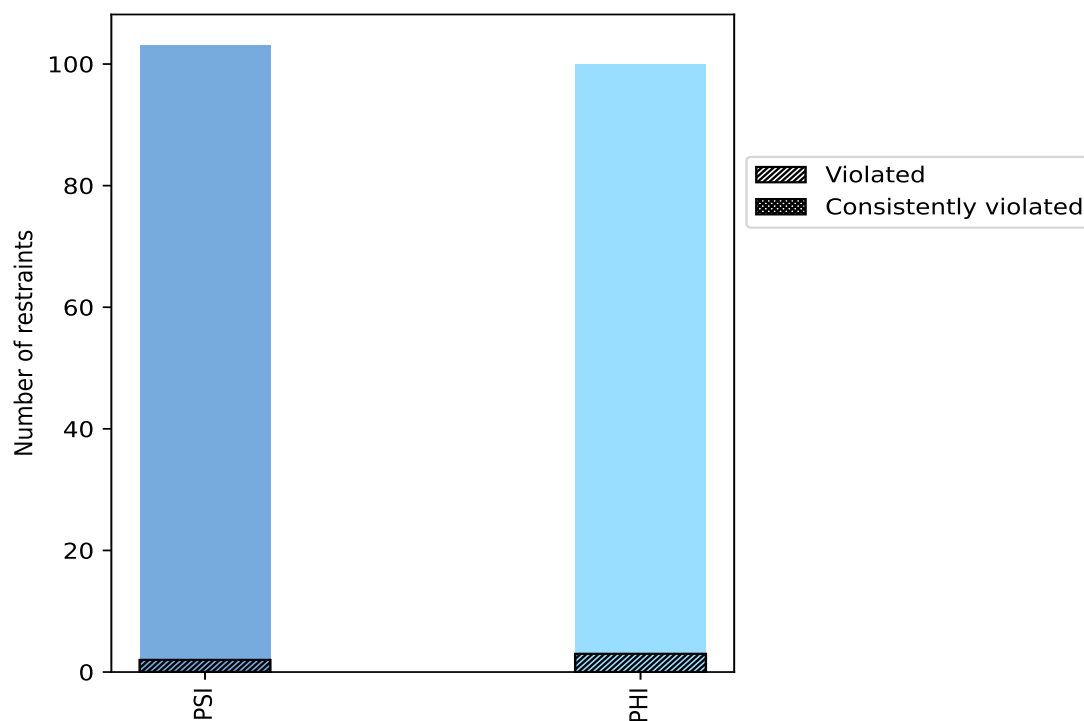
10.1 Summary of dihedral-angle violations [i](#)

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	103	50.7	2	1.9	1.0	0	0.0	0.0
PHI	100	49.3	3	3.0	1.5	0	0.0	0.0
Total	203	100.0	5	2.5	2.5	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](#)



