



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2KDD
BMRB ID : 16110
Title : Solution structure of the conserved C-terminal dimerization domain of Borealin
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Deposited on : 2009-01-06

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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 : 4.02b-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) : 2.40

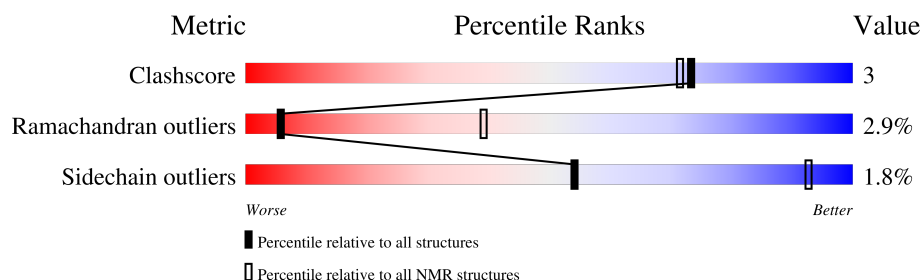
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 41%.

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	76	
1	B	76	

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:225-A:274, B:225-B:274 (100)	0.41	5

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 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1798 atoms, of which 926 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Borealin.

Mol	Chain	Residues	Atoms						Trace
1	A	57	Total	C	H	N	O	S	0
			899	271	463	82	82	1	
1	B	57	Total	C	H	N	O	S	0
			899	271	463	82	82	1	

There are 4 discrepancies between the modelled and reference sequences:

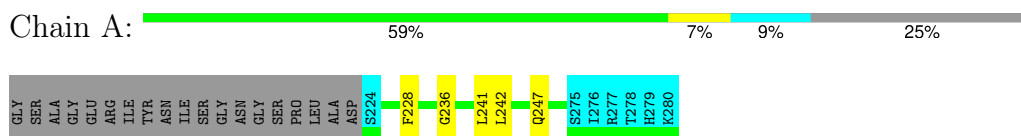
Chain	Residue	Modelled	Actual	Comment	Reference
A	205	GLY	-	expression tag	UNP Q53HL2
A	206	SER	-	expression tag	UNP Q53HL2
B	205	GLY	-	expression tag	UNP Q53HL2
B	206	SER	-	expression tag	UNP Q53HL2

4 Residue-property plots [i](#)

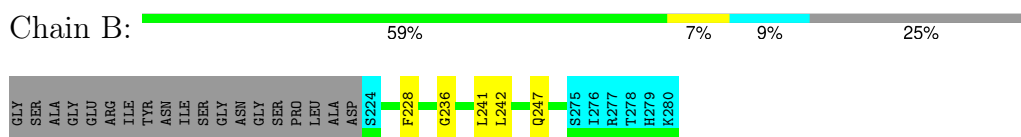
4.1 Average score per residue in the NMR ensemble

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: Borealin



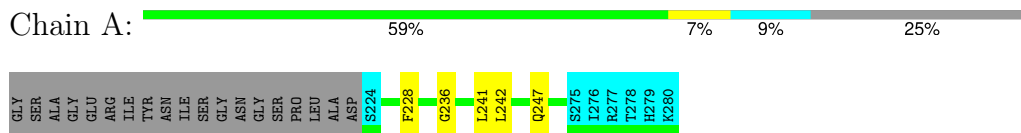
- Molecule 1: Borealin



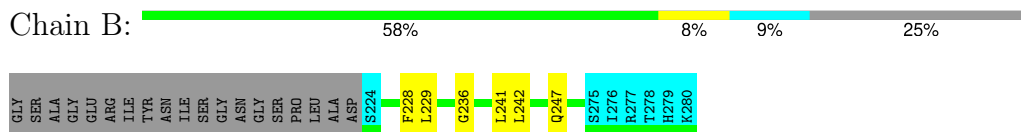
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

- Molecule 1: Borealin



- Molecule 1: Borealin



5 Refinement protocol and experimental data overview

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

Of the 100 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
ARIA	structure solution	2.2
CNS	structure solution	
CNS	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	758
Number of shifts mapped to atoms	623
Number of unparsed shifts	0
Number of shifts with mapping errors	135
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

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
1	A	378	401	400	2±1
1	B	378	401	400	3±1
All	All	7560	8020	8000	48

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 3.

5 of 12 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:PHE:HB3	1:A:242:LEU:HA	0.50	1.84	5	10
1:B:228:PHE:HB3	1:B:242:LEU:HA	0.50	1.84	5	10
1:A:241:LEU:HD11	1:A:247:GLN:H	0.49	1.66	1	8
1:B:241:LEU:HD11	1:B:247:GLN:H	0.49	1.66	1	8
1:A:231:VAL:HG11	1:A:254:LEU:HD13	0.48	1.85	6	3

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	50/76 (66%)	43±1 (86±1%)	6±1 (11±2%)	1±1 (3±2%)	6	40
1	B	50/76 (66%)	43±1 (86±1%)	6±1 (11±2%)	2±1 (3±2%)	5	38
All	All	1000/1520 (66%)	858 (86%)	113 (11%)	29 (3%)	6	39

5 of 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	236	GLY	7
1	A	236	GLY	6
1	A	235	GLY	3
1	B	235	GLY	3
1	A	234	GLY	3

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	42/62 (68%)	41±1 (98±2%)	1±1 (2±2%)	56	93
1	B	42/62 (68%)	41±1 (98±2%)	1±1 (2±2%)	52	92
All	All	840/1240 (68%)	825 (98%)	15 (2%)	54	93

5 of 6 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	226	GLU	4
1	B	226	GLU	4
1	B	229	LEU	3
1	A	229	LEU	2
1	A	256	PRO	1

