



wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 31178
Title : NMR structure of the S. pombe Slr1 La motif RNA binding domain
Authors : Donaldson, L.W.
Deposited on : 2024-06-18

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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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

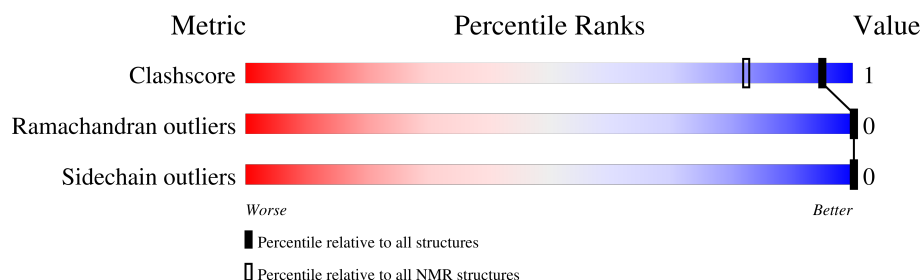
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	113	 74% 12% 13%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:2-A:83, A:90-A:92 (85)	0.58	13

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1589 atoms, of which 792 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized HTH La-type RNA-binding protein C1527.03.

Mol	Chain	Residues	Atoms						Trace
1	A	98	Total	C	H	N	O	S	0
			1589	512	792	131	150	4	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9P6K0
A	21	SER	CYS	engineered mutation	UNP Q9P6K0
A	61	ALA	CYS	engineered mutation	UNP Q9P6K0
A	71	GLU	ILE	conflict	UNP Q9P6K0
A	106	LEU	-	expression tag	UNP Q9P6K0
A	107	GLU	-	expression tag	UNP Q9P6K0
A	108	HIS	-	expression tag	UNP Q9P6K0
A	109	HIS	-	expression tag	UNP Q9P6K0
A	110	HIS	-	expression tag	UNP Q9P6K0
A	111	HIS	-	expression tag	UNP Q9P6K0
A	112	HIS	-	expression tag	UNP Q9P6K0
A	113	HIS	-	expression tag	UNP Q9P6K0

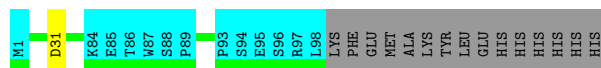
4 Residue-property plots [i](#)

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: Uncharacterized HTH La-type RNA-binding protein C1527.03

Chain A: 

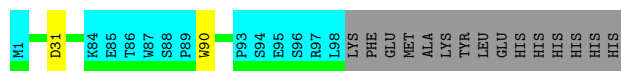


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Uncharacterized HTH La-type RNA-binding protein C1527.03

Chain A: 



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
Rosetta	refinement	
CYANA	structure calculation	3

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1269
Number of shifts mapped to atoms	1150
Number of unparsed shifts	0
Number of shifts with mapping errors	119
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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	690	686	686	1±1
All	All	13800	13720	13720	28

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 11 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:LEU:H	1:A:92:LEU:HD23	0.68	1.49	4	2
1:A:69:VAL:HG22	1:A:81:VAL:HG12	0.54	1.79	1	2
1:A:92:LEU:HD23	1:A:92:LEU:N	0.48	2.22	4	1
1:A:31:ASP:C	1:A:31:ASP:OD1	0.47	2.58	9	8
1:A:31:ASP:OD1	1:A:31:ASP:C	0.44	2.60	13	7

