wwPDB NMR Structure Validation Summary Report

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PDB ID	:	8Z4A / pdb_00008z4a
BMRB ID	:	51791
Title	:	Solution Structure of DRB4 C-terminal domain, DRB4D3
Authors	:	Deshmukh, M.V.; Paturi, S.; Patra, D.
Deposited on	:	2024-04-17

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

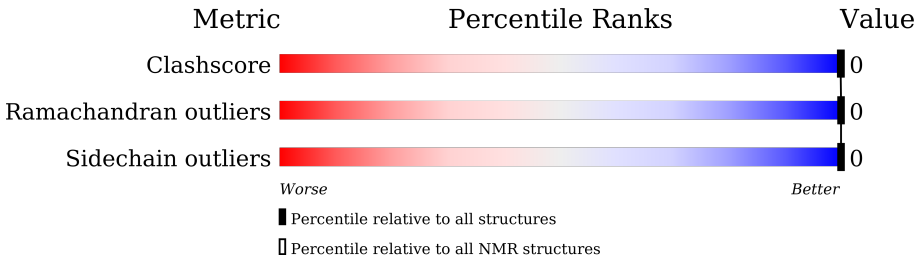
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 54%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	71	48% . 48%

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:320-A:353 (34)	0.60	8

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

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

The models can be grouped into 1 clusters and 6 single-model clusters were found.

Cluster number	Models
1	1, 7, 8, 10
Single-model clusters	2; 3; 4; 5; 6; 9

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 610 atoms, of which 303 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Double-stranded RNA-binding protein 4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	37	610	199	303	53	53	2	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	MET	-	initiating methionine	UNP Q8H1D4
A	356	LEU	-	expression tag	UNP Q8H1D4
A	357	GLU	-	expression tag	UNP Q8H1D4
A	358	HIS	-	expression tag	UNP Q8H1D4
A	359	HIS	-	expression tag	UNP Q8H1D4
A	360	HIS	-	expression tag	UNP Q8H1D4
A	361	HIS	-	expression tag	UNP Q8H1D4
A	362	HIS	-	expression tag	UNP Q8H1D4
A	363	HIS	-	expression tag	UNP Q8H1D4

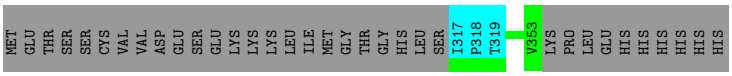
4 Residue-property plots (i)

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: Double-stranded RNA-binding protein 4

Chain A:

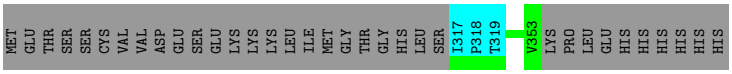


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

• Molecule 1: Double-stranded RNA-binding protein 4

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 5000 calculated structures, 10 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	structure calculation	
Rosetta	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	466
Number of shifts mapped to atoms	289
Number of unparsed shifts	0
Number of shifts with mapping errors	177
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

6 Model quality

6.1 Standard geometry

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

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
All	All	2850	2780	2790	-

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 -.

There are no clashes.