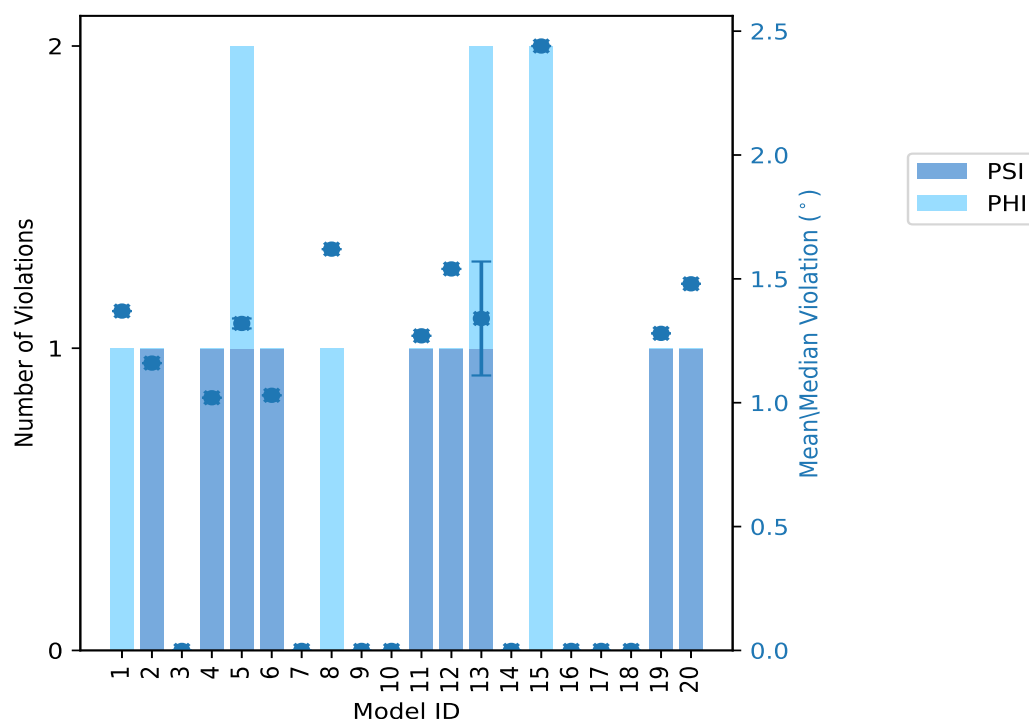
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	0	1	1	1.37	1.37	0.0	1.37
2	1	0	1	1.16	1.16	0.0	1.16
3	0	0	0	0.0	0.0	0.0	0.0
4	1	0	1	1.02	1.02	0.0	1.02
5	1	1	2	1.32	1.33	0.02	1.32
6	1	0	1	1.03	1.03	0.0	1.03
7	0	0	0	0.0	0.0	0.0	0.0
8	0	1	1	1.62	1.62	0.0	1.62
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	1	0	1	1.27	1.27	0.0	1.27
12	1	0	1	1.54	1.54	0.0	1.54
13	1	1	2	1.34	1.57	0.23	1.34
14	0	0	0	0.0	0.0	0.0	0.0
15	0	2	2	2.44	2.44	0.0	2.44
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	1	0	1	1.28	1.28	0.0	1.28
20	1	0	1	1.48	1.48	0.0	1.48

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

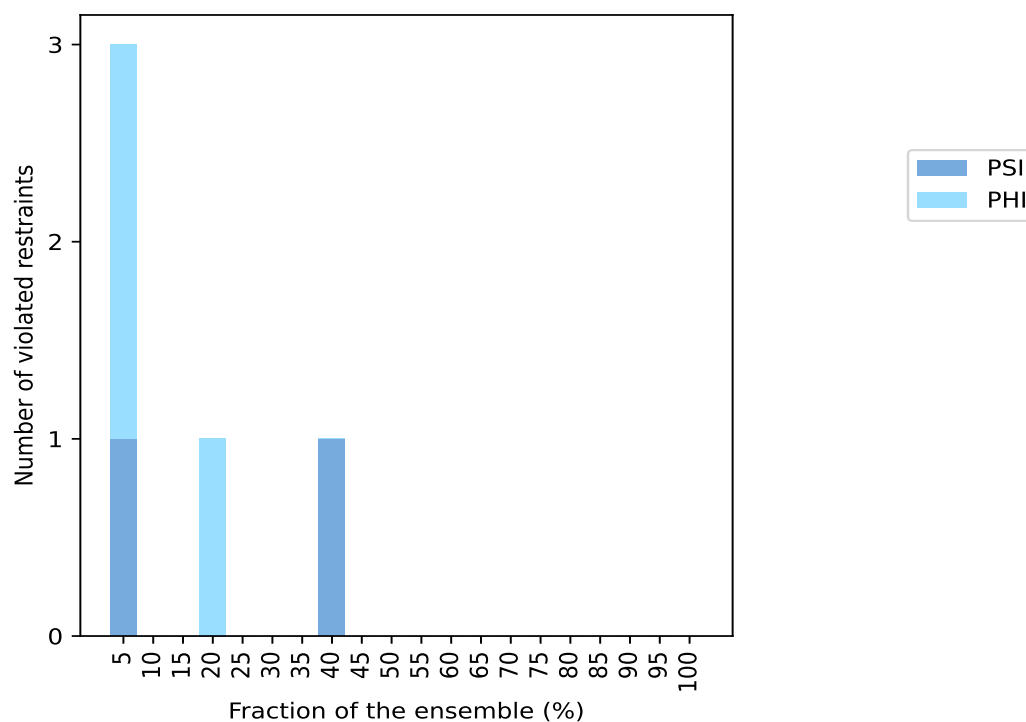
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