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	85/113 (75%)	84±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
All	All	1700/2260 (75%)	1687 (99%)	13 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	76/103 (74%)	76±0 (100±0%)	0±0 (0±0%)	100	100
All	All	1520/2060 (74%)	1520 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *my_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	1269
Number of shifts mapped to atoms	1150
Number of unparsed shifts	0
Number of shifts with mapping errors	119
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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 119) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	LYS	H	8.092	0.005	1
1	A	99	LYS	HA	4.468	0.005	1
1	A	99	LYS	HB2	1.714	0.003	2
1	A	99	LYS	HB3	1.628	0.004	2
1	A	99	LYS	HD2	1.64	0.000	1
1	A	99	LYS	HD3	1.64	0.000	1
1	A	99	LYS	HE2	2.955	0.000	1
1	A	99	LYS	HE3	2.955	0.000	1
1	A	99	LYS	HG2	1.267	0.007	2
1	A	99	LYS	HG3	1.378	0.003	2
1	A	99	LYS	C	176.171	0.012	1
1	A	99	LYS	CA	54.89	0.077	1
1	A	99	LYS	CB	33.965	0.036	1
1	A	99	LYS	CD	29.133	0.045	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	LYS	CE	42.137	0.059	1
1	A	99	LYS	CG	24.88	0.109	1
1	A	99	LYS	N	119.501	0.034	1
1	A	100	PHE	H	8.932	0.005	1
1	A	100	PHE	HA	4.656	0.010	1
1	A	100	PHE	HB2	2.936	0.000	2
1	A	100	PHE	HB3	2.881	0.000	2
1	A	100	PHE	HD1	7.175	0.000	1
1	A	100	PHE	HD2	7.175	0.000	1
1	A	100	PHE	C	174.636	0.046	1
1	A	100	PHE	CA	57.688	0.071	1
1	A	100	PHE	CB	39.826	0.035	1
1	A	100	PHE	CD1	131.692	0.000	1
1	A	100	PHE	CD2	131.692	0.000	1
1	A	100	PHE	N	125.711	0.019	1
1	A	101	GLU	H	8.016	0.004	1
1	A	101	GLU	HA	4.23	0.002	1
1	A	101	GLU	HB2	1.919	0.000	2
1	A	101	GLU	HB3	1.783	0.000	2
1	A	101	GLU	HG2	2.111	0.000	1
1	A	101	GLU	HG3	2.111	0.000	1
1	A	101	GLU	C	175.352	0.046	1
1	A	101	GLU	CA	55.355	0.077	1
1	A	101	GLU	CB	30.637	0.027	1
1	A	101	GLU	CG	36.045	0.022	1
1	A	101	GLU	N	127.647	0.033	1
1	A	102	MET	H	8.247	0.004	1
1	A	102	MET	HA	4.066	0.003	1
1	A	102	MET	HB2	2.59	0.000	2
1	A	102	MET	HB3	2.016	0.000	2
1	A	102	MET	HE1	2.122	0.000	1
1	A	102	MET	HE2	2.122	0.000	1
1	A	102	MET	HE3	2.122	0.000	1
1	A	102	MET	C	176.875	0.000	1
1	A	102	MET	CA	56.946	0.071	1
1	A	102	MET	CB	32.142	0.006	1
1	A	102	MET	CE	17.217	0.000	1
1	A	102	MET	N	124.104	0.046	1
1	A	103	ALA	H	8.506	0.004	1
1	A	103	ALA	HA	4.095	0.000	1
1	A	103	ALA	HB1	1.362	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	ALA	HB2	1.362	0.004	1
1	A	103	ALA	HB3	1.362	0.004	1
1	A	103	ALA	C	179.01	0.012	1
1	A	103	ALA	CA	54.418	0.000	1
1	A	103	ALA	CB	18.511	0.028	1
1	A	103	ALA	N	121.787	0.023	1
1	A	104	LYS	H	7.662	0.003	1
1	A	104	LYS	HA	4.079	0.000	1
1	A	104	LYS	HB2	1.723	0.000	2
1	A	104	LYS	HB3	1.72	0.000	2
1	A	104	LYS	HD2	1.622	0.000	1
1	A	104	LYS	HD3	1.622	0.000	1
1	A	104	LYS	HG2	1.384	0.000	1
1	A	104	LYS	HG3	1.384	0.000	1
1	A	104	LYS	C	177.452	0.000	1
1	A	104	LYS	CA	57.517	0.075	1
1	A	104	LYS	CB	32.493	0.066	1
1	A	104	LYS	CD	29.204	0.036	1
1	A	104	LYS	CG	24.756	0.004	1
1	A	104	LYS	N	117.353	0.021	1
1	A	105	TYR	H	7.767	0.003	1
1	A	105	TYR	HA	4.491	0.000	1
1	A	105	TYR	HB2	3.037	0.002	2
1	A	105	TYR	HB3	3.184	0.003	2
1	A	105	TYR	HD1	7.164	0.000	1
1	A	105	TYR	HD2	7.164	0.000	1
1	A	105	TYR	HE1	6.499	0.000	1
1	A	105	TYR	HE2	6.499	0.000	1
1	A	105	TYR	C	176.506	0.000	1
1	A	105	TYR	CA	59.137	0.212	1
1	A	105	TYR	CB	38.558	0.040	1
1	A	105	TYR	CE1	117.807	0.000	1
1	A	105	TYR	CE2	117.807	0.000	1
1	A	105	TYR	N	119.746	0.038	1
1	A	106	LEU	H	8.013	0.005	1
1	A	106	LEU	HA	4.172	0.000	1
1	A	106	LEU	HB2	1.712	0.000	2
1	A	106	LEU	HB3	1.648	0.000	2
1	A	106	LEU	HD11	0.867	0.000	1
1	A	106	LEU	HD12	0.867	0.000	1
1	A	106	LEU	HD13	0.867	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	LEU	HD21	0.879	0.000	1
1	A	106	LEU	HD22	0.879	0.000	1
1	A	106	LEU	HD23	0.879	0.000	1
1	A	106	LEU	C	177.636	0.000	1
1	A	106	LEU	CA	55.755	0.257	1
1	A	106	LEU	CB	42.186	0.000	1
1	A	106	LEU	CG	26.38	0.000	1
1	A	106	LEU	N	120.842	0.017	1
1	A	107	GLU	H	7.944	0.010	1
1	A	107	GLU	HA	4.105	0.000	1
1	A	107	GLU	HB2	1.908	0.000	1
1	A	107	GLU	HB3	1.908	0.000	1
1	A	107	GLU	HG2	2.219	0.000	1
1	A	107	GLU	HG3	2.219	0.000	1
1	A	107	GLU	C	176.644	0.000	1
1	A	107	GLU	CA	57.52	0.114	1
1	A	107	GLU	CB	30.097	0.074	1
1	A	107	GLU	CG	36.205	0.000	1
1	A	107	GLU	N	119.737	0.018	1
1	A	108	HIS	C	174.059	0.000	1
1	A	109	HIS	H	7.909	0.006	1
1	A	109	HIS	C	179.437	0.000	1
1	A	109	HIS	N	125.86	0.047	1