6.3 Torsion angles

6.3.1 Protein backbone

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	33/71 (46%)	33±0 (99±1%)	0±0 (1±1%)	0±0 (0±0%)	100	100
All	All	330/710 (46%)	327 (99%)	3 (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	31/66 (47%)	31±0 (100±0%)	0±0 (0±0%)	100	100
All	All	310/660 (47%)	310 (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 (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 54% for the well-defined parts and 54% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	466
Number of shifts mapped to atoms	289
Number of unparsed shifts	0
Number of shifts with mapping errors	177
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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 177) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	294	GLU	H	8.992	0.020	1
1	A	294	GLU	C	172.826	0.3	1
1	A	294	GLU	CA	57.157	0.3	1
1	A	294	GLU	CB	31.482	0.3	1
1	A	294	GLU	N	128.448	0.3	1
1	A	298	CYS	H	7.922	0.020	1
1	A	298	CYS	HA	4.824	0.020	1
1	A	298	CYS	C	174.373	0.3	1
1	A	298	CYS	CA	57.916	0.3	1
1	A	298	CYS	CB	37.708	0.3	1
1	A	298	CYS	N	125.4	0.3	1
1	A	299	VAL	H	8.068	0.020	1
1	A	299	VAL	HA	4.028	0.020	1
1	A	299	VAL	HB	1.939	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	299	VAL	HG21	0.807	0.020	1
1	A	299	VAL	HG22	0.807	0.020	1
1	A	299	VAL	HG23	0.807	0.020	1
1	A	299	VAL	C	175.852	0.3	1
1	A	299	VAL	CA	61.803	0.3	1
1	A	299	VAL	CB	31.596	0.3	1
1	A	299	VAL	CG1	20.347	0.3	1
1	A	299	VAL	N	124.648	0.3	1
1	A	300	VAL	H	8.083	0.020	1
1	A	300	VAL	HA	4.003	0.020	1
1	A	300	VAL	HB	1.92	0.020	1
1	A	300	VAL	HG21	0.792	0.020	1
1	A	300	VAL	HG22	0.792	0.020	1
1	A	300	VAL	HG23	0.792	0.020	1
1	A	300	VAL	C	175.403	0.3	1
1	A	300	VAL	CA	61.56	0.3	1
1	A	300	VAL	CB	31.789	0.3	1
1	A	300	VAL	CG1	20.336	0.3	1
1	A	300	VAL	N	125.994	0.3	1
1	A	301	ASP	H	8.279	0.020	1
1	A	301	ASP	HA	4.506	0.020	1
1	A	301	ASP	HB2	2.58	0.020	1
1	A	301	ASP	C	176.398	0.3	1
1	A	301	ASP	CA	53.545	0.3	1
1	A	301	ASP	CB	40.634	0.3	1
1	A	301	ASP	N	126.187	0.3	1
1	A	302	GLU	H	8.441	0.020	1
1	A	302	GLU	HA	4.142	0.020	1
1	A	302	GLU	HB2	1.875	0.020	1
1	A	302	GLU	HG2	2.163	0.020	1
1	A	302	GLU	C	177.05	0.3	1
1	A	302	GLU	CA	56.545	0.3	1
1	A	302	GLU	CB	28.816	0.3	1
1	A	302	GLU	CG	35.779	0.3	1
1	A	302	GLU	N	124.782	0.3	1
1	A	303	SER	H	8.285	0.020	1
1	A	303	SER	HA	4.174	0.020	1
1	A	303	SER	C	175.238	0.3	1
1	A	303	SER	CA	59.268	0.3	1
1	A	303	SER	CB	62.556	0.3	1
1	A	303	SER	N	117.742	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	304	GLU	H	8.065	0.020	1
1	A	304	GLU	HA	4.129	0.020	1
1	A	304	GLU	HB2	2.041	0.020	1
1	A	304	GLU	HG2	2.156	0.020	1
1	A	304	GLU	C	176.956	0.3	1
1	A	304	GLU	CA	56.527	0.3	1
1	A	304	GLU	CB	28.832	0.3	1
1	A	304	GLU	CG	35.728	0.3	1
1	A	304	GLU	N	123.662	0.3	1
1	A	305	LYS	H	7.901	0.020	1
1	A	305	LYS	C	175.971	0.3	1
1	A	305	LYS	CB	31.605	0.3	1
1	A	305	LYS	N	122.751	0.3	1
1	A	306	LYS	H	8.02	0.020	1
1	A	306	LYS	C	176.446	0.3	1
1	A	306	LYS	CA	55.706	0.3	1
1	A	306	LYS	CB	31.781	0.3	1
1	A	306	LYS	CE	41.662	0.3	1
1	A	306	LYS	N	123.701	0.3	1
1	A	307	LYS	H	7.941	0.020	1
1	A	307	LYS	HA	4.159	0.020	1
1	A	307	LYS	HB2	1.707	0.020	1
1	A	307	LYS	HD2	1.582	0.020	1
1	A	307	LYS	HE2	2.868	0.020	1
1	A	307	LYS	HG2	1.315	0.020	1
1	A	307	LYS	C	175.97	0.3	1
1	A	307	LYS	CA	55.922	0.3	1
1	A	307	LYS	CB	31.96	0.3	1
1	A	307	LYS	CD	28.573	0.3	1
1	A	307	LYS	CE	41.649	0.3	1
1	A	307	LYS	CG	24.205	0.3	1
1	A	307	LYS	N	123.26	0.3	1
1	A	308	LEU	H	7.727	0.020	1
1	A	308	LEU	HA	4.13	0.020	1
1	A	308	LEU	HB2	1.693	0.020	1
1	A	308	LEU	HG	1.342	0.020	1
1	A	308	LEU	C	176.522	0.3	1
1	A	308	LEU	CA	54.431	0.3	1
1	A	308	LEU	CB	42.071	0.3	1
1	A	308	LEU	CD1	24.228	0.3	1
1	A	308	LEU	CD2	24.118	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	308	LEU	N	123.452	0.3	1
1	A	309	ILE	H	7.909	0.020	1
1	A	309	ILE	HD11	0.648	0.020	1
1	A	309	ILE	HD12	0.648	0.020	1
1	A	309	ILE	HD13	0.648	0.020	1
1	A	309	ILE	C	176.9	0.3	1
1	A	309	ILE	CA	60.544	0.3	1
1	A	309	ILE	CB	37.083	0.3	1
1	A	309	ILE	CD1	12.148	0.3	1
1	A	309	ILE	CG1	27.157	0.3	1
1	A	309	ILE	CG2	16.853	0.3	1
1	A	309	ILE	N	122.959	0.3	1
1	A	310	MET	H	8.33	0.020	1
1	A	310	MET	HG2	2.581	0.020	2
1	A	310	MET	HG3	2.453	0.020	2
1	A	310	MET	C	177.152	0.3	1
1	A	310	MET	CA	54.118	0.3	1
1	A	310	MET	CB	31.185	0.3	1
1	A	310	MET	CG	31.534	0.3	1
1	A	310	MET	N	125.677	0.3	1
1	A	311	GLY	H	8.079	0.020	1
1	A	311	GLY	C	174.024	0.3	1
1	A	311	GLY	CA	44.152	0.3	1
1	A	311	GLY	N	112.127	0.3	1
1	A	312	THR	H	8.251	0.020	1
1	A	312	THR	HA	4.274	0.020	1
1	A	312	THR	HG21	1.11	0.020	1
1	A	312	THR	HG22	1.11	0.020	1
1	A	312	THR	HG23	1.11	0.020	1
1	A	312	THR	C	175.601	0.3	1
1	A	312	THR	CA	61.687	0.3	1
1	A	312	THR	CB	68.604	0.3	1
1	A	312	THR	CG2	20.999	0.3	1
1	A	312	THR	N	114.693	0.3	1
1	A	313	GLY	H	8.389	0.020	1
1	A	313	GLY	HA2	4.077	0.020	1
1	A	313	GLY	C	173.443	0.3	1
1	A	313	GLY	CA	44.79	0.3	1
1	A	313	GLY	N	111.694	0.3	1
1	A	314	HIS	H	7.975	0.020	1
1	A	314	HIS	HB2	2.98	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	314	HIS	C	173.961	0.3	1
1	A	314	HIS	CA	54.276	0.3	1
1	A	314	HIS	CB	29.563	0.3	1
1	A	314	HIS	N	119.574	0.3	1
1	A	315	LEU	H	8.02	0.020	1
1	A	315	LEU	HB2	1.301	0.020	1
1	A	315	LEU	HD11	0.707	0.020	2
1	A	315	LEU	HD12	0.707	0.020	2
1	A	315	LEU	HD13	0.707	0.020	2
1	A	315	LEU	HD21	0.649	0.020	2
1	A	315	LEU	HD22	0.649	0.020	2
1	A	315	LEU	HD23	0.649	0.020	2
1	A	315	LEU	C	176.754	0.3	1
1	A	315	LEU	CA	54.739	0.3	1
1	A	315	LEU	CB	40.598	0.3	1
1	A	315	LEU	CD1	24.449	0.3	1
1	A	315	LEU	CD2	24.408	0.3	1
1	A	315	LEU	N	124.109	0.3	1
1	A	316	SER	H	7.923	0.020	1
1	A	316	SER	HA	4.355	0.020	1
1	A	316	SER	HB2	4.018	0.020	1
1	A	316	SER	C	173.641	0.3	1
1	A	316	SER	CA	57.05	0.3	1
1	A	316	SER	CB	62.704	0.3	1
1	A	316	SER	N	116.976	0.3	1
1	A	354	LYS	H	8.111	0.020	1
1	A	354	LYS	C	174.097	0.3	1
1	A	354	LYS	CA	53.22	0.3	1
1	A	354	LYS	CB	31.571	0.3	1
1	A	354	LYS	N	127.039	0.3	1
1	A	355	PRO	HA	4.276	0.020	1
1	A	355	PRO	HB2	2.126	0.020	1
1	A	355	PRO	HD2	3.708	0.020	2
1	A	355	PRO	HD3	3.502	0.020	2
1	A	355	PRO	HG2	1.848	0.020	1
1	A	355	PRO	C	176.658	0.3	1
1	A	355	PRO	CA	62.356	0.3	1
1	A	355	PRO	CB	31.037	0.3	1
1	A	355	PRO	CD	50.166	0.3	1
1	A	355	PRO	CG	26.684	0.3	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	58	0.92 ± 0.15	Should be applied
$^{13}C_{\beta}$	56	0.80 ± 0.26	Should be applied
$^{13}C'$	59	1.01 ± 0.32	Should be applied
^{15}N	54	-1.52 ± 0.80	None needed (imprecise)

