



wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 36778
Title : Solution structure of human VAPB MSP domain
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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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 : v1.2.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

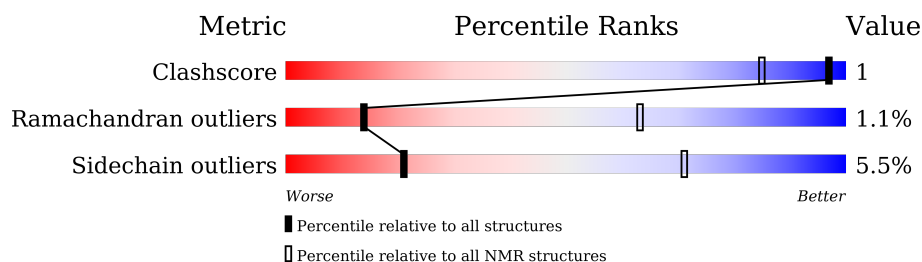
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 63%.

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	128	

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:7-A:75, A:86-A:96, A:114-A:123 (90)	0.35	4

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2017 atoms, of which 1003 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Vesicle-associated membrane protein-associated protein B/C.

Mol	Chain	Residues	Atoms						Trace
1	A	128	Total	C	H	N	O	S	0
			2017	639	1003	173	193	9	

There are 4 discrepancies between the modelled and reference sequences:

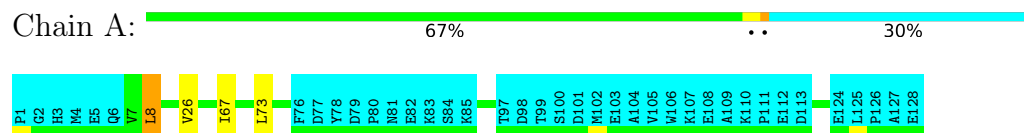
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	-	expression tag	UNP O95292
A	2	GLY	-	expression tag	UNP O95292
A	3	HIS	-	expression tag	UNP O95292
A	4	MET	-	expression tag	UNP O95292

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.

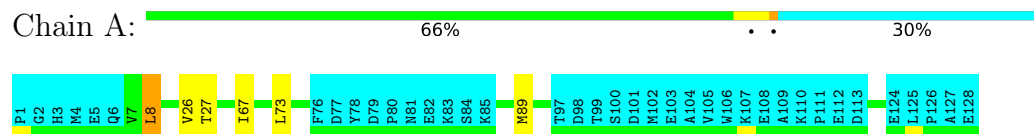
- Molecule 1: Vesicle-associated membrane protein-associated protein B/C



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

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

- Molecule 1: Vesicle-associated membrane protein-associated protein B/C



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1579
Number of shifts mapped to atoms	1579
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	63%

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	0.86±0.01	0±0/722 (0.0± 0.0%)	1.35±0.02	0±0/978 (0.0± 0.0%)
All	All	0.86	0/14440 (0.0%)	1.35	2/19560 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	TYR	N-CA-C	5.12	117.03	108.99	13	1
1	A	68	ASN	CA-CB-CG	5.06	117.66	112.60	8	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	18	PHE	Peptide	1

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	706	730	730	1±1
All	All	14120	14600	14600	20

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 1.

5 of 7 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:PHE:CZ	1:A:73:LEU:HD23	0.48	2.43	12	3
1:A:67:ILE:HD13	1:A:69:VAL:HG23	0.47	1.85	13	10
1:A:52:TYR:CB	1:A:73:LEU:HD22	0.44	2.43	11	1
1:A:32:LEU:HD23	1:A:67:ILE:HD11	0.43	1.89	3	1
1:A:67:ILE:C	1:A:67:ILE:HD12	0.43	2.39	19	2

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	90/128 (70%)	87±1 (97±1%)	2±1 (2±1%)	1±0 (1±0%)	14	63
All	All	1800/2560 (70%)	1747 (97%)	34 (2%)	19 (1%)	14	63

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	8	LEU	19

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	82/116 (71%)	77±2 (94±2%)	5±2 (6±2%)	21	71
All	All	1640/2320 (71%)	1549 (94%)	91 (6%)	21	71

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	8	LEU	19
1	A	26	VAL	18
1	A	73	LEU	18
1	A	44	VAL	6
1	A	68	ASN	5

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 63% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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	1579
Number of shifts mapped to atoms	1579
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