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
$^{13}\text{C}_\alpha$	102	-0.13 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	100	0.21 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	97	0.09 ± 0.16	None needed (< 0.5 ppm)
^{15}N	95	1.24 ± 0.47	Should be applied

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 87%, i.e. 1046 atoms were assigned a chemical shift out of a possible 1199. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	408/422 (97%)	164/169 (97%)	164/170 (96%)	80/83 (96%)
Sidechain	558/664 (84%)	376/434 (87%)	174/207 (84%)	8/23 (35%)
Aromatic	80/113 (71%)	42/56 (75%)	37/54 (69%)	1/3 (33%)
Overall	1046/1199 (87%)	582/659 (88%)	375/431 (87%)	89/109 (82%)

7.1.4 Statistically unusual chemical shifts [i](#)

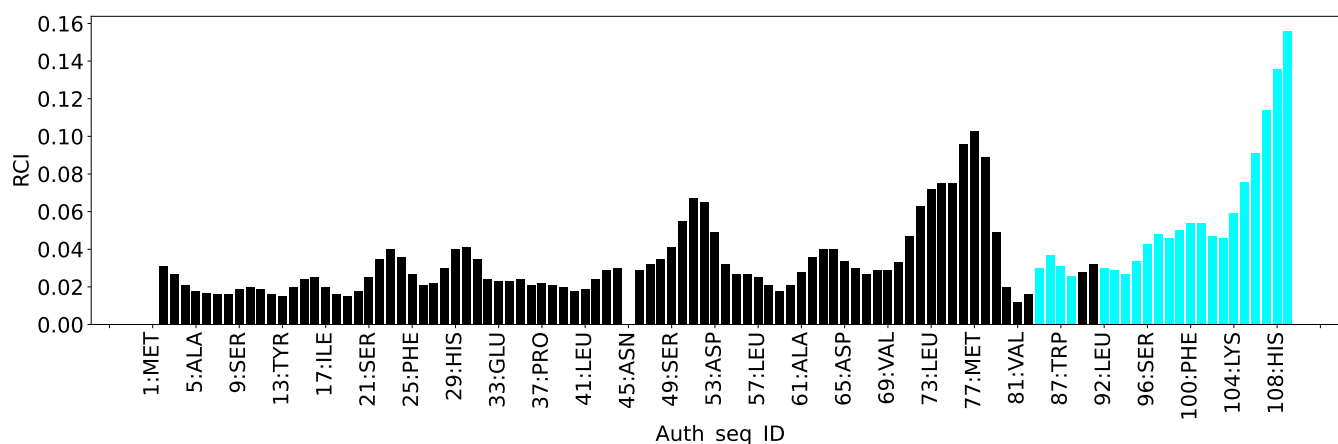
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	8	THR	HG1	5.37	0.08 – 2.19	20.0
1	A	89	PRO	HB3	-0.07	0.25 – 3.76	-5.9
1	A	34	GLY	N	129.88	91.59 – 127.52	5.7

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	2062
Intra-residue ($ i-j =0$)	927
Sequential ($ i-j =1$)	419
Medium range ($ i-j >1$ and $ i-j <5$)	284
Long range ($ i-j \geq 5$)	376
Inter-chain	0
Hydrogen bond restraints	56
Disulfide bond restraints	0
Total dihedral-angle restraints	163
Number of unmapped restraints	0
Number of restraints per residue	19.7
Number of long range restraints per residue ¹	3.4

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)	0.8	0.17
0.2-0.5 (Medium)	0.4	0.4
>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. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