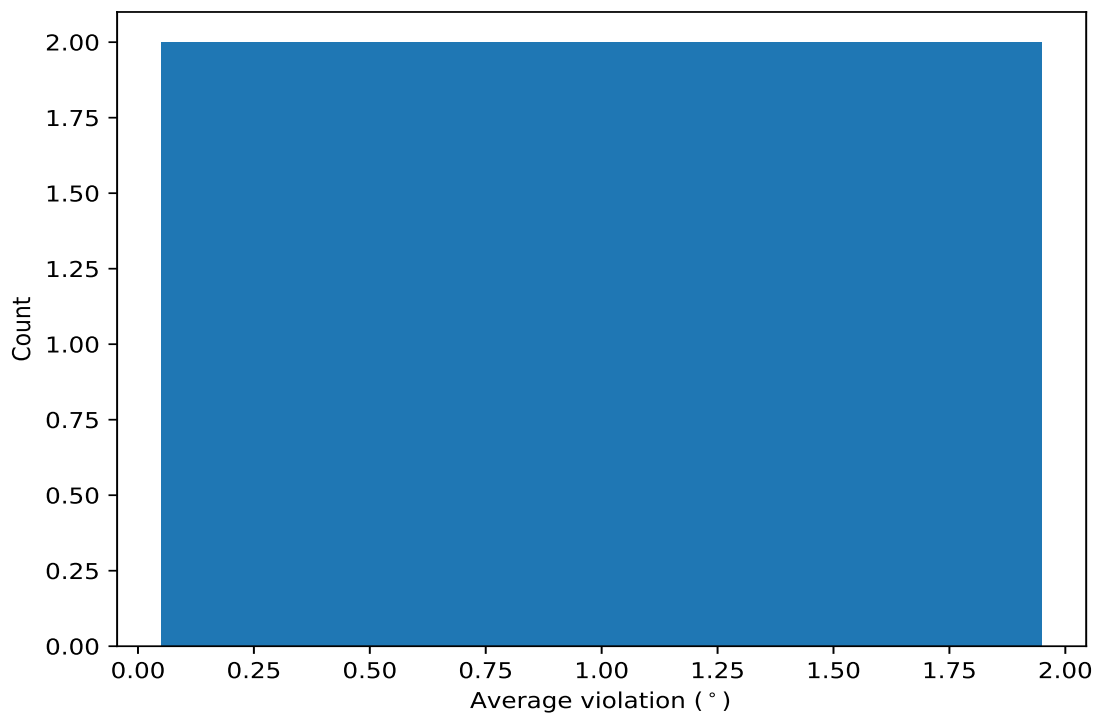


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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 violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