- Can not parse the chemical shift value. First 5 (of 445) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	PRO	HB2	1.993	.	.
1	A	1	PRO	HB3	2.326	.	.
1	A	3	HIS	HB2	3.179	.	.
1	A	3	HIS	HB3	3.277	.	.
1	A	4	MET	HG2	2.586	.	.
1	A	4	MET	HG3	2.635	.	.
1	A	5	GLU	HB2	1.913	.	.
1	A	5	GLU	HB3	2.017	.	.
1	A	6	GLN	HB2	1.933	.	.
1	A	6	GLN	HB3	2.135	.	.
1	A	6	GLN	HG2	2.487	.	.
1	A	6	GLN	HG3	2.518	.	.
1	A	7	VAL	HG11	0.699	.	.
1	A	7	VAL	HG12	0.699	.	.
1	A	7	VAL	HG13	0.699	.	.
1	A	7	VAL	HG21	1.074	.	.
1	A	7	VAL	HG22	1.074	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	VAL	HG23	1.074	.	.
1	A	7	VAL	CG1	18.815	.	.
1	A	7	VAL	CG2	21.542	.	.
1	A	8	LEU	HD11	0.586	.	.
1	A	8	LEU	HD12	0.586	.	.
1	A	8	LEU	HD13	0.586	.	.
1	A	8	LEU	HD21	0.687	.	.
1	A	8	LEU	HD22	0.687	.	.
1	A	8	LEU	HD23	0.687	.	.
1	A	8	LEU	CD1	26.016	.	.
1	A	8	LEU	CD2	22.508	.	.
1	A	9	SER	HB2	3.679	.	.
1	A	9	SER	HB3	3.743	.	.
1	A	10	LEU	HB2	1.381	.	.
1	A	10	LEU	HB3	1.780	.	.
1	A	10	LEU	HD11	0.705	.	.
1	A	10	LEU	HD12	0.705	.	.
1	A	10	LEU	HD13	0.705	.	.
1	A	10	LEU	HD21	0.758	.	.
1	A	10	LEU	HD22	0.758	.	.
1	A	10	LEU	HD23	0.758	.	.
1	A	10	LEU	CD1	24.828	.	.
1	A	10	LEU	CD2	26.888	.	.
1	A	11	GLU	HB2	1.860	.	.
1	A	11	GLU	HB3	1.910	.	.
1	A	12	PRO	HB2	2.173	.	.
1	A	12	PRO	HB3	2.545	.	.
1	A	12	PRO	HD2	3.522	.	.
1	A	12	PRO	HD3	3.691	.	.
1	A	12	PRO	HG2	1.792	.	.
1	A	12	PRO	HG3	2.018	.	.
1	A	13	GLN	HB2	1.451	.	.
1	A	13	GLN	HB3	1.779	.	.
1	A	13	GLN	HG2	2.104	.	.
1	A	13	GLN	HG3	2.228	.	.
1	A	14	HIS	HB2	3.123	.	.
1	A	14	HIS	HB3	3.241	.	.
1	A	16	LEU	HB2	0.917	.	.
1	A	16	LEU	HB3	1.444	.	.
1	A	16	LEU	HD11	0.399	.	.
1	A	16	LEU	HD12	0.399	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	LEU	HD13	0.399	.	.
1	A	16	LEU	HD21	0.106	.	.
1	A	16	LEU	HD22	0.106	.	.
1	A	16	LEU	HD23	0.106	.	.
1	A	16	LEU	CD1	23.935	.	.
1	A	16	LEU	CD2	25.511	.	.
1	A	18	PHE	HB2	3.047	.	.
1	A	18	PHE	HB3	3.225	.	.
1	A	18	PHE	CD1	132.892	.	.
1	A	18	PHE	CD2	132.892	.	.
1	A	18	PHE	CE1	130.296	.	.
1	A	18	PHE	CE2	130.296	.	.
1	A	19	ARG	HB2	1.731	.	.
1	A	19	ARG	HB3	1.862	.	.
1	A	19	ARG	HG2	1.549	.	.
1	A	19	ARG	HG3	1.804	.	.
1	A	20	GLY	HA3	3.900	.	.
1	A	21	PRO	HB2	2.034	.	.
1	A	21	PRO	HB3	2.413	.	.
1	A	22	PHE	HB2	2.206	.	.
1	A	22	PHE	HB3	3.413	.	.
1	A	22	PHE	CD1	132.699	.	.
1	A	22	PHE	CD2	132.699	.	.
1	A	22	PHE	CE1	130.659	.	.
1	A	22	PHE	CE2	130.659	.	.
1	A	24	ASP	HB2	2.512	.	.
1	A	24	ASP	HB3	2.738	.	.
1	A	25	VAL	HG11	0.868	.	.
1	A	25	VAL	HG12	0.868	.	.
1	A	25	VAL	HG13	0.868	.	.
1	A	25	VAL	HG21	1.082	.	.
1	A	25	VAL	HG22	1.082	.	.
1	A	25	VAL	HG23	1.082	.	.
1	A	25	VAL	CG1	21.527	.	.
1	A	25	VAL	CG2	22.566	.	.
1	A	26	VAL	HG11	1.292	.	.
1	A	26	VAL	HG12	1.292	.	.
1	A	26	VAL	HG13	1.292	.	.
1	A	26	VAL	HG21	1.345	.	.
1	A	26	VAL	HG22	1.345	.	.
1	A	26	VAL	HG23	1.345	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	VAL	CG1	22.015	.	.
1	A	26	VAL	CG2	22.961	.	.
1	A	29	ASN	HB2	2.464	.	.
1	A	29	ASN	HB3	2.715	.	.
1	A	29	ASN	HD21	6.854	.	.
1	A	29	ASN	HD22	7.470	.	.
1	A	30	LEU	HB2	0.963	.	.
1	A	30	LEU	HB3	1.563	.	.
1	A	30	LEU	HD11	0.679	.	.
1	A	30	LEU	HD12	0.679	.	.
1	A	30	LEU	HD13	0.679	.	.
1	A	30	LEU	HD21	0.505	.	.
1	A	30	LEU	HD22	0.505	.	.
1	A	30	LEU	HD23	0.505	.	.
1	A	30	LEU	CD1	23.876	.	.
1	A	30	LEU	CD2	26.277	.	.
1	A	31	LYS	HB2	1.627	.	.
1	A	31	LYS	HB3	1.815	.	.
1	A	31	LYS	HG2	1.085	.	.
1	A	31	LYS	HG3	1.245	.	.
1	A	32	LEU	HB2	0.779	.	.
1	A	32	LEU	HB3	1.423	.	.
1	A	32	LEU	HD11	0.451	.	.
1	A	32	LEU	HD12	0.451	.	.
1	A	32	LEU	HD13	0.451	.	.
1	A	32	LEU	HD21	-0.018	.	.
1	A	32	LEU	HD22	-0.018	.	.
1	A	32	LEU	HD23	-0.018	.	.
1	A	32	LEU	CD1	25.110	.	.
1	A	32	LEU	CD2	25.523	.	.
1	A	34	ASN	HB2	2.089	.	.
1	A	34	ASN	HB3	3.530	.	.
1	A	34	ASN	HD21	6.479	.	.
1	A	34	ASN	HD22	8.636	.	.
1	A	35	PRO	HD2	3.900	.	.
1	A	35	PRO	HD3	4.027	.	.
1	A	35	PRO	HG2	1.929	.	.
1	A	35	PRO	HG3	2.100	.	.
1	A	37	ASP	HB2	2.654	.	.
1	A	37	ASP	HB3	2.884	.	.
1	A	38	ARG	HB2	1.692	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	38	ARG	HB3	2.041	.	.
1	A	38	ARG	HD2	2.537	.	.
1	A	38	ARG	HD3	2.784	.	.
1	A	39	ASN	HB2	2.432	.	.
1	A	39	ASN	HB3	2.796	.	.
1	A	39	ASN	HD21	6.910	.	.
1	A	39	ASN	HD22	7.568	.	.
1	A	40	VAL	HG11	0.758	.	.
1	A	40	VAL	HG12	0.758	.	.
1	A	40	VAL	HG13	0.758	.	.
1	A	40	VAL	HG21	0.761	.	.
1	A	40	VAL	HG22	0.761	.	.
1	A	40	VAL	HG23	0.761	.	.
1	A	40	VAL	CG1	22.453	.	.
1	A	40	VAL	CG2	22.453	.	.
1	A	41	CYS	HB2	2.719	.	.
1	A	41	CYS	HB3	3.091	.	.
1	A	42	PHE	HB2	2.569	.	.
1	A	42	PHE	HB3	2.825	.	.
1	A	42	PHE	HE1	6.725	.	.
1	A	42	PHE	HE2	6.825	.	.
1	A	42	PHE	CD1	131.722	.	.
1	A	42	PHE	CD2	131.722	.	.
1	A	42	PHE	CE1	131.724	.	.
1	A	42	PHE	CE2	129.780	.	.
1	A	43	LYS	HB2	1.051	.	.
1	A	43	LYS	HB3	1.207	.	.
1	A	43	LYS	HD2	0.522	.	.
1	A	43	LYS	HD3	0.689	.	.
1	A	43	LYS	HE2	1.561	.	.
1	A	43	LYS	HE3	1.830	.	.
1	A	43	LYS	HG2	0.635	.	.
1	A	43	LYS	HG3	0.705	.	.
1	A	44	VAL	HG11	1.007	.	.
1	A	44	VAL	HG12	1.007	.	.
1	A	44	VAL	HG13	1.007	.	.
1	A	44	VAL	HG21	0.839	.	.
1	A	44	VAL	HG22	0.839	.	.
1	A	44	VAL	HG23	0.839	.	.
1	A	44	VAL	CG1	20.945	.	.
1	A	44	VAL	CG2	22.265	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	LYS	HB2	1.586	.	.
1	A	45	LYS	HB3	1.799	.	.
1	A	45	LYS	HG2	1.162	.	.
1	A	45	LYS	HG3	1.273	.	.
1	A	49	PRO	HB2	1.998	.	.
1	A	49	PRO	HB3	2.334	.	.
1	A	49	PRO	HD2	3.364	.	.
1	A	49	PRO	HD3	3.638	.	.
1	A	50	ARG	HB2	1.738	.	.
1	A	50	ARG	HB3	1.860	.	.
1	A	51	ARG	HB2	1.768	.	.
1	A	51	ARG	HB3	1.924	.	.
1	A	51	ARG	HG2	1.708	.	.
1	A	51	ARG	HG3	1.513	.	.
1	A	52	TYR	HB2	2.604	.	.
1	A	52	TYR	HB3	2.712	.	.
1	A	52	TYR	CD1	133.407	.	.
1	A	52	TYR	CD2	133.407	.	.
1	A	52	TYR	CE1	118.537	.	.
1	A	52	TYR	CE2	118.537	.	.
1	A	54	VAL	HG11	0.941	.	.
1	A	54	VAL	HG12	0.941	.	.
1	A	54	VAL	HG13	0.941	.	.
1	A	54	VAL	HG21	0.852	.	.
1	A	54	VAL	HG22	0.852	.	.
1	A	54	VAL	HG23	0.852	.	.
1	A	54	VAL	CG1	21.568	.	.
1	A	54	VAL	CG2	22.041	.	.
1	A	55	ARG	HB2	1.770	.	.
1	A	55	ARG	HB3	1.858	.	.
1	A	55	ARG	HG2	1.582	.	.
1	A	55	ARG	HG3	1.706	.	.
1	A	56	PRO	HB2	2.413	.	.
1	A	56	PRO	HB3	2.666	.	.
1	A	56	PRO	HD2	3.734	.	.
1	A	56	PRO	HD3	4.157	.	.
1	A	56	PRO	HG2	2.088	.	.
1	A	56	PRO	HG3	2.272	.	.
1	A	57	ASN	HB2	2.797	.	.
1	A	57	ASN	HB3	3.241	.	.
1	A	58	SER	HB2	3.792	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	SER	HB3	3.840	.	.