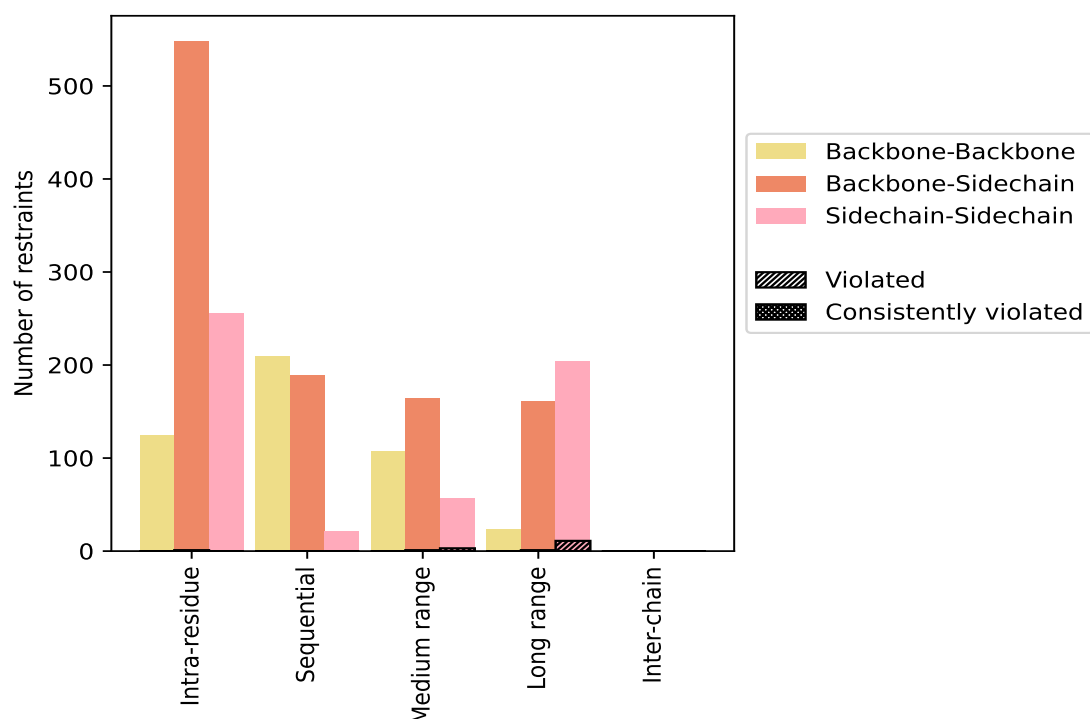
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	927	45.0	1	0.1	0.0	0	0.0	0.0
Backbone-Backbone	124	6.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	548	26.6	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	255	12.4	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	419	20.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	209	10.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	189	9.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	21	1.0	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	284	13.8	4	1.4	0.2	0	0.0	0.0
Backbone-Backbone	107	5.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	120	5.8	1	0.8	0.0	0	0.0	0.0
Sidechain-Sidechain	57	2.8	3	5.3	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	376	18.2	12	3.2	0.6	0	0.0	0.0
Backbone-Backbone	23	1.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	149	7.2	1	0.7	0.0	0	0.0	0.0
Sidechain-Sidechain	204	9.9	11	5.4	0.5	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	56	2.7	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	2062	100.0	17	0.8	0.8	0	0.0	0.0
Backbone-Backbone	463	22.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1062	51.5	3	0.3	0.1	0	0.0	0.0
Sidechain-Sidechain	537	26.0	14	2.6	0.7	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	0	0	1	2	0	3	0.11	0.12	0.0	0.11
2	0	0	0	1	0	1	0.13	0.13	0.0	0.13
3	0	0	0	1	0	1	0.11	0.11	0.0	0.11
4	0	0	0	2	0	2	0.19	0.28	0.09	0.19
5	0	0	0	2	0	2	0.19	0.24	0.05	0.19
6	0	0	1	1	0	2	0.19	0.22	0.03	0.19
7	0	0	0	2	0	2	0.1	0.1	0.0	0.1
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	1	0	1	0.11	0.11	0.0	0.11
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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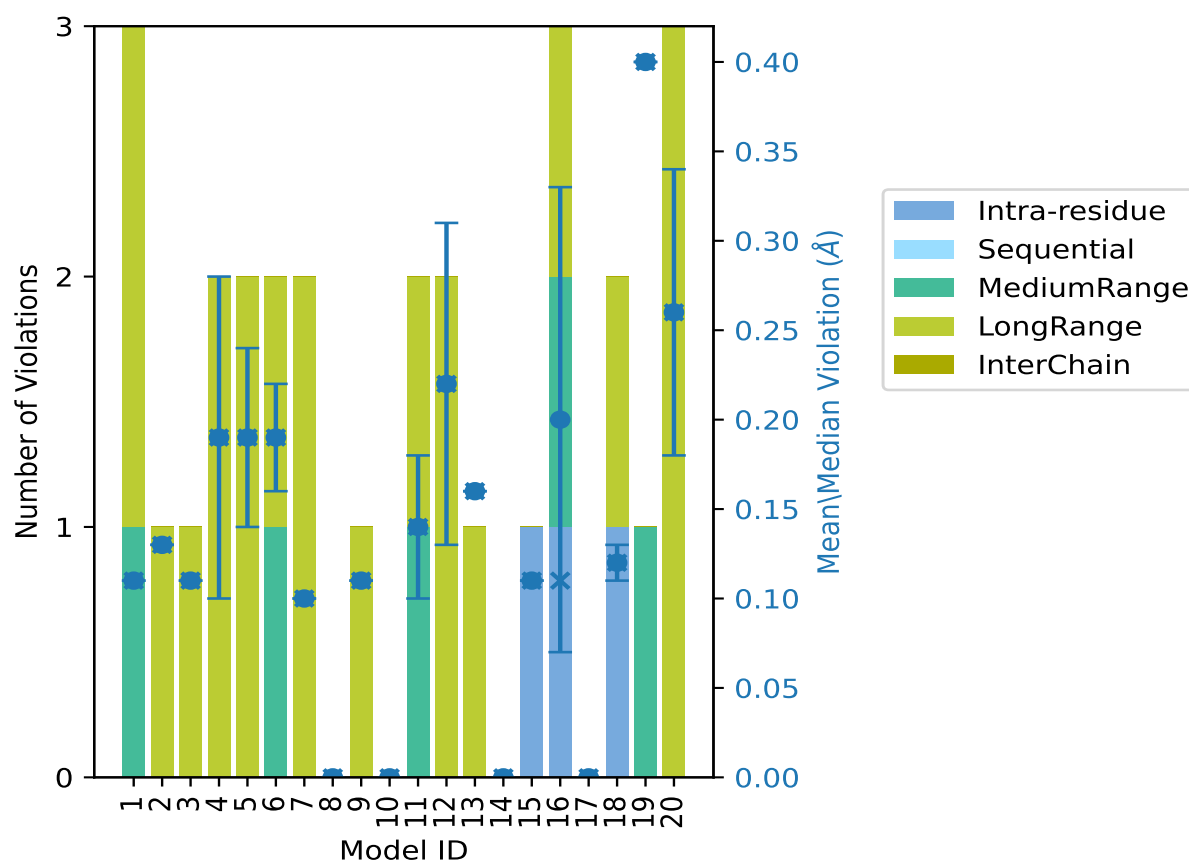
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	1	1	0	2	0.14	0.17	0.04	0.14
12	0	0	0	2	0	2	0.22	0.31	0.09	0.22
13	0	0	0	1	0	1	0.16	0.16	0.0	0.16
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	1	0	0	0	0	1	0.11	0.11	0.0	0.11
16	1	0	1	1	0	3	0.2	0.38	0.13	0.11
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	1	0	0	1	0	2	0.12	0.13	0.01	0.12
19	0	0	1	0	0	1	0.4	0.4	0.0	0.4
20	0	0	0	3	0	3	0.26	0.36	0.08	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