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 54%, i.e. 268 atoms were assigned a chemical shift out of a possible 496. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	150/165 (91%)	51/66 (77%)	68/68 (100%)	31/31 (100%)
Sidechain	118/284 (42%)	65/184 (35%)	53/87 (61%)	0/13 (0%)
Aromatic	0/47 (0%)	0/24 (0%)	0/22 (0%)	0/1 (0%)
Overall	268/496 (54%)	116/274 (42%)	121/177 (68%)	31/45 (69%)

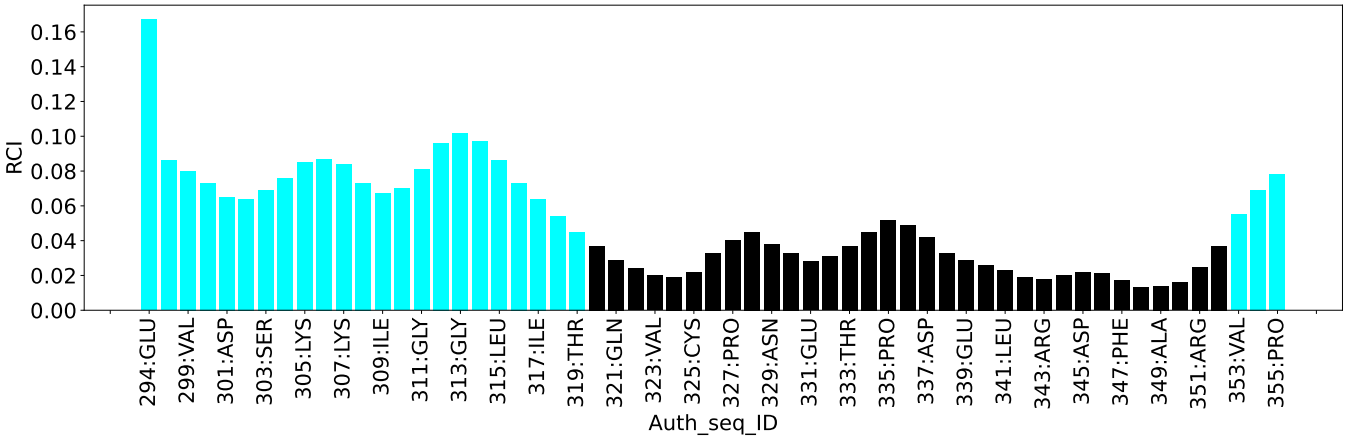
7.1.4 Statistically unusual chemical shifts (i)

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:


RCI
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
294:GLU
299:VAL
301:ASP
303:SER
305:LYS
307:LYS
309:ILE
311:GLY
313:GLY
315:LEU
317:ILE
319:THR
321:GLN
323:VAL
325:CYS
327:PRO
329:ASN
331:GLU
333:THR
335:PRO
337:ASP
339:GLU
341:LEU
343:ARG
345:ASP
347:PHE
349:ALA
351:ARG
353:VAL
355:PRO
Auth_seq_ID

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	38
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	12
Medium range (|i-j|>1 and |i-j|<5)	6
Long range (|i-j|≥5)	20
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	60
Number of unmapped restraints	0
Number of restraints per residue	1.4
Number of long range restraints per residue[1]	0.3

[1]Long 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)	1.4	0.2
0.2-0.5 (Medium)	3.4	0.5
>0.5 (Large)	2.5	1.18

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	11.8	9.98
10.0-20.0 (Medium)	5.8	18.73
>20.0 (Large)	2.8	70.06

9 Distance violation analysis (i)

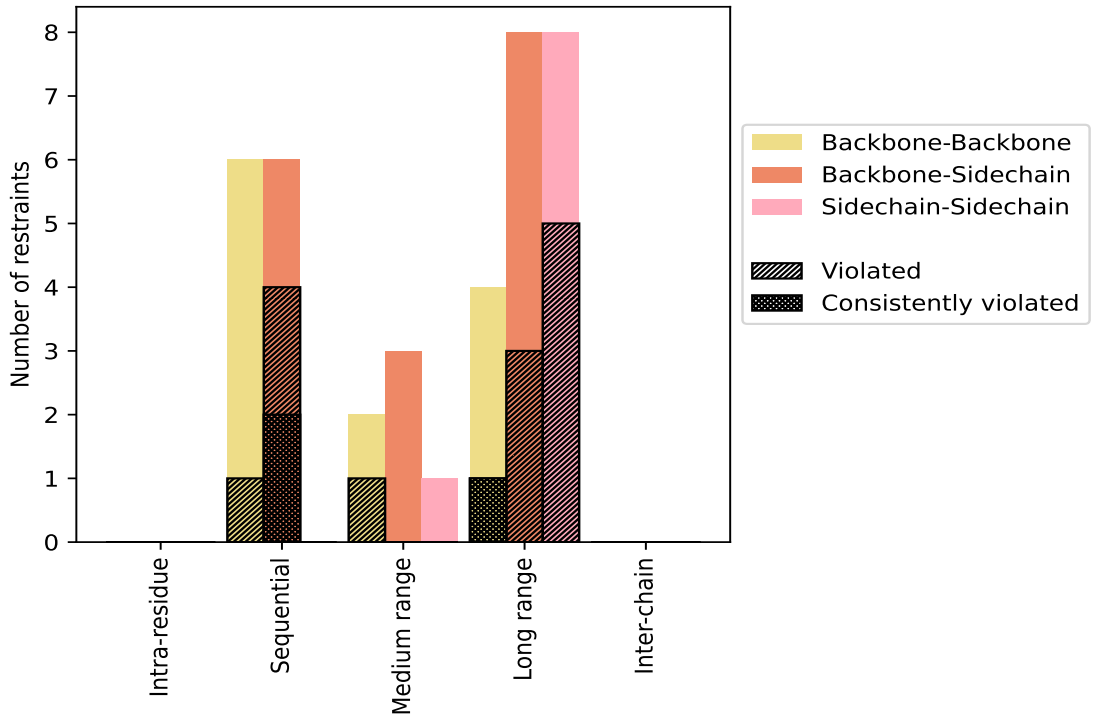
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	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
Sequential (|i-j|=1)	12	31.6	5	41.7	13.2	2	16.7	5.3
Backbone-Backbone	6	15.8	1	16.7	2.6	0	0.0	0.0
Backbone-Sidechain	6	15.8	4	66.7	10.5	2	33.3	5.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	6	15.8	1	16.7	2.6	0	0.0	0.0
Backbone-Backbone	2	5.3	1	50.0	2.6	0	0.0	0.0
Backbone-Sidechain	3	7.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1	2.6	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	20	52.6	9	45.0	23.7	1	5.0	2.6
Backbone-Backbone	4	10.5	1	25.0	2.6	1	25.0	2.6
Backbone-Sidechain	8	21.1	3	37.5	7.9	0	0.0	0.0
Sidechain-Sidechain	8	21.1	5	62.5	13.2	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	38	100.0	15	39.5	39.5	3	7.9	7.9
Backbone-Backbone	12	31.6	3	25.0	7.9	1	8.3	2.6
Backbone-Sidechain	17	44.7	7	41.2	18.4	2	11.8	5.3
Sidechain-Sidechain	9	23.7	5	55.6	13.2	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