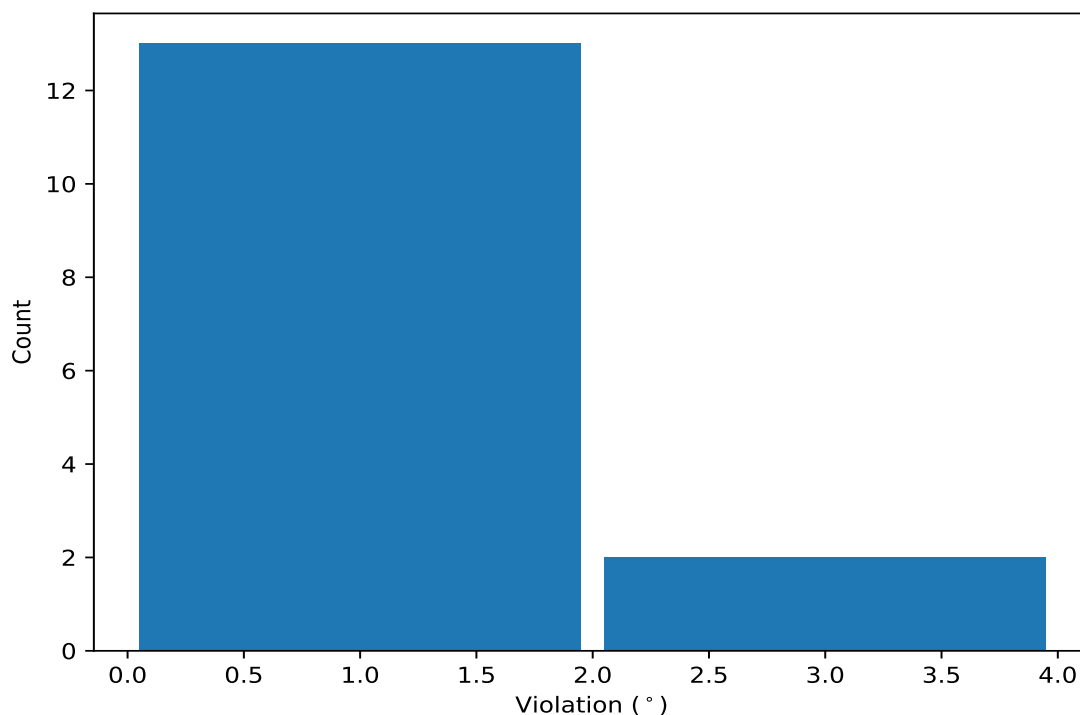
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,48)	1:419:A:LEU:N	1:419:A:LEU:CA	1:419:A:LEU:C	1:420:A:GLY:N	8	1.27	0.18	1.27
(1,15)	1:402:A:ALA:C	1:403:A:ARG:N	1:403:A:ARG:CA	1:403:A:ARG:C	4	1.68	0.45	1.5

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 (°)
(1,187)	1:536:A:ARG:C	1:537:A:LYS:N	1:537:A:LYS:CA	1:537:A:LYS:C	15	2.44
(1,15)	1:402:A:ALA:C	1:403:A:ARG:N	1:403:A:ARG:CA	1:403:A:ARG:C	15	2.43
(1,15)	1:402:A:ALA:C	1:403:A:ARG:N	1:403:A:ARG:CA	1:403:A:ARG:C	8	1.62
(1,48)	1:419:A:LEU:N	1:419:A:LEU:CA	1:419:A:LEU:C	1:420:A:GLY:N	13	1.57
(1,18)	1:404:A:ALA:N	1:404:A:ALA:CA	1:404:A:ALA:C	1:405:A:ASP:N	12	1.54
(1,48)	1:419:A:LEU:N	1:419:A:LEU:CA	1:419:A:LEU:C	1:420:A:GLY:N	20	1.48
(1,15)	1:402:A:ALA:C	1:403:A:ARG:N	1:403:A:ARG:CA	1:403:A:ARG:C	1	1.37
(1,48)	1:419:A:LEU:N	1:419:A:LEU:CA	1:419:A:LEU:C	1:420:A:GLY:N	5	1.33
(1,15)	1:402:A:ALA:C	1:403:A:ARG:N	1:403:A:ARG:CA	1:403:A:ARG:C	5	1.3
(1,48)	1:419:A:LEU:N	1:419:A:LEU:CA	1:419:A:LEU:C	1:420:A:GLY:N	19	1.28