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 41% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	758
Number of shifts mapped to atoms	623
Number of unparsed shifts	0
Number of shifts with mapping errors	135
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 135) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	208	GLY	H	8.317	0.02	1
1	A	209	GLU	H	8.106	0.02	1
1	A	209	GLU	HA	4.244	0.02	1
1	A	209	GLU	HB2	1.893	0.02	2
1	A	209	GLU	HB3	1.989	0.02	2
1	A	209	GLU	HG2	2.206	0.02	2
1	A	209	GLU	CA	55.728	0.2	1
1	A	209	GLU	CB	29.946	0.2	1
1	A	209	GLU	CG	35.618	0.2	1
1	A	209	GLU	N	120.266	0.1	1
1	A	210	ARG	H	8.279	0.02	1
1	A	210	ARG	HA	4.26	0.02	1
1	A	210	ARG	HB2	1.668	0.02	2
1	A	210	ARG	HD2	3.106	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	210	ARG	HG2	1.444	0.02	2
1	A	210	ARG	HG3	1.512	0.02	2
1	A	210	ARG	CA	55.728	0.2	1
1	A	210	ARG	CB	29.946	0.2	1
1	A	210	ARG	CD	42.837	0.2	1
1	A	210	ARG	CG	26.853	0.2	1
1	A	210	ARG	N	122.148	0.1	1
1	A	211	ILE	H	8.042	0.02	1
1	A	211	ILE	HA	4.081	0.02	1
1	A	211	ILE	HB	1.699	0.02	1
1	A	211	ILE	HD11	0.755	0.02	1
1	A	211	ILE	HD12	0.755	0.02	1
1	A	211	ILE	HD13	0.755	0.02	1
1	A	211	ILE	HG12	1.042	0.02	2
1	A	211	ILE	HG13	1.288	0.02	2
1	A	211	ILE	HG21	0.734	0.02	1
1	A	211	ILE	HG22	0.734	0.02	1
1	A	211	ILE	HG23	0.734	0.02	1
1	A	211	ILE	CA	60.306	0.2	1
1	A	211	ILE	CB	38.221	0.2	1
1	A	211	ILE	CD1	12.388	0.2	1
1	A	211	ILE	CG1	26.809	0.2	1
1	A	211	ILE	CG2	17.093	0.2	1
1	A	211	ILE	N	121.663	0.1	1
1	A	212	TYR	H	8.225	0.02	1
1	A	212	TYR	HA	4.571	0.02	1
1	A	212	TYR	HB2	2.818	0.02	2
1	A	212	TYR	HB3	2.987	0.02	2
1	A	212	TYR	HD1	7.049	0.02	3
1	A	212	TYR	HD2	7.049	0.02	3
1	A	212	TYR	HE1	6.747	0.02	3
1	A	212	TYR	HE2	6.747	0.02	3
1	A	212	TYR	CA	57.159	0.2	1
1	A	212	TYR	CB	38.596	0.2	1
1	A	212	TYR	CD1	132.469	0.2	3
1	A	212	TYR	CD2	132.469	0.2	3
1	A	212	TYR	CE1	116.501	0.2	3
1	A	212	TYR	CE2	116.501	0.2	3
1	A	212	TYR	N	123.846	0.1	1
1	A	213	ASN	H	8.332	0.02	1
1	A	213	ASN	HA	4.679	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	213	ASN	HB2	2.646	0.02	2
1	A	213	ASN	HB3	2.752	0.02	2
1	A	213	ASN	CA	52.659	0.2	1
1	A	213	ASN	CB	38.221	0.2	1
1	A	213	ASN	N	120.61	0.1	1
1	A	214	ILE	H	8.075	0.02	1
1	A	214	ILE	HA	4.158	0.02	1
1	A	214	ILE	HB	1.842	0.02	1
1	A	214	ILE	HD11	0.808	0.02	1
1	A	214	ILE	HD12	0.808	0.02	1
1	A	214	ILE	HD13	0.808	0.02	1
1	A	214	ILE	HG12	1.117	0.02	2
1	A	214	ILE	HG13	1.384	0.02	2
1	A	214	ILE	HG21	0.858	0.02	1
1	A	214	ILE	HG22	0.858	0.02	1
1	A	214	ILE	HG23	0.858	0.02	1
1	A	214	ILE	CA	60.74	0.2	1
1	A	214	ILE	CB	38.052	0.2	1
1	A	214	ILE	CD1	12.807	0.2	1
1	A	214	ILE	CG1	26.708	0.2	1
1	A	214	ILE	CG2	16.902	0.2	1
1	A	214	ILE	N	120.796	0.1	1
1	A	215	SER	H	8.33	0.02	1
1	A	215	SER	HA	4.424	0.02	1
1	A	215	SER	HB2	3.821	0.02	2
1	A	215	SER	HB3	3.856	0.02	2
1	A	215	SER	CA	57.436	0.2	1
1	A	215	SER	CB	63.197	0.2	1
1	A	215	SER	N	118.792	0.1	1
1	A	218	GLY	H	8.372	0.02	1
1	A	218	GLY	HA2	3.906	0.02	2
1	A	218	GLY	N	109.059	0.1	1
1	A	219	SER	H	7.823	0.02	1
1	A	219	SER	HA	4.714	0.02	1
1	A	219	SER	HB2	3.805	0.02	2
1	A	219	SER	CA	55.583	0.2	1
1	A	219	SER	CB	62.838	0.2	1
1	A	219	SER	N	114.991	0.1	1
1	A	220	PRO	HA	4.402	0.02	1
1	A	220	PRO	HB2	1.851	0.02	2
1	A	220	PRO	HB3	2.228	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	220	PRO	HD2	3.659	0.02	2
1	A	220	PRO	HD3	3.761	0.02	2
1	A	220	PRO	HG2	1.937	0.02	2
1	A	220	PRO	CA	62.762	0.2	1
1	A	220	PRO	CB	31.349	0.2	1
1	A	220	PRO	CD	49.912	0.2	1
1	A	220	PRO	CG	26.698	0.2	1
1	A	221	LEU	H	8.183	0.02	1
1	A	221	LEU	HA	4.231	0.02	1
1	A	221	LEU	HB2	1.523	0.02	2
1	A	221	LEU	HB3	1.543	0.02	2
1	A	221	LEU	HD11	0.793	0.02	1
1	A	221	LEU	HD12	0.793	0.02	1
1	A	221	LEU	HD13	0.793	0.02	1
1	A	221	LEU	HD21	0.833	0.02	1
1	A	221	LEU	HD22	0.833	0.02	1
1	A	221	LEU	HD23	0.833	0.02	1
1	A	221	LEU	HG	1.545	0.02	1
1	A	221	LEU	CA	54.552	0.2	1
1	A	221	LEU	CB	41.662	0.2	1
1	A	221	LEU	CD1	23.099	0.2	2
1	A	221	LEU	CD2	24.13	0.2	2
1	A	221	LEU	CG	26.708	0.2	1
1	A	221	LEU	N	121.747	0.1	1
1	A	222	ALA	H	8.146	0.02	1
1	A	222	ALA	HA	4.207	0.02	1
1	A	222	ALA	HB1	1.325	0.02	1
1	A	222	ALA	HB2	1.325	0.02	1
1	A	222	ALA	HB3	1.325	0.02	1
1	A	222	ALA	CA	52.273	0.2	1
1	A	222	ALA	CB	18.758	0.2	1
1	A	222	ALA	N	124.243	0.1	1
1	A	223	ASP	H	8.205	0.02	1
1	A	223	ASP	HA	4.544	0.02	1
1	A	223	ASP	HB2	2.582	0.02	2
1	A	223	ASP	HB3	2.669	0.02	2
1	A	223	ASP	CA	53.324	0.2	1
1	A	223	ASP	CB	40.433	0.2	1
1	A	223	ASP	N	119.284	0.1	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	66	0.48 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	63	0.86 ± 0.10	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	63	0.18 ± 0.41	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 41%, i.e. 569 atoms were assigned a chemical shift out of a possible 1374. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	193/500 (39%)	98/204 (48%)	49/200 (24%)	46/96 (48%)
Sidechain	364/838 (43%)	245/548 (45%)	114/256 (45%)	5/34 (15%)
Aromatic	12/36 (33%)	7/18 (39%)	5/14 (36%)	0/4 (0%)
Overall	569/1374 (41%)	350/770 (45%)	168/470 (36%)	51/134 (38%)