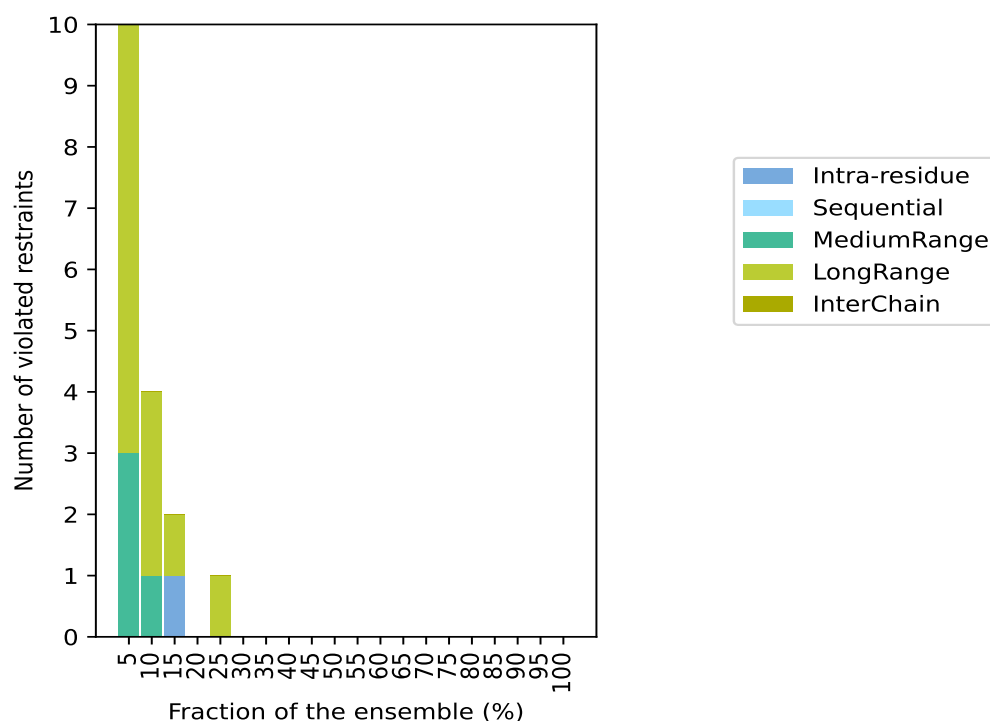
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1989(IR:926, SQ:419, MR:280, LR:364, IC:0) restraints are 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	%
0	0	3	7	0	10	1	5.0
0	0	1	3	0	4	2	10.0
1	0	0	1	0	2	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	1	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
0	0	0	0	0	0	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
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