1	A	59	GLY	HA2	4.034	.	.
1	A	60	ILE	HG12	1.152	.	.
1	A	60	ILE	HG13	1.646	.	.
1	A	61	ILE	HG12	0.771	.	.
1	A	61	ILE	HG13	1.758	.	.
1	A	62	ASP	HB2	2.442	.	.
1	A	62	ASP	HB3	2.649	.	.
1	A	64	GLY	HA2	3.903	.	.
1	A	64	GLY	HA3	4.115	.	.
1	A	66	SER	HB2	3.561	.	.
1	A	66	SER	HB3	3.670	.	.
1	A	67	ILE	HG12	1.081	.	.
1	A	67	ILE	HG13	1.408	.	.
1	A	68	ASN	HB2	2.536	.	.
1	A	68	ASN	HB3	2.873	.	.
1	A	68	ASN	HD21	6.733	.	.
1	A	68	ASN	HD22	7.351	.	.
1	A	69	VAL	HG11	0.751	.	.
1	A	69	VAL	HG12	0.751	.	.
1	A	69	VAL	HG13	0.751	.	.
1	A	69	VAL	HG21	0.849	.	.
1	A	69	VAL	HG22	0.849	.	.
1	A	69	VAL	HG23	0.849	.	.
1	A	69	VAL	CG1	21.012	.	.
1	A	69	VAL	CG2	21.602	.	.
1	A	70	SER	HB2	3.902	.	.
1	A	70	SER	HB3	3.959	.	.
1	A	71	VAL	HG11	0.660	.	.
1	A	71	VAL	HG12	0.660	.	.
1	A	71	VAL	HG13	0.660	.	.
1	A	71	VAL	HG21	0.991	.	.
1	A	71	VAL	HG22	0.991	.	.
1	A	71	VAL	HG23	0.991	.	.
1	A	71	VAL	CG1	20.267	.	.
1	A	71	VAL	CG2	23.534	.	.
1	A	72	MET	HB2	1.790	.	.
1	A	72	MET	HB3	2.226	.	.
1	A	72	MET	HG2	2.405	.	.
1	A	72	MET	HG3	2.726	.	.
1	A	73	LEU	HB2	0.930	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	73	LEU	HB3	2.017	.	.
1	A	73	LEU	HD11	0.119	.	.
1	A	73	LEU	HD12	0.119	.	.
1	A	73	LEU	HD13	0.119	.	.
1	A	73	LEU	CD1	22.708	.	.
1	A	74	GLN	HB2	1.735	.	.
1	A	74	GLN	HB3	2.211	.	.
1	A	74	GLN	HE21	6.790	.	.
1	A	74	GLN	HE22	7.074	.	.
1	A	75	PRO	HD2	3.416	.	.
1	A	75	PRO	HD3	3.652	.	.
1	A	75	PRO	HG2	1.652	.	.
1	A	75	PRO	HG3	2.043	.	.
1	A	76	PHE	HB2	3.126	.	.
1	A	76	PHE	HB3	3.286	.	.
1	A	76	PHE	CD1	132.690	.	.
1	A	76	PHE	CD2	132.690	.	.
1	A	76	PHE	CE1	130.700	.	.
1	A	76	PHE	CE2	130.700	.	.
1	A	77	ASP	HB2	2.528	.	.
1	A	77	ASP	HB3	2.630	.	.
1	A	78	TYR	HB2	2.385	.	.
1	A	78	TYR	HB3	2.674	.	.
1	A	78	TYR	CD1	133.141	.	.
1	A	78	TYR	CD2	133.141	.	.
1	A	78	TYR	CE1	117.920	.	.
1	A	78	TYR	CE2	117.920	.	.
1	A	79	ASP	HB2	2.514	.	.
1	A	79	ASP	HB3	2.782	.	.
1	A	80	PRO	HD2	3.439	.	.
1	A	80	PRO	HD3	3.879	.	.
1	A	80	PRO	HG2	1.916	.	.
1	A	80	PRO	HG3	2.023	.	.
1	A	81	ASN	HB2	2.781	.	.
1	A	81	ASN	HB3	2.801	.	.
1	A	81	ASN	HD21	6.985	.	.
1	A	81	ASN	HD22	7.935	.	.
1	A	82	GLU	HB3	2.104	.	.
1	A	83	LYS	HG2	1.436	.	.
1	A	83	LYS	HG3	1.524	.	.
1	A	84	SER	HB2	3.535	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	84	SER	HB3	3.649	.	.
1	A	85	LYS	HB2	1.686	.	.
1	A	85	LYS	HB3	1.878	.	.
1	A	85	LYS	HG2	1.364	.	.
1	A	85	LYS	HG3	1.417	.	.
1	A	86	HIS	HB2	3.022	.	.
1	A	86	HIS	HB3	3.148	.	.
1	A	87	LYS	HB2	1.688	.	.
1	A	87	LYS	HB3	1.797	.	.
1	A	88	PHE	HB2	2.628	.	.
1	A	88	PHE	HB3	2.688	.	.
1	A	88	PHE	CD1	130.627	.	.
1	A	88	PHE	CD2	130.627	.	.
1	A	88	PHE	CE1	130.630	.	.
1	A	88	PHE	CE2	130.630	.	.
1	A	89	MET	HB2	1.774	.	.
1	A	89	MET	HB3	2.036	.	.
1	A	89	MET	HG2	2.313	.	.
1	A	89	MET	HG3	2.460	.	.
1	A	90	VAL	HG11	0.766	.	.
1	A	90	VAL	HG12	0.766	.	.
1	A	90	VAL	HG13	0.766	.	.
1	A	90	VAL	HG21	0.851	.	.
1	A	90	VAL	HG22	0.851	.	.
1	A	90	VAL	HG23	0.851	.	.
1	A	90	VAL	CG1	20.808	.	.
1	A	90	VAL	CG2	21.267	.	.
1	A	91	GLN	HB2	1.891	.	.
1	A	91	GLN	HB3	2.014	.	.
1	A	91	GLN	HE21	6.670	.	.
1	A	91	GLN	HE22	8.074	.	.
1	A	92	SER	HB2	3.736	.	.
1	A	92	SER	HB3	3.905	.	.
1	A	93	MET	HB2	1.892	.	.
1	A	93	MET	HB3	2.094	.	.
1	A	94	PHE	HB2	2.759	.	.
1	A	94	PHE	HB3	3.133	.	.
1	A	94	PHE	CD1	131.642	.	.
1	A	94	PHE	CD2	131.642	.	.
1	A	94	PHE	CE1	131.716	.	.
1	A	94	PHE	CE2	131.716	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	96	PRO	HB2	2.156	.	.
1	A	96	PRO	HB3	2.264	.	.
1	A	96	PRO	HG2	1.780	.	.
1	A	96	PRO	HG3	1.995	.	.
1	A	98	ASP	HB2	2.523	.	.
1	A	98	ASP	HB3	2.848	.	.
1	A	101	ASP	HB2	2.432	.	.
1	A	101	ASP	HB3	2.880	.	.
1	A	102	MET	HG2	2.673	.	.
1	A	102	MET	HG3	2.823	.	.
1	A	103	GLU	HG2	2.309	.	.
1	A	103	GLU	HG3	2.399	.	.
1	A	105	VAL	HG11	0.554	.	.
1	A	105	VAL	HG12	0.554	.	.
1	A	105	VAL	HG13	0.554	.	.
1	A	105	VAL	HG21	0.962	.	.
1	A	105	VAL	HG22	0.962	.	.
1	A	105	VAL	HG23	0.962	.	.
1	A	105	VAL	CG1	21.444	.	.
1	A	105	VAL	CG2	22.785	.	.
1	A	106	TRP	HB2	3.121	.	.
1	A	106	TRP	HB3	3.287	.	.
1	A	107	LYS	HB2	1.981	.	.
1	A	107	LYS	HB3	2.004	.	.
1	A	107	LYS	HG2	1.532	.	.
1	A	107	LYS	HG3	1.616	.	.
1	A	108	GLU	HB2	1.871	.	.
1	A	108	GLU	HB3	2.213	.	.
1	A	110	LYS	HB2	1.687	.	.
1	A	110	LYS	HB3	2.058	.	.
1	A	110	LYS	HG2	1.601	.	.
1	A	110	LYS	HG3	1.678	.	.
1	A	111	PRO	HB2	1.943	.	.
1	A	111	PRO	HB3	2.406	.	.
1	A	111	PRO	HD2	3.854	.	.
1	A	111	PRO	HD3	3.942	.	.
1	A	111	PRO	HG2	2.095	.	.
1	A	111	PRO	HG3	2.247	.	.
1	A	114	LEU	HB2	1.432	.	.
1	A	114	LEU	HB3	1.899	.	.
1	A	114	LEU	HD11	0.865	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	114	LEU	HD12	0.865	.	.
1	A	114	LEU	HD13	0.865	.	.
1	A	114	LEU	HD21	0.899	.	.
1	A	114	LEU	HD22	0.899	.	.
1	A	114	LEU	HD23	0.899	.	.
1	A	114	LEU	CD1	24.552	.	.
1	A	114	LEU	CD2	25.450	.	.
1	A	116	ASP	HB2	2.483	.	.
1	A	116	ASP	HB3	2.609	.	.
1	A	117	SER	HB2	3.386	.	.
1	A	117	SER	HB3	4.031	.	.
1	A	119	LEU	HB2	1.276	.	.
1	A	119	LEU	HB3	1.416	.	.
1	A	119	LEU	HD11	0.628	.	.
1	A	119	LEU	HD12	0.628	.	.
1	A	119	LEU	HD13	0.628	.	.
1	A	119	LEU	HD21	0.493	.	.
1	A	119	LEU	HD22	0.493	.	.
1	A	119	LEU	HD23	0.493	.	.
1	A	119	LEU	CD1	25.666	.	.
1	A	119	LEU	CD2	26.284	.	.
1	A	120	ARG	HD2	3.254	.	.
1	A	120	ARG	HD3	3.292	.	.
1	A	120	ARG	HG2	1.694	.	.
1	A	120	ARG	HG3	1.722	.	.
1	A	121	CYS	HB2	2.749	.	.
1	A	121	CYS	HB3	2.845	.	.
1	A	122	VAL	HG11	0.802	.	.
1	A	122	VAL	HG12	0.802	.	.
1	A	122	VAL	HG13	0.802	.	.
1	A	122	VAL	HG21	0.923	.	.
1	A	122	VAL	HG22	0.923	.	.
1	A	122	VAL	HG23	0.923	.	.
1	A	122	VAL	CG1	20.749	.	.
1	A	122	VAL	CG2	21.300	.	.
1	A	123	PHE	HB2	3.011	.	.
1	A	123	PHE	HB3	3.130	.	.
1	A	123	PHE	CD1	132.976	.	.
1	A	123	PHE	CD2	132.976	.	.
1	A	123	PHE	CE1	131.516	.	.
1	A	123	PHE	CE2	131.516	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	LEU	HB2	1.486	.	.
1	A	125	LEU	HB3	1.679	.	.
1	A	125	LEU	HD11	0.828	.	.
1	A	125	LEU	HD12	0.828	.	.
1	A	125	LEU	HD13	0.828	.	.
1	A	125	LEU	HD21	0.910	.	.
1	A	125	LEU	HD22	0.910	.	.
1	A	125	LEU	HD23	0.910	.	.
1	A	125	LEU	CD1	23.997	.	.
1	A	125	LEU	CD2	25.052	.	.
1	A	126	PRO	HB2	1.922	.	.
1	A	126	PRO	HB3	2.253	.	.
1	A	126	PRO	HD2	3.452	.	.
1	A	126	PRO	HD3	3.478	.	.
1	A	126	PRO	HG2	1.826	.	.
1	A	126	PRO	HG3	2.034	.	.
1	A	128	GLU	HB2	1.890	.	.
1	A	128	GLU	HB3	2.052	.	.