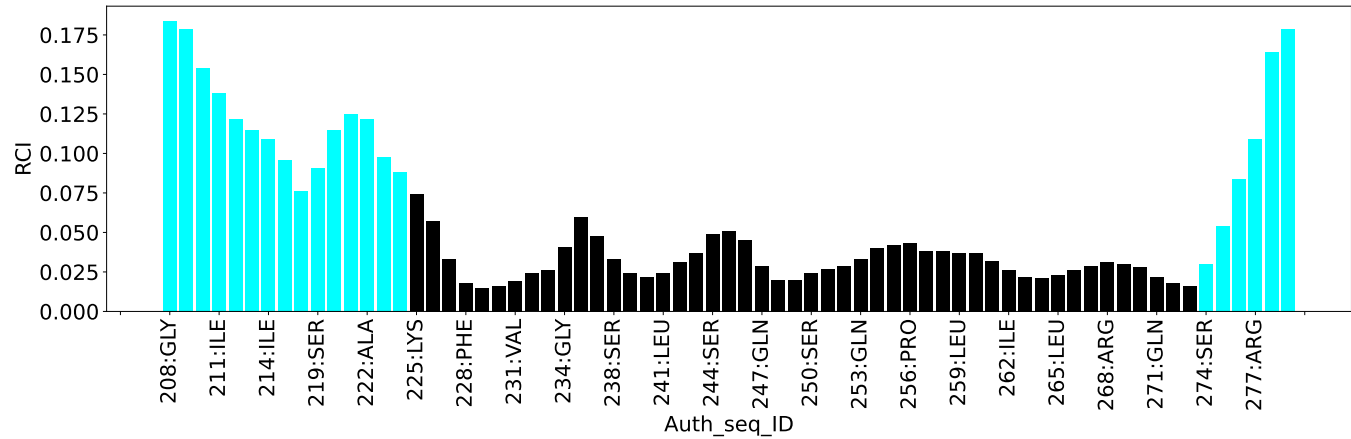
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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	3800
Intra-residue ($ i-j =0$)	1690
Sequential ($ i-j =1$)	794
Medium range ($ i-j >1$ and $ i-j <5$)	618
Long range ($ i-j \geq 5$)	358
Inter-chain	340
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	172
Number of unmapped restraints	388
Number of restraints per residue	26.1
Number of long range restraints per residue ¹	2.4

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)	53.6	0.2
0.2-0.5 (Medium)	113.3	0.5
>0.5 (Large)	101.9	3.13

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.9	1.38
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