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

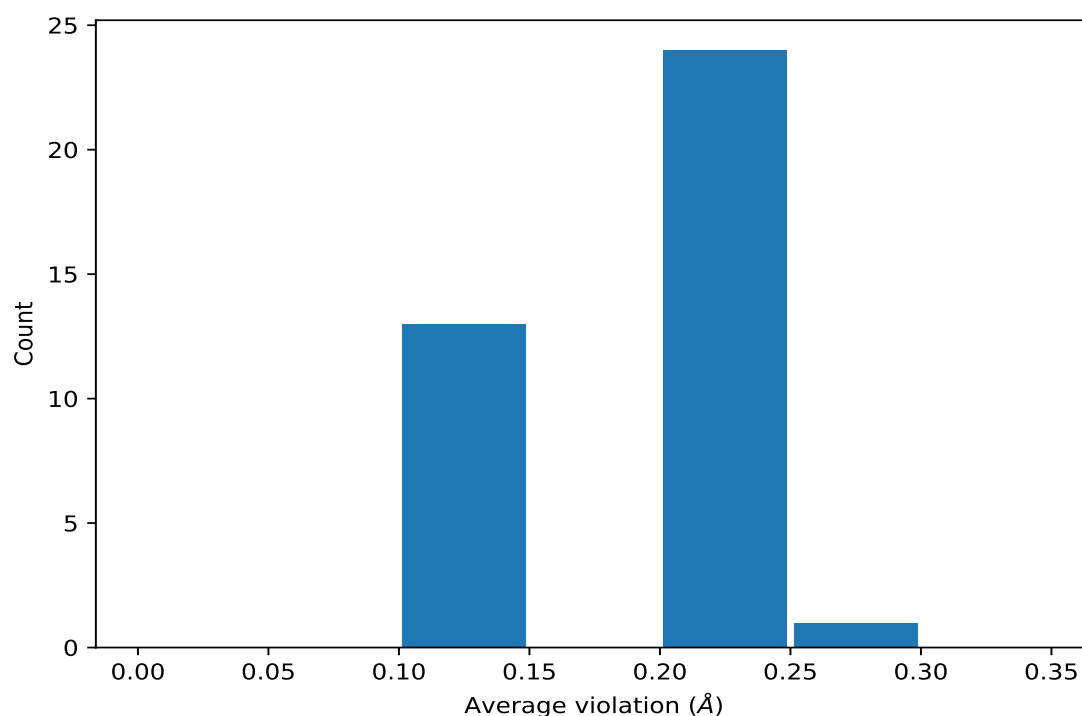
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 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. 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)
(1,161)	1:79:A:ILE:HG21	1:38:A:LEU:HB3	5	0.14	0.03	0.16
(1,161)	1:79:A:ILE:HG22	1:38:A:LEU:HB3	5	0.14	0.03	0.16
(1,161)	1:79:A:ILE:HG23	1:38:A:LEU:HB3	5	0.14	0.03	0.16
(1,815)	1:17:A:ILE:HD11	1:86:A:THR:HG21	3	0.23	0.11	0.24
(1,815)	1:17:A:ILE:HD11	1:86:A:THR:HG22	3	0.23	0.11	0.24
(1,815)	1:17:A:ILE:HD11	1:86:A:THR:HG23	3	0.23	0.11	0.24
(1,815)	1:17:A:ILE:HD12	1:86:A:THR:HG21	3	0.23	0.11	0.24
(1,815)	1:17:A:ILE:HD12	1:86:A:THR:HG22	3	0.23	0.11	0.24
(1,815)	1:17:A:ILE:HD12	1:86:A:THR:HG23	3	0.23	0.11	0.24
(1,815)	1:17:A:ILE:HD13	1:86:A:THR:HG21	3	0.23	0.11	0.24
(1,815)	1:17:A:ILE:HD13	1:86:A:THR:HG22	3	0.23	0.11	0.24
(1,815)	1:17:A:ILE:HD13	1:86:A:THR:HG23	3	0.23	0.11	0.24
(3,767)	1:98:A:LEU:H	1:98:A:LEU:HG	3	0.12	0.01	0.11
(3,740)	1:19:A:ASN:HD22	1:23:A:ASP:HB3	2	0.29	0.12	0.29
(1,65)	1:50:A:PHE:HE1	1:7:A:LEU:HD11	2	0.2	0.08	0.2
(1,65)	1:50:A:PHE:HE1	1:7:A:LEU:HD12	2	0.2	0.08	0.2