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
$^{13}\text{C}_\alpha$	126	-0.01 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	123	-0.34 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	128	0.40 ± 0.11	None needed (< 0.5 ppm)
^{15}N	117	-0.39 ± 0.29	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 63%, i.e. 795 atoms were assigned a chemical shift out of a possible 1256. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	433/440 (98%)	171/177 (97%)	179/180 (99%)	83/83 (100%)
Sidechain	328/733 (45%)	159/479 (33%)	162/222 (73%)	7/32 (22%)
Aromatic	34/83 (41%)	29/42 (69%)	5/39 (13%)	0/2 (0%)
Overall	795/1256 (63%)	359/698 (51%)	346/441 (78%)	90/117 (77%)

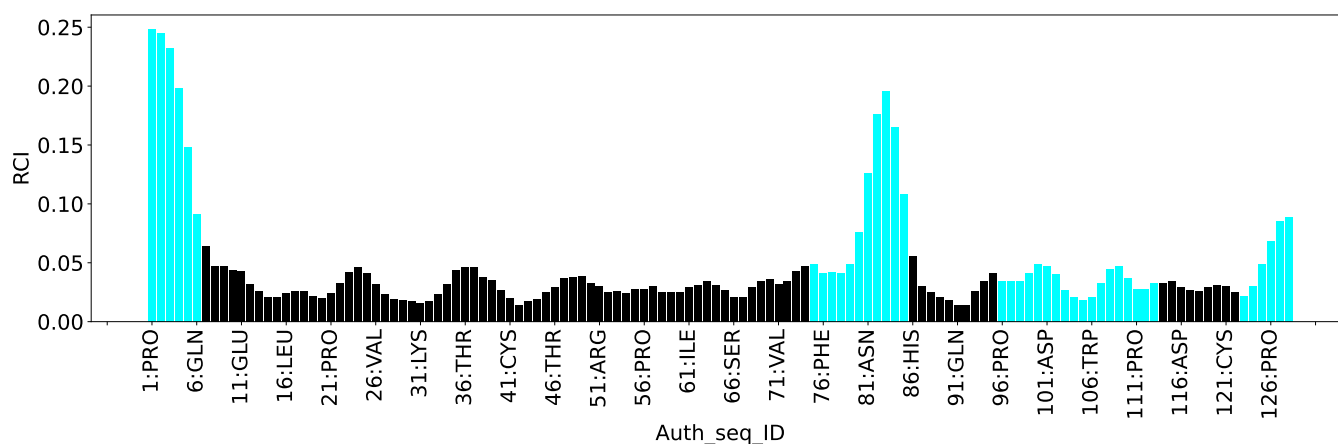
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