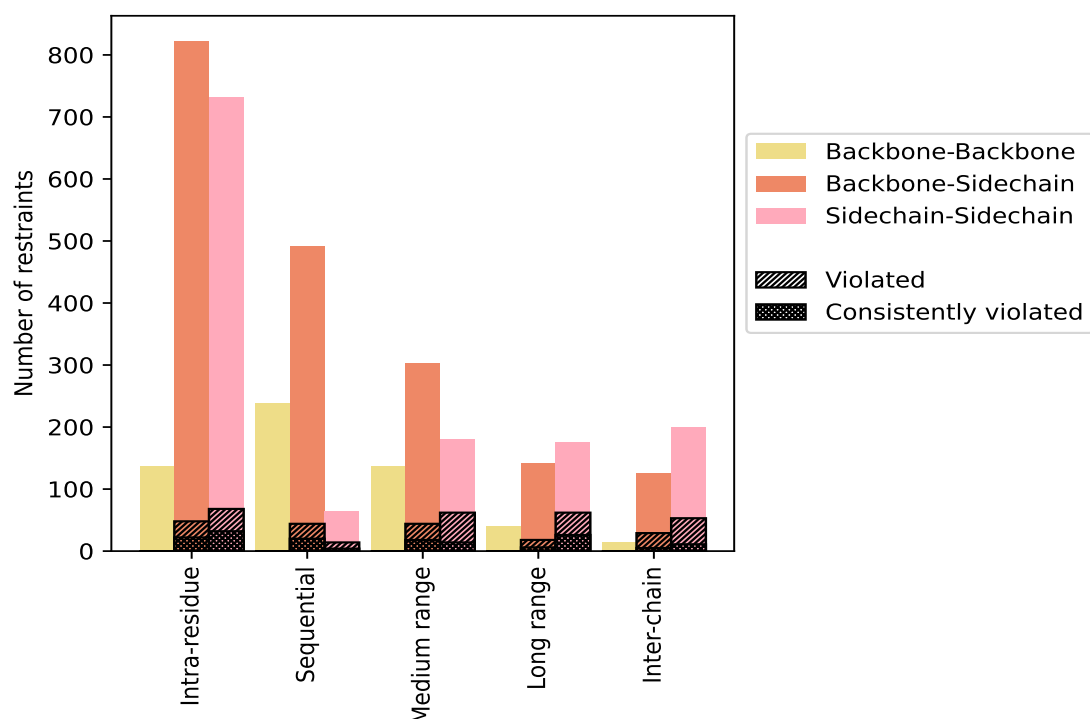
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1690	44.5	116	6.9	3.1	54	3.2	1.4
Backbone-Backbone	136	3.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	822	21.6	48	5.8	1.3	22	2.7	0.6
Sidechain-Sidechain	732	19.3	68	9.3	1.8	32	4.4	0.8
Sequential ($i-j =1$)	794	20.9	58	7.3	1.5	24	3.0	0.6
Backbone-Backbone	238	6.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	492	12.9	44	8.9	1.2	20	4.1	0.5
Sidechain-Sidechain	64	1.7	14	21.9	0.4	4	6.2	0.1
Medium range ($i-j >1$ & $i-j <5$)	618	16.3	106	17.2	2.8	32	5.2	0.8
Backbone-Backbone	136	3.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	302	7.9	44	14.6	1.2	18	6.0	0.5
Sidechain-Sidechain	180	4.7	62	34.4	1.6	14	7.8	0.4
Long range ($i-j \geq 5$)	358	9.4	80	22.3	2.1	32	8.9	0.8
Backbone-Backbone	40	1.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	142	3.7	18	12.7	0.5	6	4.2	0.2
Sidechain-Sidechain	176	4.6	62	35.2	1.6	26	14.8	0.7
Inter-chain	340	8.9	82	24.1	2.2	16	4.7	0.4
Backbone-Backbone	14	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	126	3.3	29	23.0	0.8	5	4.0	0.1
Sidechain-Sidechain	200	5.3	53	26.5	1.4	11	5.5	0.3
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	3800	100.0	442	11.6	11.6	158	4.2	4.2
Backbone-Backbone	564	14.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1884	49.6	183	9.7	4.8	71	3.8	1.9
Sidechain-Sidechain	1352	35.6	259	19.2	6.8	87	6.4	2.3

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

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



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

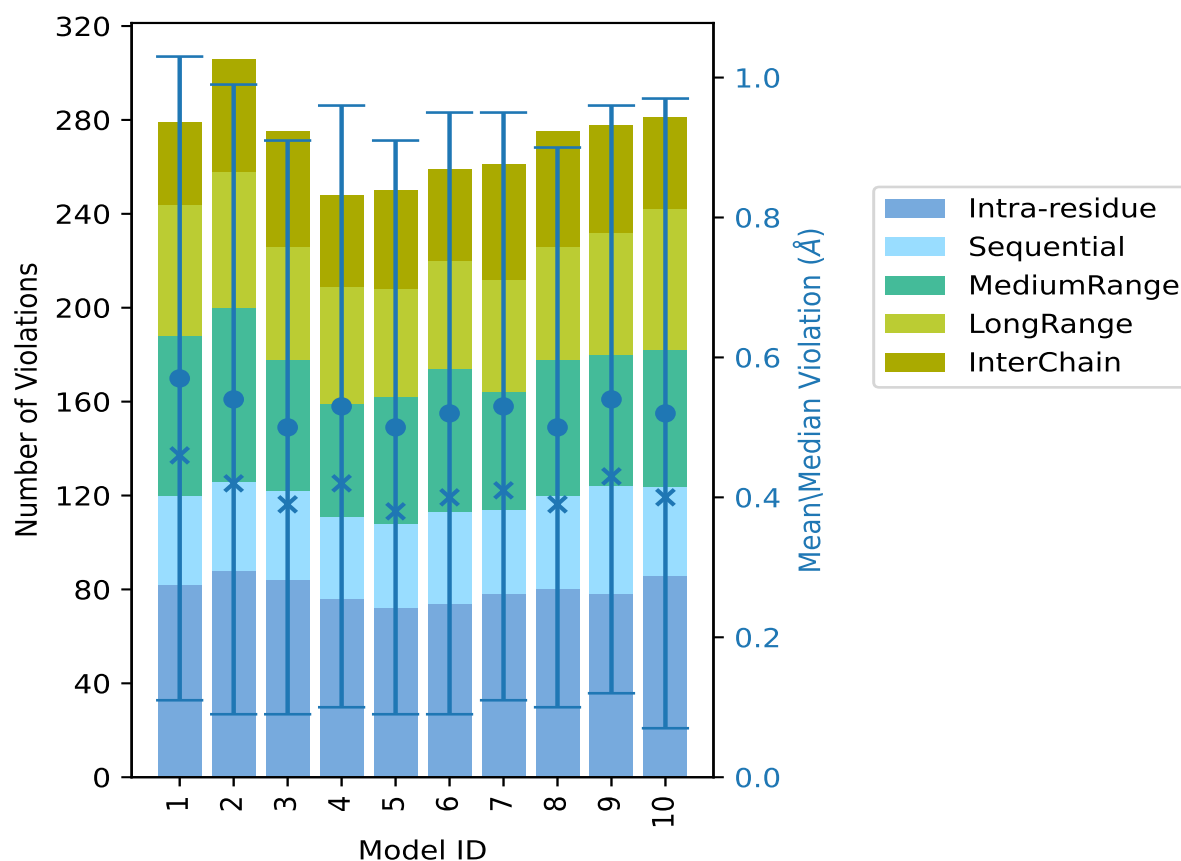
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	82	38	68	56	35	279	0.57	3.02	0.46	0.46
2	88	38	74	58	48	306	0.54	3.13	0.45	0.42
3	84	38	56	48	49	275	0.5	2.41	0.41	0.39
4	76	35	48	50	39	248	0.53	2.53	0.43	0.42
5	72	36	54	46	42	250	0.5	2.48	0.41	0.38
6	74	39	61	46	39	259	0.52	2.52	0.43	0.4
7	78	36	50	48	49	261	0.53	2.57	0.42	0.41
8	80	40	58	48	49	275	0.5	2.3	0.4	0.39
9	78	46	56	52	46	278	0.54	2.56	0.42	0.43
10	86	38	58	60	39	281	0.52	3.08	0.45	0.4