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

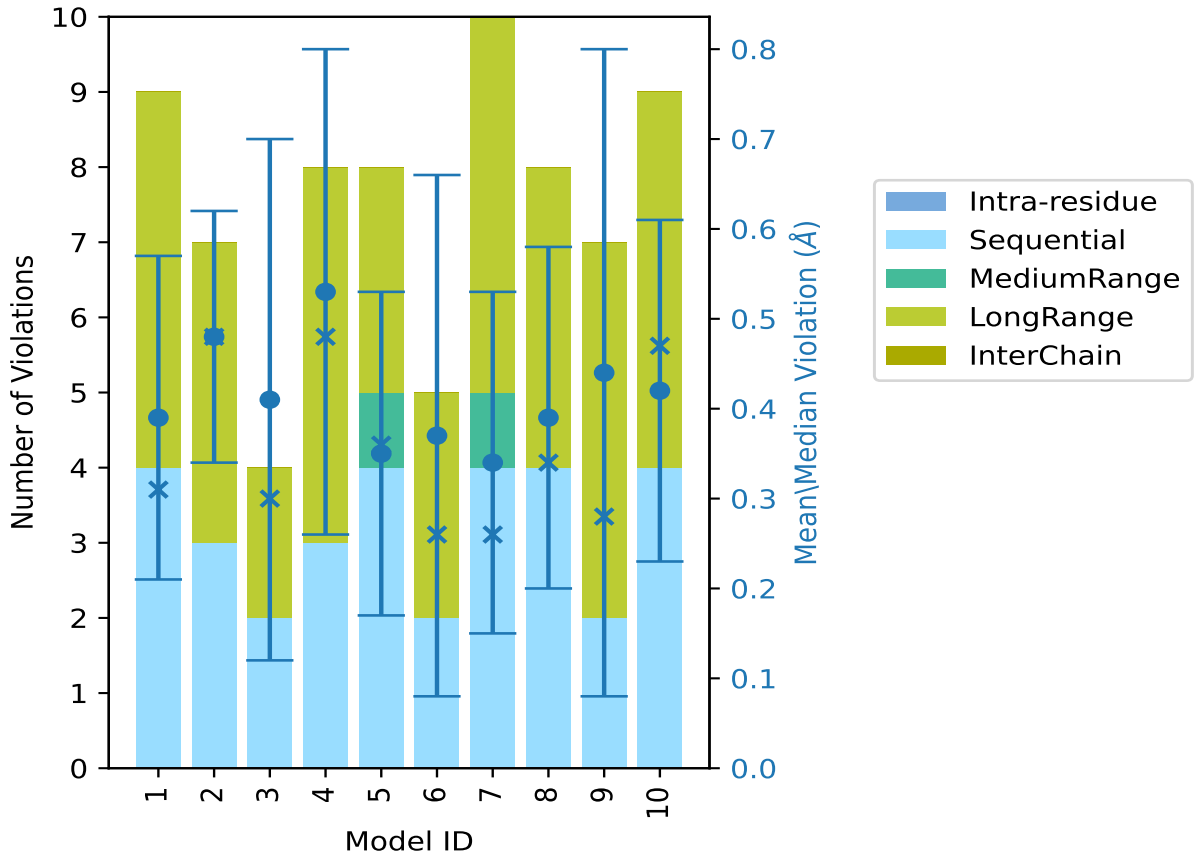
9.2 Distance violation statistics for each model

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	4	0	5	0	9	0.39	0.71	0.18	0.31
2	0	3	0	4	0	7	0.48	0.72	0.14	0.48
3	0	2	0	2	0	4	0.41	0.88	0.29	0.3
4	0	3	0	5	0	8	0.53	0.98	0.27	0.48
5	0	4	1	3	0	8	0.35	0.64	0.18	0.36
6	0	2	0	3	0	5	0.37	0.93	0.29	0.26
7	0	4	1	5	0	10	0.34	0.63	0.19	0.26
8	0	4	0	4	0	8	0.39	0.72	0.19	0.34
9	0	2	0	5	0	7	0.44	1.18	0.36	0.28
10	0	4	0	5	0	9	0.42	0.64	0.19	0.47

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance 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

9.3 Distance violation statistics for the ensemble (i)

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, 23(IR:0, SQ:7, MR:5, LR:11, 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	0	4	0	4	1	10.0
0	1	1	0	0	2	2	20.0
0	1	0	0	0	1	3	30.0

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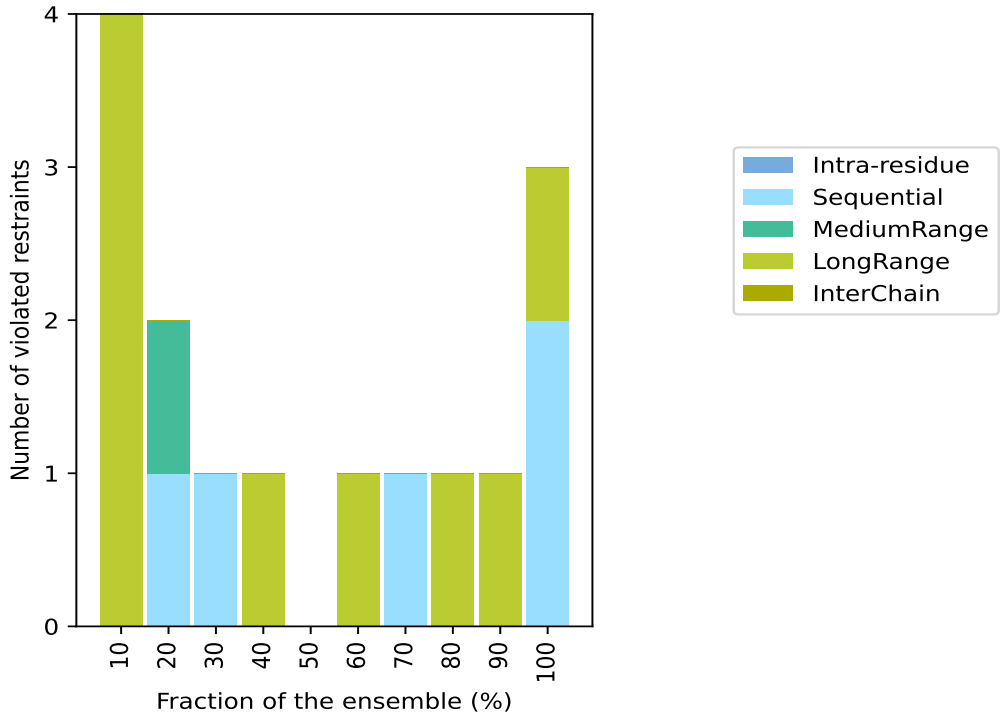
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	1	0	1	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	1	0	1	6	60.0
0	1	0	0	0	1	7	70.0
0	0	0	1	0	1	8	80.0
0	0	0	1	0	1	9	90.0
0	2	0	1	0	3	10	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble