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	2239
Intra-residue ($ i-j =0$)	484
Sequential ($ i-j =1$)	669
Medium range ($ i-j >1$ and $ i-j <5$)	237
Long range ($ i-j \geq 5$)	849
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	191
Number of unmapped restraints	0
Number of restraints per residue	19.0
Number of long range restraints per residue ¹	6.6

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)	16.9	0.2
0.2-0.5 (Medium)	3.7	0.5
>0.5 (Large)	2.1	0.98

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

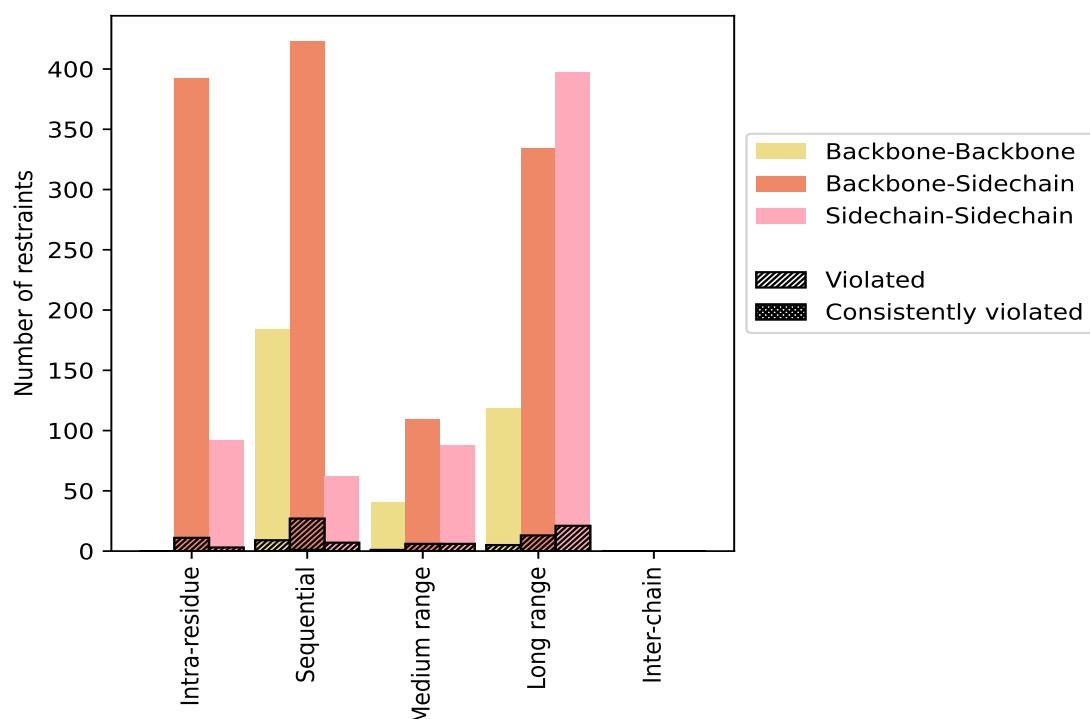
9.1 Summary of distance violations ⓘ

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$)	484	21.6	14	2.9	0.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	392	17.5	11	2.8	0.5	0	0.0	0.0
Sidechain-Sidechain	92	4.1	3	3.3	0.1	0	0.0	0.0
Sequential ($ i-j =1$)	669	29.9	43	6.4	1.9	1	0.1	0.0
Backbone-Backbone	184	8.2	9	4.9	0.4	0	0.0	0.0
Backbone-Sidechain	423	18.9	27	6.4	1.2	1	0.2	0.0
Sidechain-Sidechain	62	2.8	7	11.3	0.3	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	237	10.6	13	5.5	0.6	0	0.0	0.0
Backbone-Backbone	40	1.8	1	2.5	0.0	0	0.0	0.0
Backbone-Sidechain	109	4.9	6	5.5	0.3	0	0.0	0.0
Sidechain-Sidechain	88	3.9	6	6.8	0.3	0	0.0	0.0
Long range ($ i-j \geq 5$)	849	37.9	39	4.6	1.7	0	0.0	0.0
Backbone-Backbone	118	5.3	5	4.2	0.2	0	0.0	0.0
Backbone-Sidechain	334	14.9	13	3.9	0.6	0	0.0	0.0
Sidechain-Sidechain	397	17.7	21	5.3	0.9	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	2239	100.0	109	4.9	4.9	1	0.0	0.0
Backbone-Backbone	342	15.3	15	4.4	0.7	0	0.0	0.0
Backbone-Sidechain	1258	56.2	57	4.5	2.5	1	0.1	0.0
Sidechain-Sidechain	639	28.5	37	5.8	1.7	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	13	5	9	0	28	0.23	0.98	0.21	0.15
2	2	13	3	13	0	31	0.19	0.81	0.16	0.13
3	3	12	1	12	0	28	0.19	0.8	0.17	0.13
4	2	11	1	10	0	24	0.21	0.77	0.19	0.13
5	1	8	3	9	0	21	0.17	0.41	0.1	0.13
6	3	10	2	13	0	28	0.2	0.83	0.18	0.13
7	1	4	4	7	0	16	0.26	0.78	0.22	0.15
8	2	7	1	11	0	21	0.24	0.81	0.21	0.16
9	4	9	3	17	0	33	0.2	0.76	0.16	0.14
10	2	11	3	7	0	23	0.19	0.74	0.16	0.13