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 [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, 3358(IR:1574, SQ:736, MR:512, LR:278, IC:258) 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	%
14	8	22	22	17	83	1	10.0
14	0	13	0	8	35	2	20.0
4	6	7	6	13	36	3	30.0

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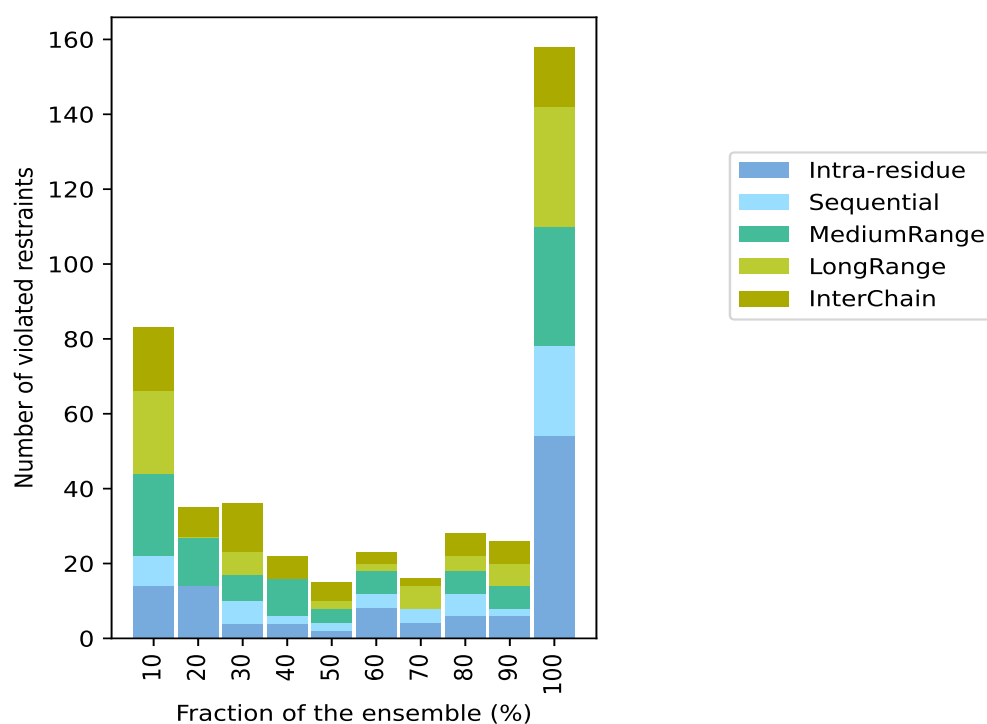
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
4	2	10	0	6	22	4	40.0
2	2	4	2	5	15	5	50.0
8	4	6	2	3	23	6	60.0
4	4	0	6	2	16	7	70.0
6	6	6	4	6	28	8	80.0
6	2	6	6	6	26	9	90.0
54	24	32	32	16	158	10	100.0