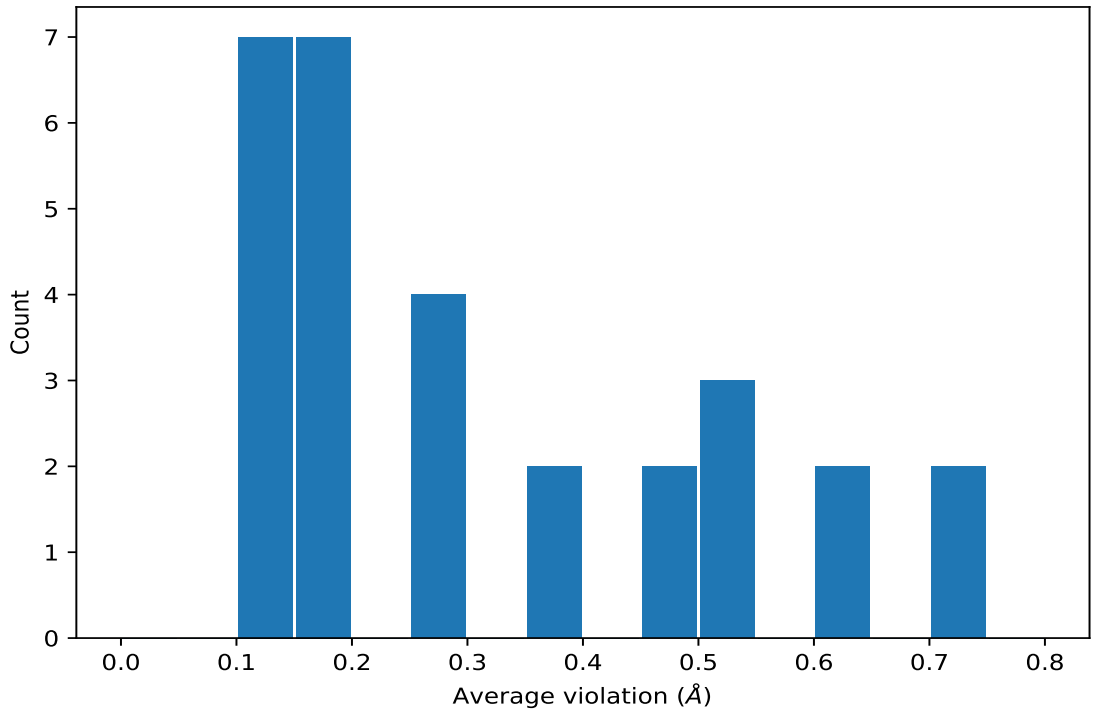


9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance 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



9.4.2 Table: Most violated distance restraints

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)
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB2	10	0.73	0.16	0.72
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB3	10	0.73	0.16	0.72
(1,3)	1:339:A:GLU:H	1:351:A:ARG:H	10	0.29	0.12	0.26
(1,18)	1:339:A:GLU:H	1:338:A:ALA:HB1	10	0.28	0.08	0.29
(1,18)	1:339:A:GLU:H	1:338:A:ALA:HB2	10	0.28	0.08	0.29
(1,18)	1:339:A:GLU:H	1:338:A:ALA:HB3	10	0.28	0.08	0.29
(1,16)	1:326:A:ARG:H	1:348:A:ILE:HG12	9	0.48	0.16	0.52
(1,16)	1:326:A:ARG:H	1:348:A:ILE:HG13	9	0.48	0.16	0.52
(1,20)	1:342:A:PHE:H	1:348:A:ILE:HG12	8	0.64	0.25	0.56
(1,20)	1:342:A:PHE:H	1:348:A:ILE:HG13	8	0.64	0.25	0.56
(1,22)	1:349:A:ALA:H	1:348:A:ILE:HD11	7	0.52	0.06	0.49
(1,22)	1:349:A:ALA:H	1:348:A:ILE:HD12	7	0.52	0.06	0.49
(1,22)	1:349:A:ALA:H	1:348:A:ILE:HD13	7	0.52	0.06	0.49
(1,23)	1:328:A:TRP:HB2	1:348:A:ILE:HB	6	0.36	0.14	0.32
(1,23)	1:328:A:TRP:HB3	1:348:A:ILE:HB	6	0.36	0.14	0.32