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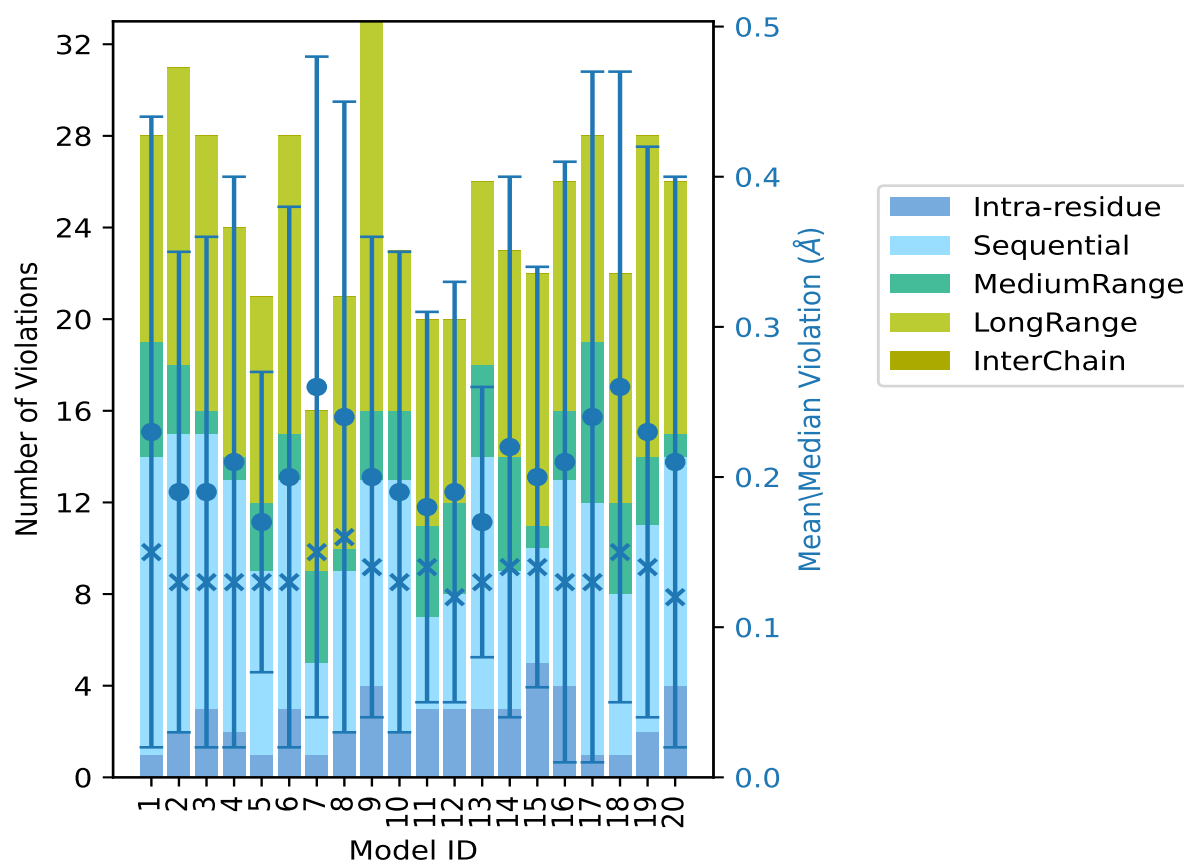
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	4	4	9	0	20	0.18	0.65	0.13	0.14
12	3	5	4	8	0	20	0.19	0.63	0.14	0.12
13	3	11	4	8	0	26	0.17	0.47	0.09	0.13
14	3	6	5	9	0	23	0.22	0.78	0.18	0.14
15	5	5	1	11	0	22	0.2	0.61	0.14	0.14
16	4	9	3	10	0	26	0.21	0.89	0.2	0.13
17	1	11	7	9	0	28	0.24	0.93	0.23	0.13
18	1	7	4	10	0	22	0.26	0.85	0.21	0.15
19	2	9	3	14	0	28	0.23	0.82	0.19	0.14
20	4	10	1	11	0	26	0.21	0.84	0.19	0.12

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

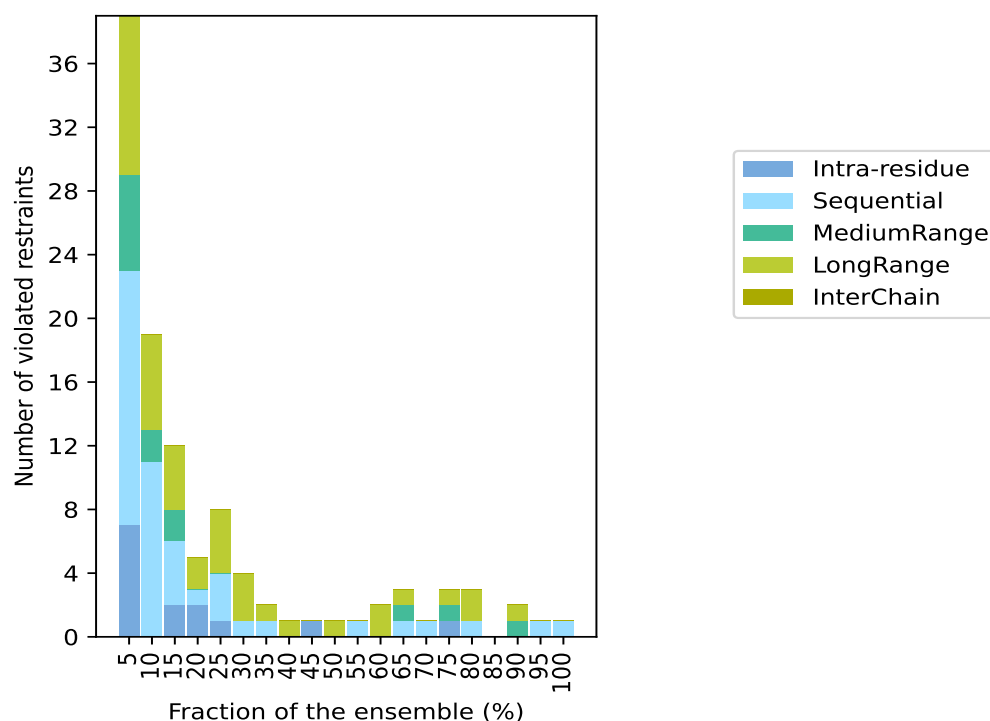
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2130(IR:470, SQ:626, MR:224, LR:810, IC:0) restraints are 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	%
7	16	6	10	0	39	1	5.0
0	11	2	6	0	19	2	10.0
2	4	2	4	0	12	3	15.0
2	1	0	2	0	5	4	20.0
1	3	0	4	0	8	5	25.0
0	1	0	3	0	4	6	30.0
0	1	0	1	0	2	7	35.0
0	0	0	1	0	1	8	40.0
1	0	0	0	0	1	9	45.0
0	0	0	1	0	1	10	50.0
0	1	0	0	0	1	11	55.0
0	0	0	2	0	2	12	60.0
0	1	1	1	0	3	13	65.0
0	1	0	0	0	1	14	70.0
1	0	1	1	0	3	15	75.0
0	1	0	2	0	3	16	80.0
0	0	0	0	0	0	17	85.0
0	0	1	1	0	2	18	90.0
0	1	0	0	0	1	19	95.0
0	1	0	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