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 ⓘ

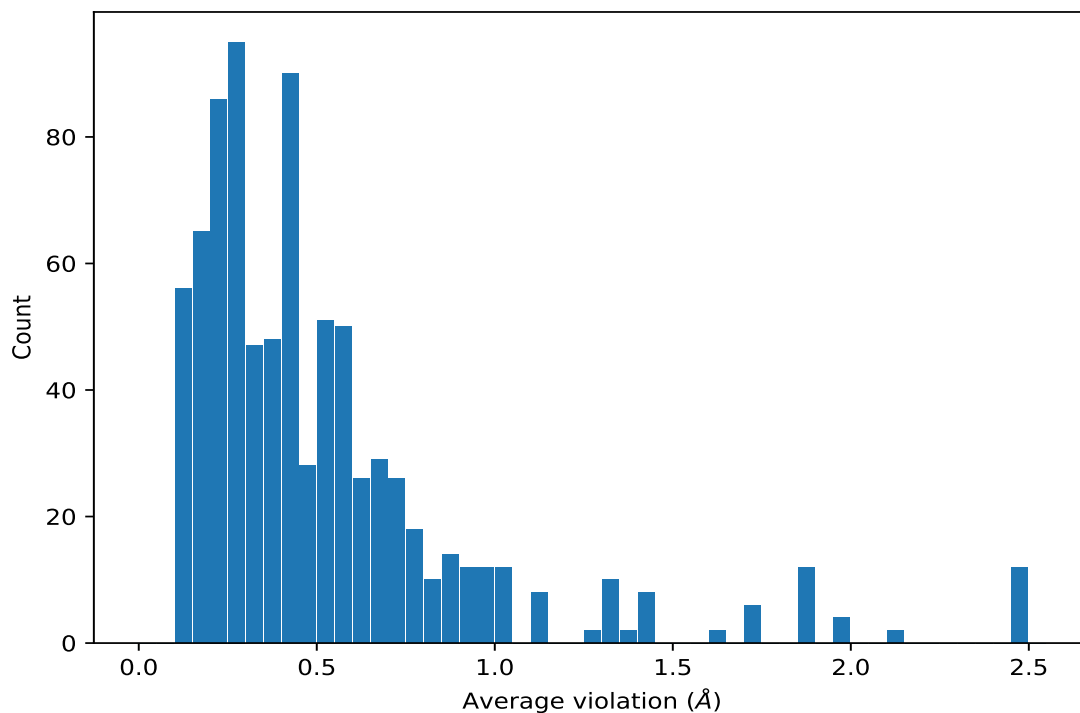


9.4 Most violated distance restraints in the ensemble ⓘ

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 [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)
(1,3733)	1:228:A:PHE:HE2	1:229:A:LEU:HD22	10	2.46	0.09	2.5
(1,3733)	1:228:A:PHE:HE2	1:229:A:LEU:HD23	10	2.46	0.09	2.5
(1,3733)	1:228:A:PHE:HE1	1:229:A:LEU:HD22	10	2.46	0.09	2.5
(1,3733)	1:228:A:PHE:HE1	1:229:A:LEU:HD21	10	2.46	0.09	2.5
(1,3733)	1:228:A:PHE:HE1	1:229:A:LEU:HD23	10	2.46	0.09	2.5
(1,3733)	1:228:A:PHE:HE2	1:229:A:LEU:HD21	10	2.46	0.09	2.5
(1,3734)	1:228:B:PHE:HE2	1:229:B:LEU:HD22	10	2.46	0.09	2.5
(1,3734)	1:228:B:PHE:HE2	1:229:B:LEU:HD23	10	2.46	0.09	2.5
(1,3734)	1:228:B:PHE:HE1	1:229:B:LEU:HD22	10	2.46	0.09	2.5
(1,3734)	1:228:B:PHE:HE1	1:229:B:LEU:HD21	10	2.46	0.09	2.5
(1,3734)	1:228:B:PHE:HE1	1:229:B:LEU:HD23	10	2.46	0.09	2.5
(1,3734)	1:228:B:PHE:HE2	1:229:B:LEU:HD21	10	2.46	0.09	2.5
(1,1873)	1:247:A:GLN:HG2	1:242:A:LEU:HB3	10	2.1	0.64	1.69
(1,1874)	1:247:B:GLN:HG2	1:242:B:LEU:HB3	10	2.1	0.64	1.69
(1,3743)	1:228:A:PHE:HE2	1:229:A:LEU:HD22	10	1.85	0.1	1.88

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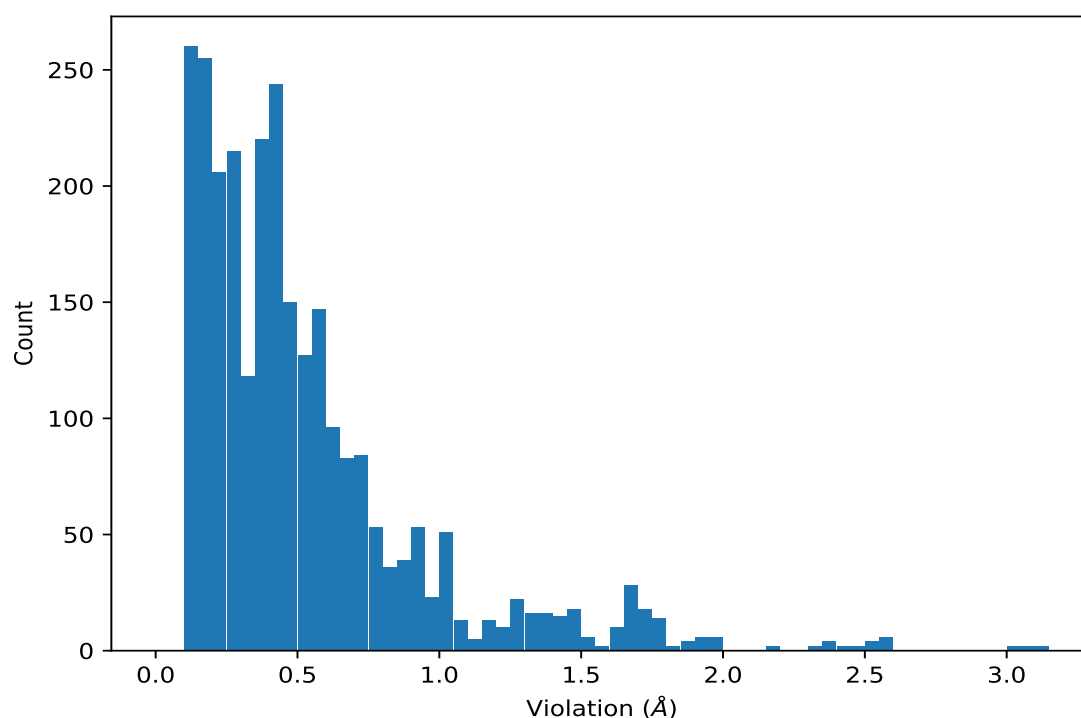
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3743)	1:228:A:PHE:HE2	1:229:A:LEU:HD23	10	1.85	0.1	1.88
(1,3743)	1:228:A:PHE:HE1	1:229:A:LEU:HD22	10	1.85	0.1	1.88
(1,3743)	1:228:A:PHE:HE1	1:229:A:LEU:HD21	10	1.85	0.1	1.88
(1,3743)	1:228:A:PHE:HE1	1:229:A:LEU:HD23	10	1.85	0.1	1.88
(1,3743)	1:228:A:PHE:HE2	1:229:A:LEU:HD21	10	1.85	0.1	1.88
(1,3744)	1:228:B:PHE:HE2	1:229:B:LEU:HD22	10	1.85	0.09	1.88
(1,3744)	1:228:B:PHE:HE2	1:229:B:LEU:HD23	10	1.85	0.09	1.88
(1,3744)	1:228:B:PHE:HE1	1:229:B:LEU:HD22	10	1.85	0.09	1.88
(1,3744)	1:228:B:PHE:HE1	1:229:B:LEU:HD21	10	1.85	0.09	1.88
(1,3744)	1:228:B:PHE:HE1	1:229:B:LEU:HD23	10	1.85	0.09	1.88
(1,3744)	1:228:B:PHE:HE2	1:229:B:LEU:HD21	10	1.85	0.09	1.88
(1,1893)	1:262:A:ILE:HD13	1:251:A:ILE:HG12	10	1.74	0.06	1.72
(1,1893)	1:262:A:ILE:HD12	1:251:A:ILE:HG12	10	1.74	0.06	1.72
(1,1893)	1:262:A:ILE:HD11	1:251:A:ILE:HG12	10	1.74	0.06	1.72
(1,1894)	1:262:B:ILE:HD13	1:251:B:ILE:HG12	10	1.74	0.06	1.72
(1,1894)	1:262:B:ILE:HD12	1:251:B:ILE:HG12	10	1.74	0.06	1.72
(1,1894)	1:262:B:ILE:HD11	1:251:B:ILE:HG12	10	1.74	0.06	1.72
(1,2819)	1:261:A:ASN:H	1:263:A:LYS:HB3	10	1.64	0.07	1.65
(1,2820)	1:261:B:ASN:H	1:263:B:LYS:HB3	10	1.64	0.07	1.65