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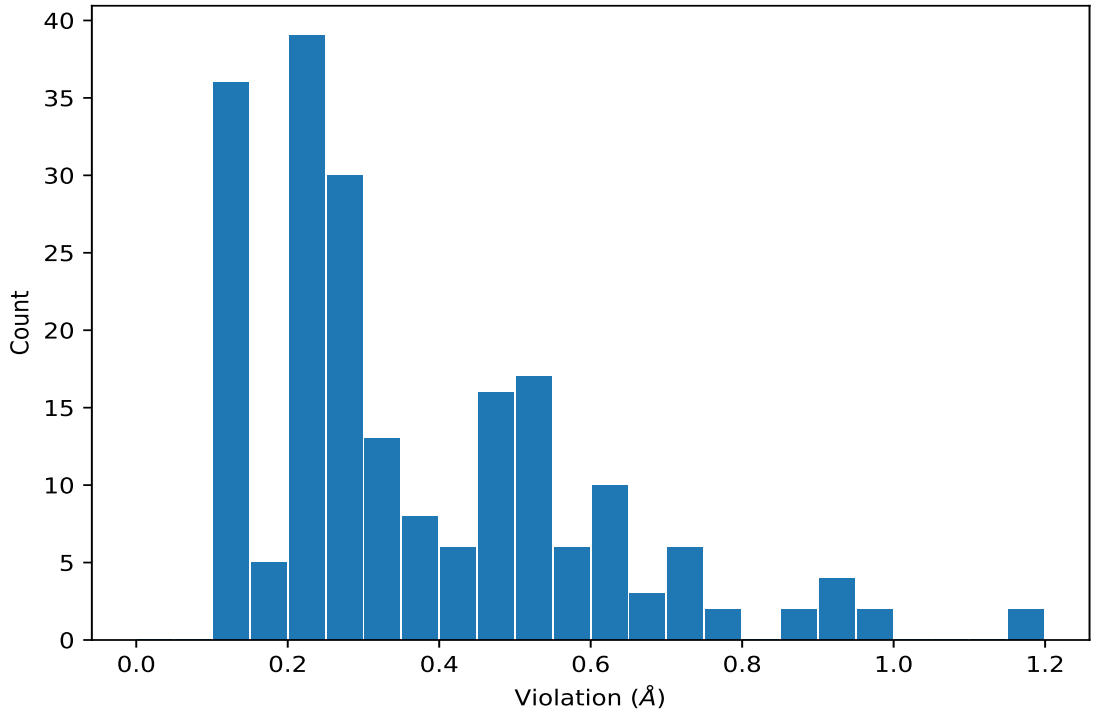
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,26)	1:350:A:TYR:H	1:323:A:VAL:HG11	4	0.19	0.04	0.21
(1,26)	1:350:A:TYR:H	1:323:A:VAL:HG12	4	0.19	0.04	0.21
(1,26)	1:350:A:TYR:H	1:323:A:VAL:HG13	4	0.19	0.04	0.21
(1,26)	1:350:A:TYR:H	1:323:A:VAL:HG21	4	0.19	0.04	0.21
(1,26)	1:350:A:TYR:H	1:323:A:VAL:HG22	4	0.19	0.04	0.21
(1,26)	1:350:A:TYR:H	1:323:A:VAL:HG23	4	0.19	0.04	0.21
(1,12)	1:324:A:VAL:H	1:323:A:VAL:HG11	3	0.11	0.01	0.11
(1,12)	1:324:A:VAL:H	1:323:A:VAL:HG12	3	0.11	0.01	0.11
(1,12)	1:324:A:VAL:H	1:323:A:VAL:HG13	3	0.11	0.01	0.11
(1,12)	1:324:A:VAL:H	1:323:A:VAL:HG21	3	0.11	0.01	0.11
(1,12)	1:324:A:VAL:H	1:323:A:VAL:HG22	3	0.11	0.01	0.11
(1,12)	1:324:A:VAL:H	1:323:A:VAL:HG23	3	0.11	0.01	0.11
(1,7)	1:332:A:ILE:H	1:331:A:GLU:H	2	0.16	0.01	0.16

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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)
(1,20)	1:342:A:PHE:H	1:348:A:ILE:HG12	9	1.18
(1,20)	1:342:A:PHE:H	1:348:A:ILE:HG13	9	1.18
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB2	4	0.98
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB3	4	0.98
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB2	6	0.93
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB3	6	0.93
(1,20)	1:342:A:PHE:H	1:348:A:ILE:HG12	4	0.9
(1,20)	1:342:A:PHE:H	1:348:A:ILE:HG13	4	0.9
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB2	3	0.88
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB3	3	0.88
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB2	9	0.75
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB3	9	0.75
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB2	2	0.72
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB3	2	0.72
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB2	8	0.72
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB3	8	0.72
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB2	1	0.71
(1,21)	1:346:A:LYS:H	1:345:A:ASP:HB3	1	0.71
(1,22)	1:349:A:ALA:H	1:348:A:ILE:HD11	4	0.65

10 Dihedral-angle violation analysis

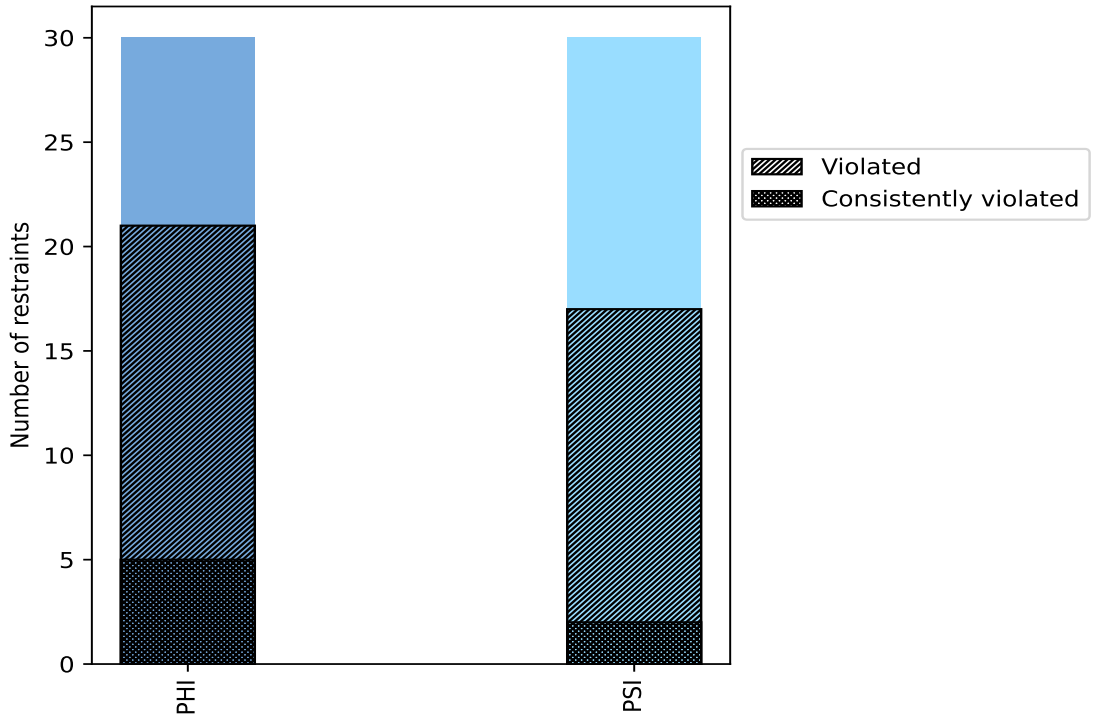
10.1 Summary of dihedral-angle violations

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	30	50.0	21	70.0	35.0	5	16.7	8.3
PSI	30	50.0	17	56.7	28.3	2	6.7	3.3
Total	60	100.0	38	63.3	63.3	7	11.7	11.7