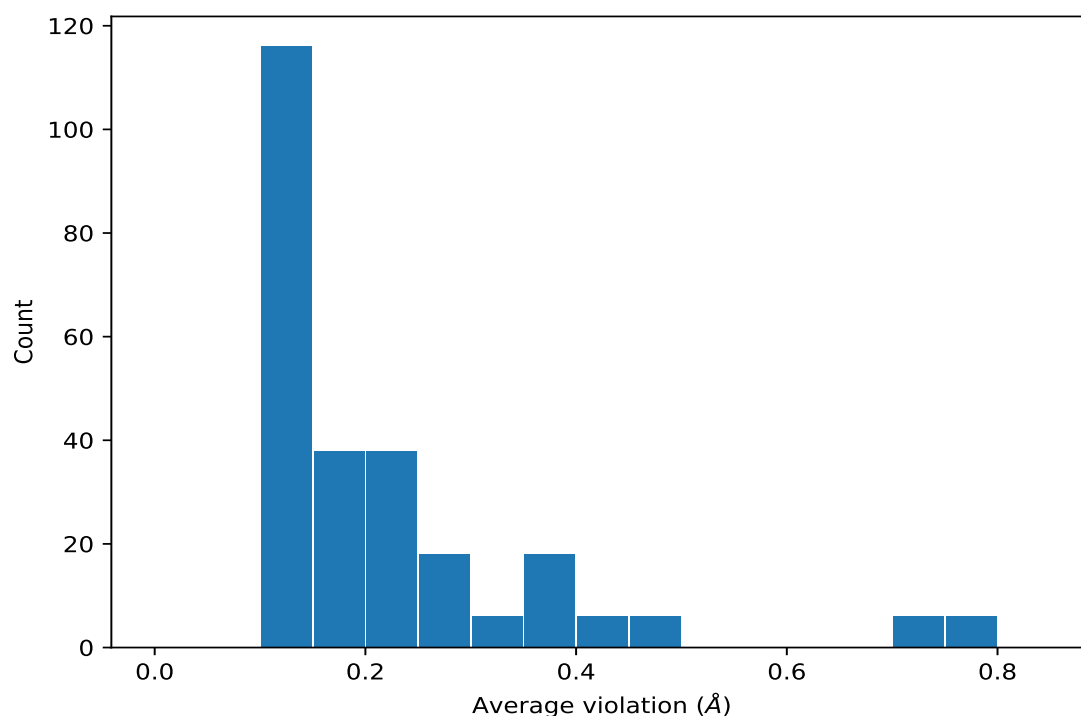
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,647)	1:10:A:LEU:HA	1:11:A:GLU:HG2	20	0.13	0.02	0.13
(1,647)	1:10:A:LEU:HA	1:11:A:GLU:HG3	20	0.13	0.02	0.13
(1,612)	1:45:A:LYS:HB2	1:46:A:THR:HA	19	0.13	0.02	0.13
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG11	18	0.79	0.1	0.79
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG12	18	0.79	0.1	0.79
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG13	18	0.79	0.1	0.79
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG21	18	0.79	0.1	0.79
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG22	18	0.79	0.1	0.79
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG23	18	0.79	0.1	0.79
(1,625)	1:67:A:ILE:HG12	1:69:A:VAL:HB	18	0.12	0.01	0.11
(1,1946)	1:30:A:LEU:HD11	1:67:A:ILE:HD11	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD11	1:67:A:ILE:HD12	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD11	1:67:A:ILE:HD13	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD12	1:67:A:ILE:HD11	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD12	1:67:A:ILE:HD12	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD12	1:67:A:ILE:HD13	16	0.36	0.13	0.38