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)
(1,1874)	1:247:B:GLN:HG2	1:242:B:LEU:HB3	2	3.13
(1,1873)	1:247:A:GLN:HG2	1:242:A:LEU:HB3	2	3.13
(1,1874)	1:247:B:GLN:HG2	1:242:B:LEU:HB3	10	3.08
(1,1873)	1:247:A:GLN:HG2	1:242:A:LEU:HB3	10	3.08
(1,1874)	1:247:B:GLN:HG2	1:242:B:LEU:HB3	1	3.02
(1,1873)	1:247:A:GLN:HG2	1:242:A:LEU:HB3	1	3.02
(1,3734)	1:228:B:PHE:HE1	1:229:B:LEU:HD23	7	2.57
(1,3733)	1:228:A:PHE:HE1	1:229:A:LEU:HD23	7	2.57
(1,3734)	1:228:B:PHE:HE2	1:229:B:LEU:HD22	1	2.56
(1,3734)	1:228:B:PHE:HE2	1:229:B:LEU:HD21	9	2.56

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

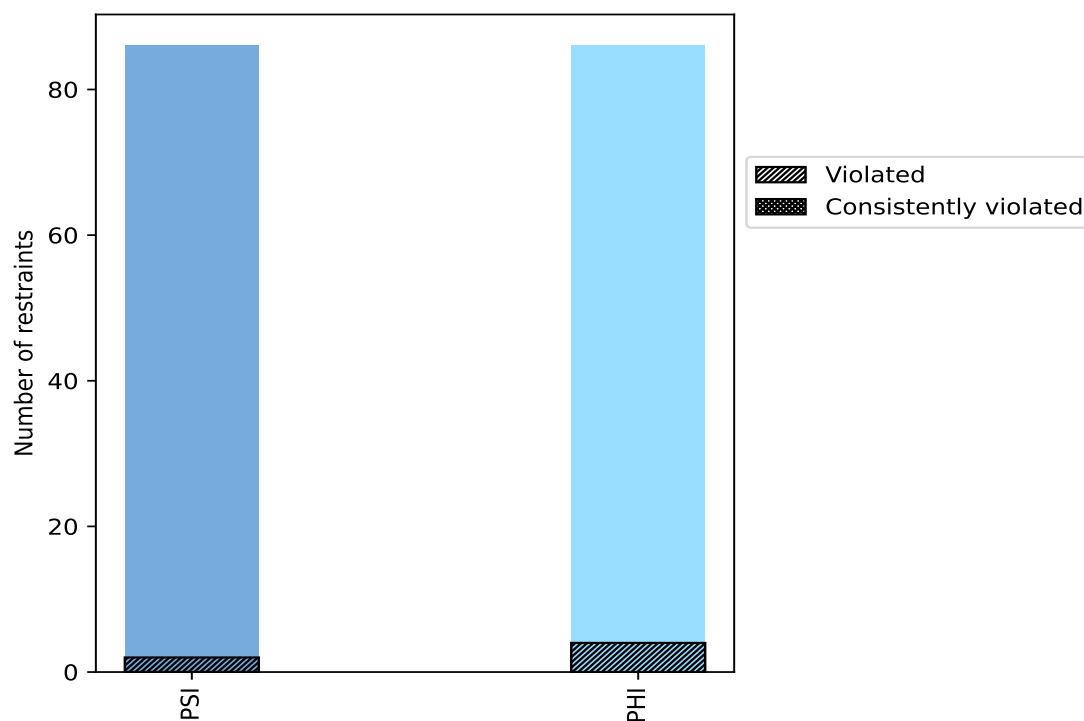
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	86	50.0	2	2.3	1.2	0	0.0	0.0
PHI	86	50.0	4	4.7	2.3	0	0.0	0.0
Total	172	100.0	6	3.5	3.5	0	0.0	0.0

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

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



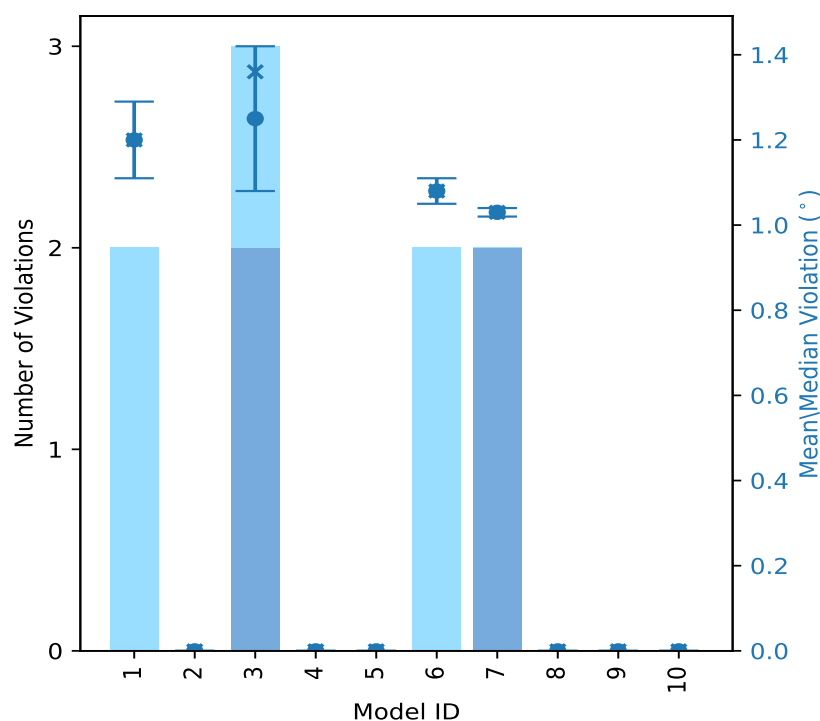
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [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 (°)
	PSI	PHI	Total				
1	0	2	2	1.2	1.29	0.09	1.2
2	0	0	0	0.0	0.0	0.0	0.0
3	2	1	3	1.25	1.38	0.17	1.36
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	2	2	1.08	1.11	0.03	1.08
7	2	0	2	1.03	1.04	0.01	1.03
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