[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



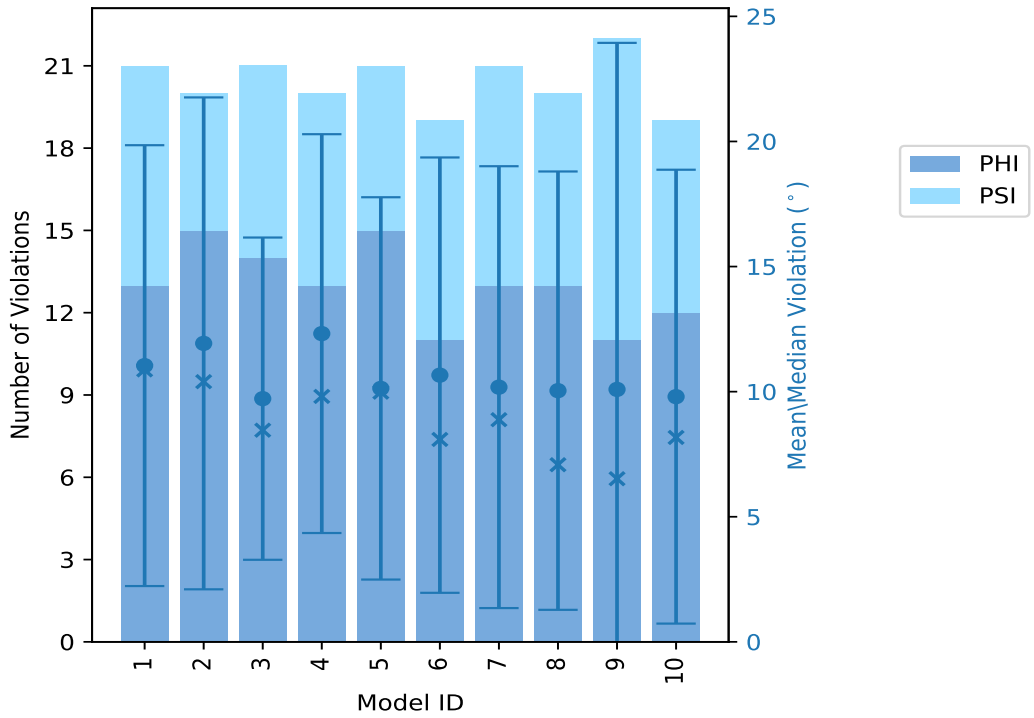
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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 (°)
	PHI	PSI	Total				
1	13	8	21	11.04	33.1	8.81	10.87
2	15	5	20	11.93	34.14	9.83	10.4
3	14	7	21	9.72	26.52	6.44	8.46
4	13	7	20	12.32	32.99	7.97	9.81
5	15	6	21	10.13	31.17	7.64	9.98
6	11	8	19	10.66	34.11	8.7	8.09
7	13	8	21	10.18	31.12	8.83	8.88
8	13	7	20	10.04	30.74	8.76	7.08
9	11	11	22	10.09	70.06	13.85	6.52
10	12	7	19	9.8	36.78	9.07	8.17

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

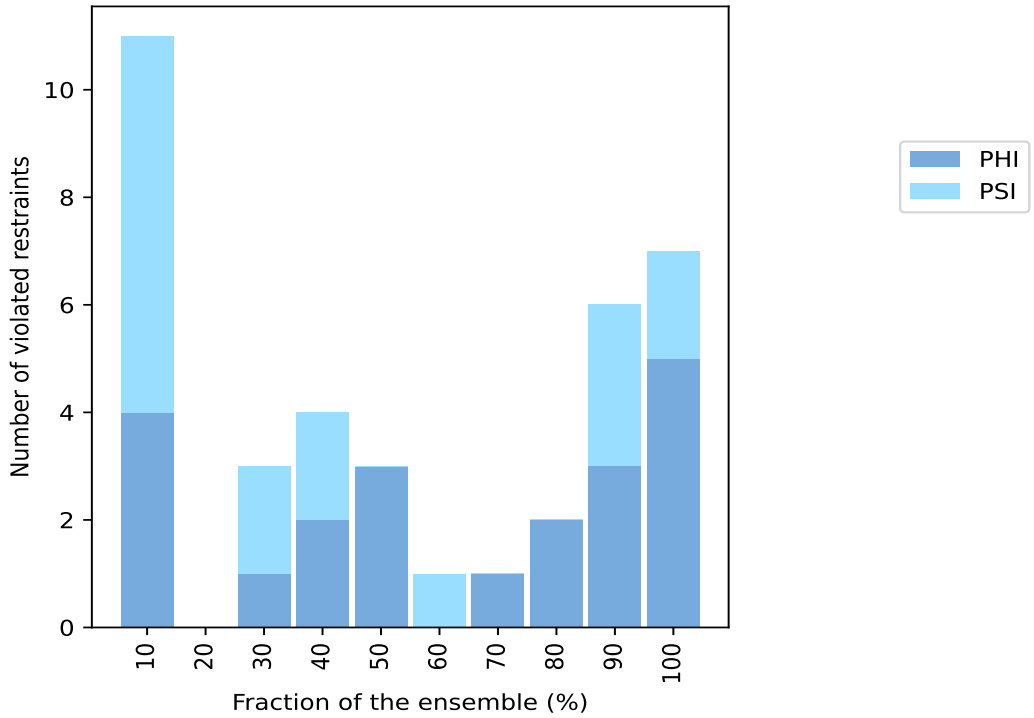
10.3 Dihedral-angle violation statistics for the ensemble

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	
PHI	PSI	Total	Count[1]	%
4	7	11	1	10.0
0	0	0	2	20.0
1	2	3	3	30.0
2	2	4	4	40.0
3	0	3	5	50.0
0	1	1	6	60.0
1	0	1	7	70.0
2	0	2	8	80.0
3	3	6	9	90.0
5	2	7	10	100.0

[1] Number of models with violations

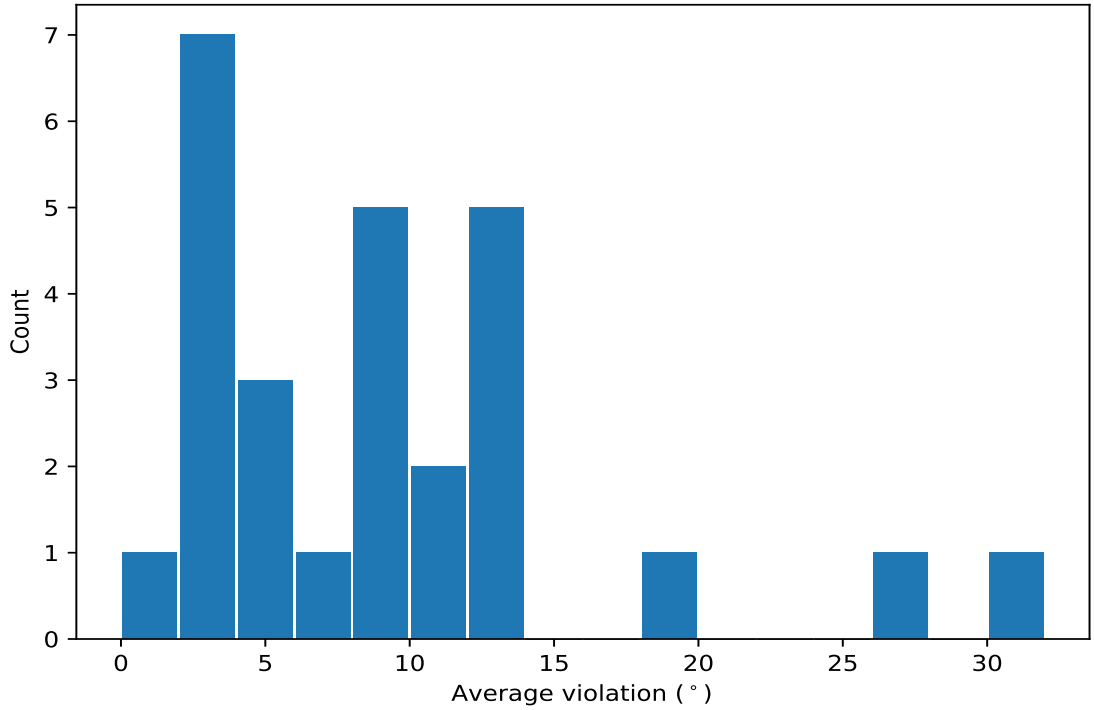
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