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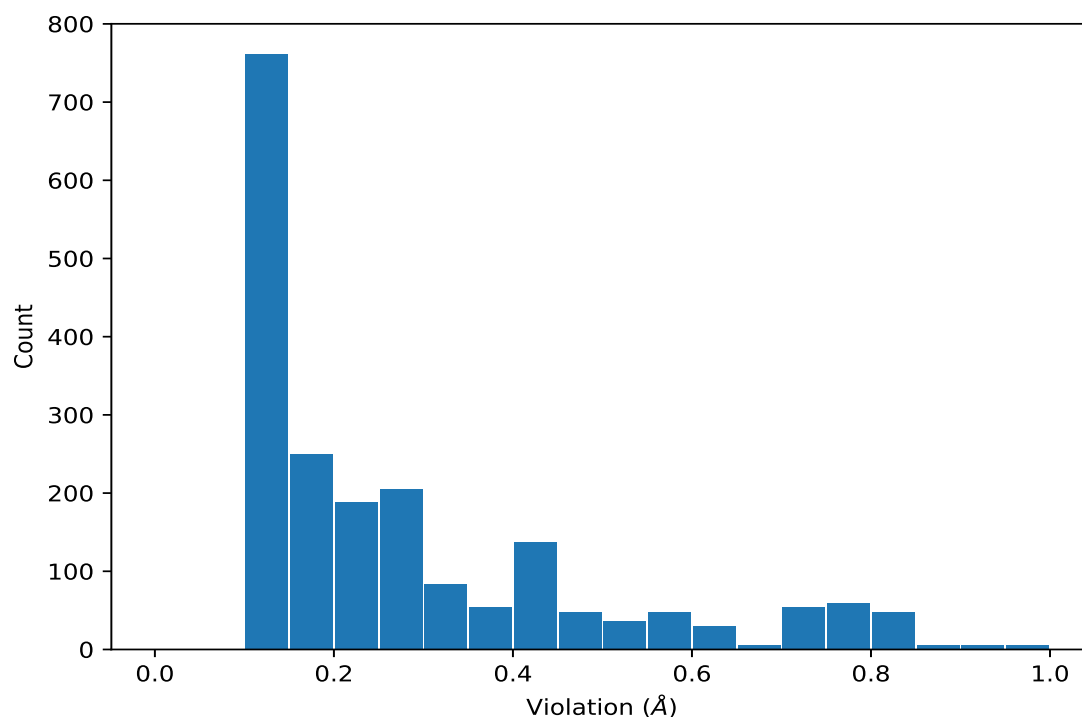
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1946)	1:30:A:LEU:HD13	1:67:A:ILE:HD11	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD13	1:67:A:ILE:HD12	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD13	1:67:A:ILE:HD13	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD21	1:67:A:ILE:HD11	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD21	1:67:A:ILE:HD12	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD21	1:67:A:ILE:HD13	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD22	1:67:A:ILE:HD11	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD22	1:67:A:ILE:HD12	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD22	1:67:A:ILE:HD13	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD23	1:67:A:ILE:HD11	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD23	1:67:A:ILE:HD12	16	0.36	0.13	0.38
(1,1946)	1:30:A:LEU:HD23	1:67:A:ILE:HD13	16	0.36	0.13	0.38
(1,1863)	1:16:A:LEU:HD11	1:123:A:PHE:HE1	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD11	1:123:A:PHE:HE2	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD12	1:123:A:PHE:HE1	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD12	1:123:A:PHE:HE2	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD13	1:123:A:PHE:HE1	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD13	1:123:A:PHE:HE2	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD21	1:123:A:PHE:HE1	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD21	1:123:A:PHE:HE2	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD22	1:123:A:PHE:HE1	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD22	1:123:A:PHE:HE2	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD23	1:123:A:PHE:HE1	16	0.29	0.1	0.3
(1,1863)	1:16:A:LEU:HD23	1:123:A:PHE:HE2	16	0.29	0.1	0.3
(1,1158)	1:23:A:THR:HG21	1:24:A:ASP:H	16	0.12	0.01	0.12
(1,1158)	1:23:A:THR:HG22	1:24:A:ASP:H	16	0.12	0.01	0.12
(1,1158)	1:23:A:THR:HG23	1:24:A:ASP:H	16	0.12	0.01	0.12
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG11	15	0.74	0.06	0.75
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG12	15	0.74	0.06	0.75
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG13	15	0.74	0.06	0.75
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG21	15	0.74	0.06	0.75
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG22	15	0.74	0.06	0.75
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG23	15	0.74	0.06	0.75
(1,1941)	1:30:A:LEU:HA	1:32:A:LEU:HD11	15	0.47	0.09	0.45
(1,1941)	1:30:A:LEU:HA	1:32:A:LEU:HD12	15	0.47	0.09	0.45
(1,1941)	1:30:A:LEU:HA	1:32:A:LEU:HD13	15	0.47	0.09	0.45
(1,1941)	1:30:A:LEU:HA	1:32:A:LEU:HD21	15	0.47	0.09	0.45
(1,1941)	1:30:A:LEU:HA	1:32:A:LEU:HD22	15	0.47	0.09	0.45
(1,1941)	1:30:A:LEU:HA	1:32:A:LEU:HD23	15	0.47	0.09	0.45
(1,1028)	1:27:A:THR:H	1:27:A:THR:HB	15	0.14	0.01	0.14

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)
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG11	1	0.98
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG12	1	0.98
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG13	1	0.98
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG21	1	0.98
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG22	1	0.98
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG23	1	0.98
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG11	17	0.93
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG12	17	0.93
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG13	17	0.93
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG21	17	0.93
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG22	17	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG23	17	0.93
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG11	16	0.89
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG12	16	0.89
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG13	16	0.89
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG21	16	0.89
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG22	16	0.89
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG23	16	0.89
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG11	18	0.85
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG12	18	0.85
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG13	18	0.85
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG21	18	0.85
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG22	18	0.85
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG23	18	0.85
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG11	20	0.84
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG12	20	0.84
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG13	20	0.84
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG21	20	0.84
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG22	20	0.84
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG23	20	0.84
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG11	6	0.83
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG12	6	0.83
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG13	6	0.83
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG21	6	0.83
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG22	6	0.83
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG23	6	0.83
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG11	19	0.82
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG12	19	0.82
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG13	19	0.82
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG21	19	0.82
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG22	19	0.82
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG23	19	0.82
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG11	8	0.81
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG12	8	0.81
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG13	8	0.81
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG21	8	0.81
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG22	8	0.81
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG23	8	0.81
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG11	2	0.81
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG12	2	0.81
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG13	2	0.81
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG21	2	0.81
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG22	2	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1864)	1:18:A:PHE:HA	1:26:A:VAL:HG23	2	0.81
(1,1871)	1:19:A:ARG:H	1:26:A:VAL:HG11	16	0.8

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

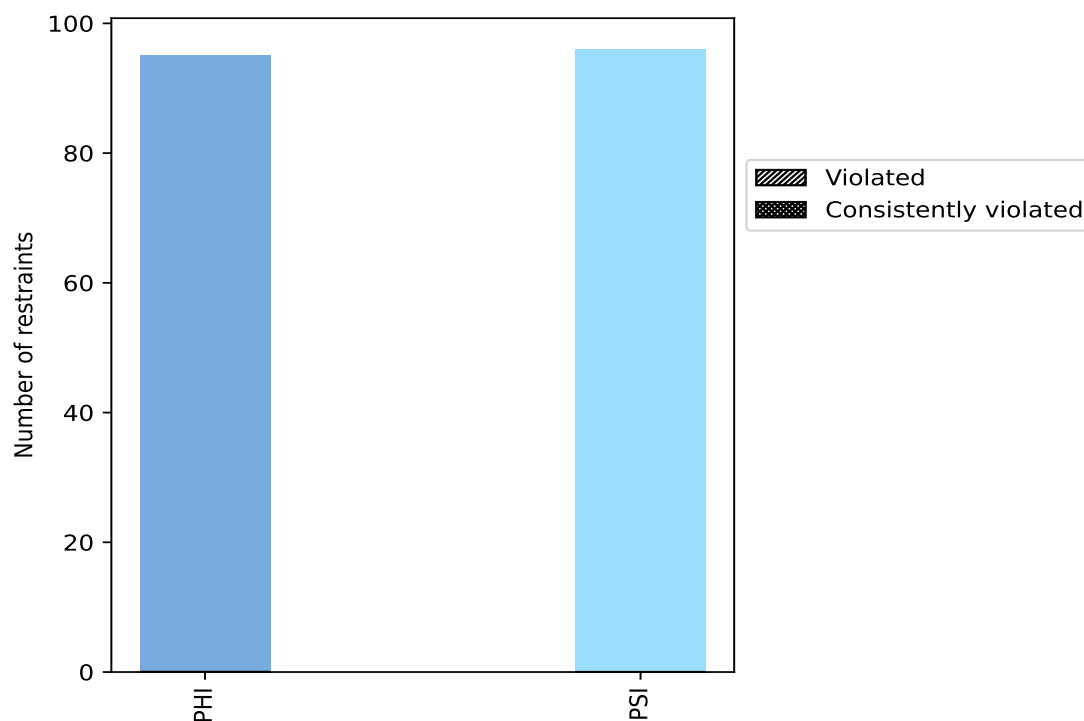
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	95	49.7	0	0.0	0.0	0	0.0	0.0
PSI	96	50.3	0	0.0	0.0	0	0.0	0.0
Total	191	100.0	0	0.0	0.0	0	0.0	0.0

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

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



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

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

No violations found

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

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

No violations found

10.5 All violated dihedral-angle restraints [i](#)

No violations found