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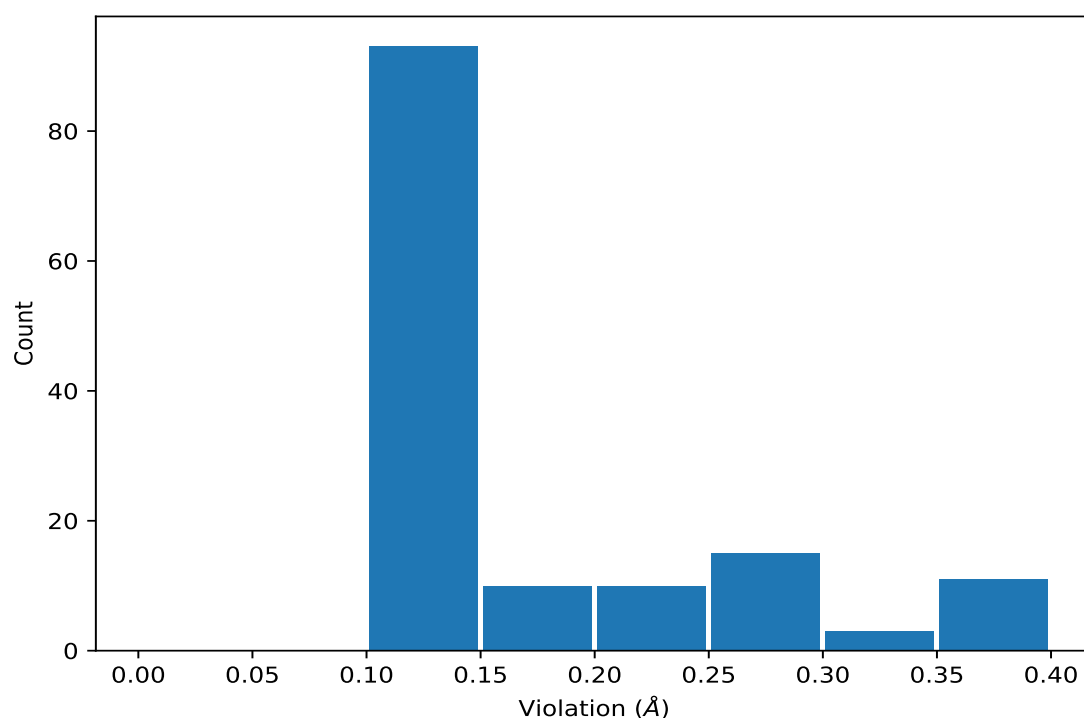
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,65)	1:50:A:PHE:HE1	1:7:A:LEU:HD13	2	0.2	0.08	0.2
(1,65)	1:50:A:PHE:HE2	1:7:A:LEU:HD11	2	0.2	0.08	0.2
(1,65)	1:50:A:PHE:HE2	1:7:A:LEU:HD12	2	0.2	0.08	0.2
(1,65)	1:50:A:PHE:HE2	1:7:A:LEU:HD13	2	0.2	0.08	0.2
(1,76)	1:17:A:ILE:HD11	1:86:A:THR:HG21	2	0.2	0.06	0.2
(1,76)	1:17:A:ILE:HD11	1:86:A:THR:HG22	2	0.2	0.06	0.2
(1,76)	1:17:A:ILE:HD11	1:86:A:THR:HG23	2	0.2	0.06	0.2
(1,76)	1:17:A:ILE:HD12	1:86:A:THR:HG21	2	0.2	0.06	0.2
(1,76)	1:17:A:ILE:HD12	1:86:A:THR:HG22	2	0.2	0.06	0.2
(1,76)	1:17:A:ILE:HD12	1:86:A:THR:HG23	2	0.2	0.06	0.2
(1,76)	1:17:A:ILE:HD13	1:86:A:THR:HG21	2	0.2	0.06	0.2
(1,76)	1:17:A:ILE:HD13	1:86:A:THR:HG22	2	0.2	0.06	0.2
(1,76)	1:17:A:ILE:HD13	1:86:A:THR:HG23	2	0.2	0.06	0.2
(1,1146)	1:47:A:ILE:HG21	1:42:A:ALA:HB1	2	0.13	0.0	0.13
(1,1146)	1:47:A:ILE:HG21	1:42:A:ALA:HB2	2	0.13	0.0	0.13
(1,1146)	1:47:A:ILE:HG21	1:42:A:ALA:HB3	2	0.13	0.0	0.13
(1,1146)	1:47:A:ILE:HG22	1:42:A:ALA:HB1	2	0.13	0.0	0.13
(1,1146)	1:47:A:ILE:HG22	1:42:A:ALA:HB2	2	0.13	0.0	0.13
(1,1146)	1:47:A:ILE:HG22	1:42:A:ALA:HB3	2	0.13	0.0	0.13
(1,1146)	1:47:A:ILE:HG23	1:42:A:ALA:HB1	2	0.13	0.0	0.13
(1,1146)	1:47:A:ILE:HG23	1:42:A:ALA:HB2	2	0.13	0.0	0.13
(1,1146)	1:47:A:ILE:HG23	1:42:A:ALA:HB3	2	0.13	0.0	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)
(3,740)	1:19:A:ASN:HD22	1:23:A:ASP:HB3	19	0.4
(1,946)	1:97:A:ARG:HD3	1:94:A:SER:HA	16	0.38
(1,815)	1:17:A:ILE:HD11	1:86:A:THR:HG21	20	0.36
(1,815)	1:17:A:ILE:HD11	1:86:A:THR:HG22	20	0.36
(1,815)	1:17:A:ILE:HD11	1:86:A:THR:HG23	20	0.36
(1,815)	1:17:A:ILE:HD12	1:86:A:THR:HG21	20	0.36
(1,815)	1:17:A:ILE:HD12	1:86:A:THR:HG22	20	0.36
(1,815)	1:17:A:ILE:HD12	1:86:A:THR:HG23	20	0.36
(1,815)	1:17:A:ILE:HD13	1:86:A:THR:HG21	20	0.36
(1,815)	1:17:A:ILE:HD13	1:86:A:THR:HG22	20	0.36
(1,815)	1:17:A:ILE:HD13	1:86:A:THR:HG23	20	0.36
(1,257)	1:8:A:THR:HG21	1:64:A:SER:HB2	12	0.31
(1,257)	1:8:A:THR:HG22	1:64:A:SER:HB2	12	0.31
(1,257)	1:8:A:THR:HG23	1:64:A:SER:HB2	12	0.31
(1,65)	1:50:A:PHE:HE1	1:7:A:LEU:HD11	4	0.28
(1,65)	1:50:A:PHE:HE1	1:7:A:LEU:HD12	4	0.28
(1,65)	1:50:A:PHE:HE1	1:7:A:LEU:HD13	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:50:A:PHE:HE2	1:7:A:LEU:HD11	4	0.28
(1,65)	1:50:A:PHE:HE2	1:7:A:LEU:HD12	4	0.28
(1,65)	1:50:A:PHE:HE2	1:7:A:LEU:HD13	4	0.28
(1,76)	1:17:A:ILE:HD11	1:86:A:THR:HG21	20	0.26
(1,76)	1:17:A:ILE:HD11	1:86:A:THR:HG22	20	0.26
(1,76)	1:17:A:ILE:HD11	1:86:A:THR:HG23	20	0.26
(1,76)	1:17:A:ILE:HD12	1:86:A:THR:HG21	20	0.26
(1,76)	1:17:A:ILE:HD12	1:86:A:THR:HG22	20	0.26
(1,76)	1:17:A:ILE:HD12	1:86:A:THR:HG23	20	0.26
(1,76)	1:17:A:ILE:HD13	1:86:A:THR:HG21	20	0.26
(1,76)	1:17:A:ILE:HD13	1:86:A:THR:HG22	20	0.26
(1,76)	1:17:A:ILE:HD13	1:86:A:THR:HG23	20	0.26
(1,815)	1:17:A:ILE:HD11	1:86:A:THR:HG21	5	0.24
(1,815)	1:17:A:ILE:HD11	1:86:A:THR:HG22	5	0.24
(1,815)	1:17:A:ILE:HD11	1:86:A:THR:HG23	5	0.24
(1,815)	1:17:A:ILE:HD12	1:86:A:THR:HG21	5	0.24
(1,815)	1:17:A:ILE:HD12	1:86:A:THR:HG22	5	0.24
(1,815)	1:17:A:ILE:HD12	1:86:A:THR:HG23	5	0.24
(1,815)	1:17:A:ILE:HD13	1:86:A:THR:HG21	5	0.24
(1,815)	1:17:A:ILE:HD13	1:86:A:THR:HG22	5	0.24
(1,815)	1:17:A:ILE:HD13	1:86:A:THR:HG23	5	0.24
(1,923)	1:92:A:LEU:HB2	1:96:A:SER:HB2	6	0.22
(3,740)	1:19:A:ASN:HD22	1:23:A:ASP:HB3	11	0.17
(1,161)	1:79:A:ILE:HG21	1:38:A:LEU:HB3	20	0.17