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

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

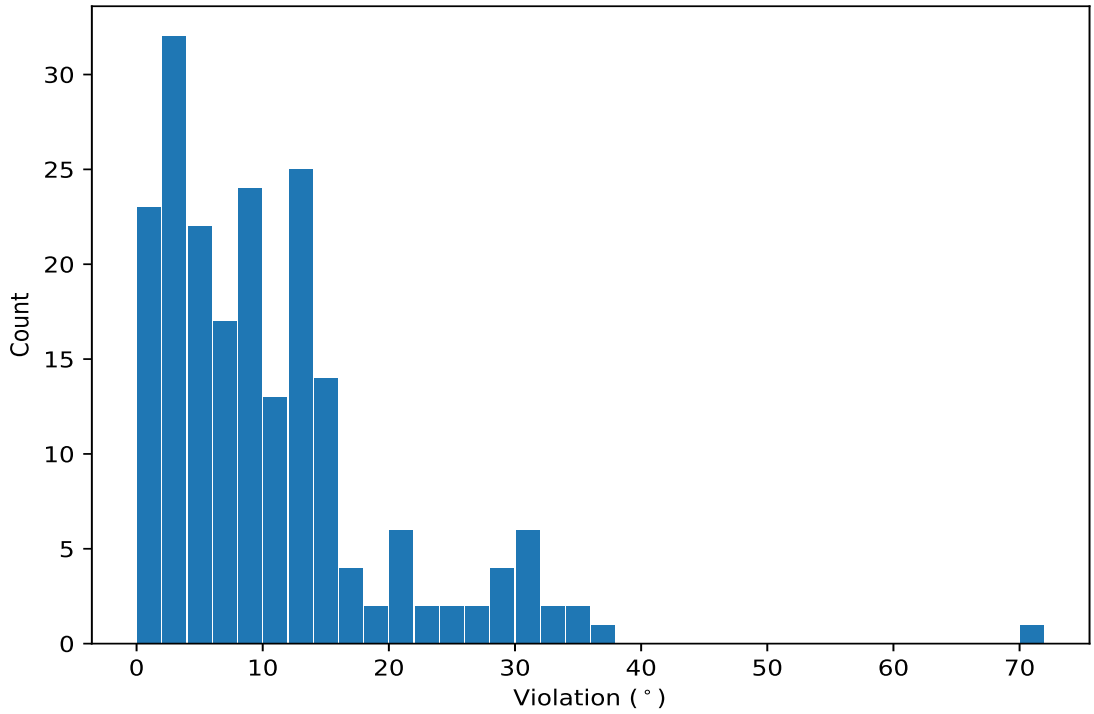
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,21)	1:328:A:TRP:C	1:329:A:ASN:N	1:329:A:ASN:CA	1:329:A:ASN:C	10	26.52	7.61	28.49
(1,7)	1:321:A:GLN:C	1:322:A:HIS:N	1:322:A:HIS:CA	1:322:A:HIS:C	10	19.53	6.18	21.0
(1,16)	1:326:A:ARG:N	1:326:A:ARG:CA	1:326:A:ARG:C	1:327:A:PRO:N	10	13.88	3.34	14.7
(1,51)	1:347:A:PHE:C	1:348:A:ILE:N	1:348:A:ILE:CA	1:348:A:ILE:C	10	11.73	4.94	12.44
(1,3)	1:318:A:PRO:C	1:319:A:THR:N	1:319:A:THR:CA	1:319:A:THR:C	10	8.4	0.76	8.3
(1,40)	1:340:A:MET:N	1:340:A:MET:CA	1:340:A:MET:C	1:341:A:LEU:N	10	5.98	2.08	5.84
(1,31)	1:334:A:LEU:C	1:335:A:PRO:N	1:335:A:PRO:CA	1:335:A:PRO:C	10	2.91	0.93	3.12
(1,26)	1:331:A:GLU:N	1:331:A:GLU:CA	1:331:A:GLU:C	1:332:A:ILE:N	9	13.62	3.69	13.28
(1,17)	1:326:A:ARG:C	1:327:A:PRO:N	1:327:A:PRO:CA	1:327:A:PRO:C	9	11.8	0.51	12.01
(1,29)	1:333:A:THR:C	1:334:A:LEU:N	1:334:A:LEU:CA	1:334:A:LEU:C	9	9.01	3.26	8.88

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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

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 (°)
(1,18)	1:327:A:PRO:N	1:327:A:PRO:CA	1:327:A:PRO:C	1:328:A:TRP:N	9	70.06
(1,19)	1:327:A:PRO:C	1:328:A:TRP:N	1:328:A:TRP:CA	1:328:A:TRP:C	10	36.78
(1,19)	1:327:A:PRO:C	1:328:A:TRP:N	1:328:A:TRP:CA	1:328:A:TRP:C	2	34.14
(1,28)	1:333:A:THR:N	1:333:A:THR:CA	1:333:A:THR:C	1:334:A:LEU:N	6	34.11
(1,19)	1:327:A:PRO:C	1:328:A:TRP:N	1:328:A:TRP:CA	1:328:A:TRP:C	1	33.1
(1,19)	1:327:A:PRO:C	1:328:A:TRP:N	1:328:A:TRP:CA	1:328:A:TRP:C	4	32.99
(1,21)	1:328:A:TRP:C	1:329:A:ASN:N	1:329:A:ASN:CA	1:329:A:ASN:C	5	31.17
(1,19)	1:327:A:PRO:C	1:328:A:TRP:N	1:328:A:TRP:CA	1:328:A:TRP:C	7	31.12
(1,59)	1:351:A:ARG:C	1:352:A:LEU:N	1:352:A:LEU:CA	1:352:A:LEU:C	2	30.74
(1,19)	1:327:A:PRO:C	1:328:A:TRP:N	1:328:A:TRP:CA	1:328:A:TRP:C	8	30.74