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

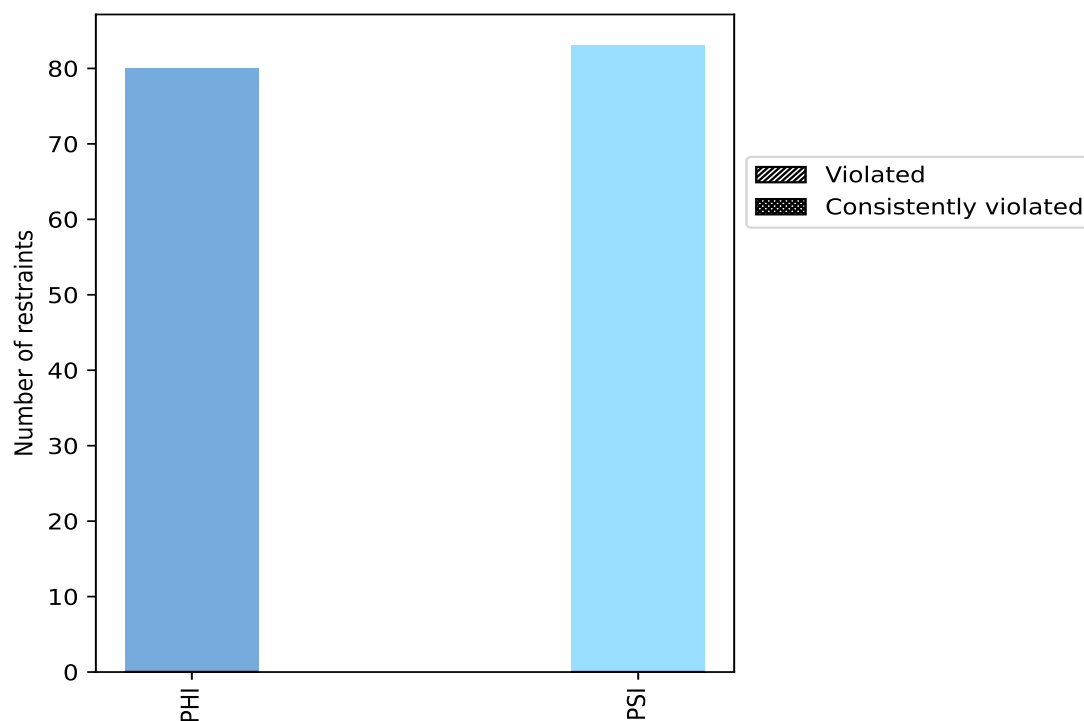
10.1 Summary of dihedral-angle violations [i](#)

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	80	49.1	0	0.0	0.0	0	0.0	0.0
PSI	83	50.9	0	0.0	0.0	0	0.0	0.0
Total	163	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