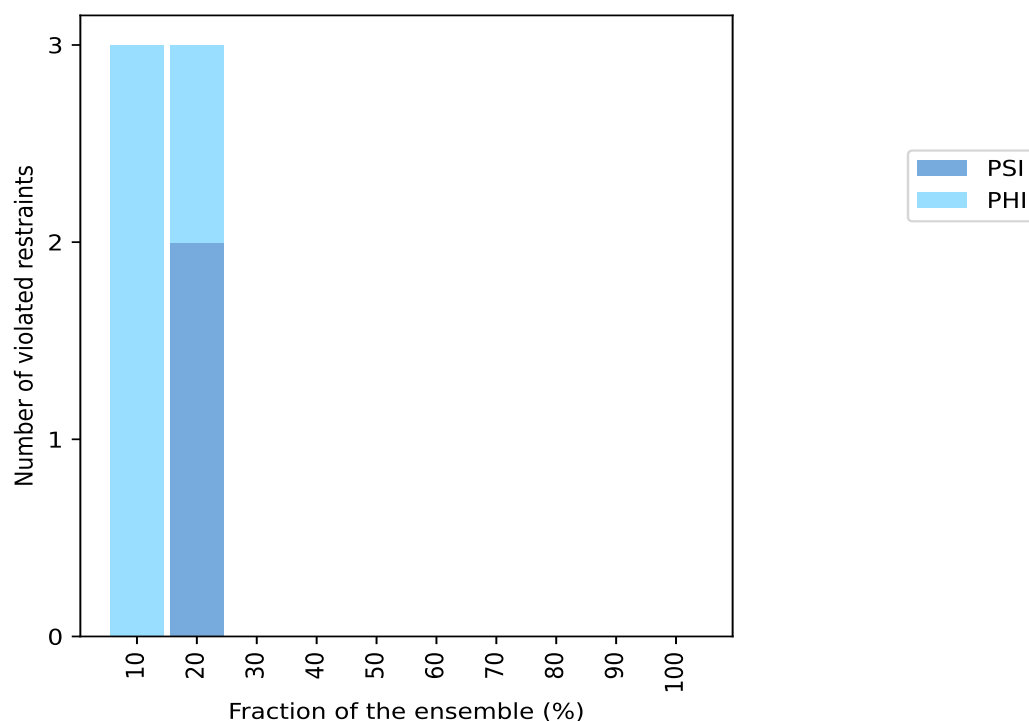
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	3	3	1	10.0
2	1	3	2	20.0
0	0	0	3	30.0
0	0	0	4	40.0
0	0	0	5	50.0
0	0	0	6	60.0
0	0	0	7	70.0
0	0	0	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

¹ Number of models with violations

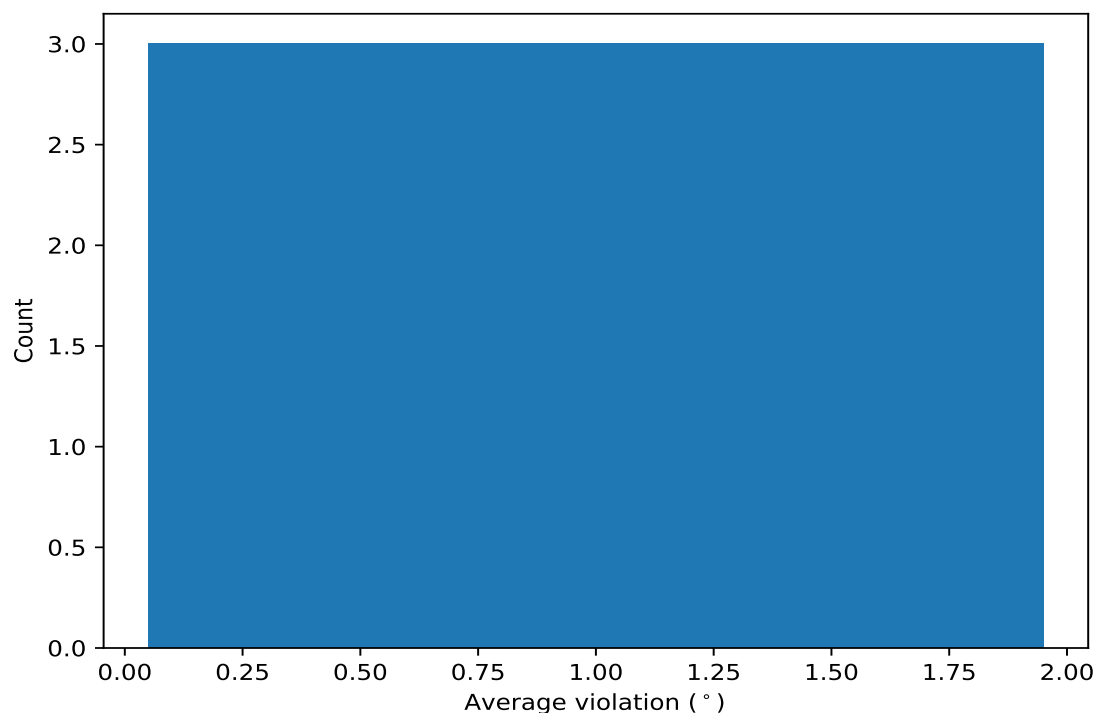
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

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

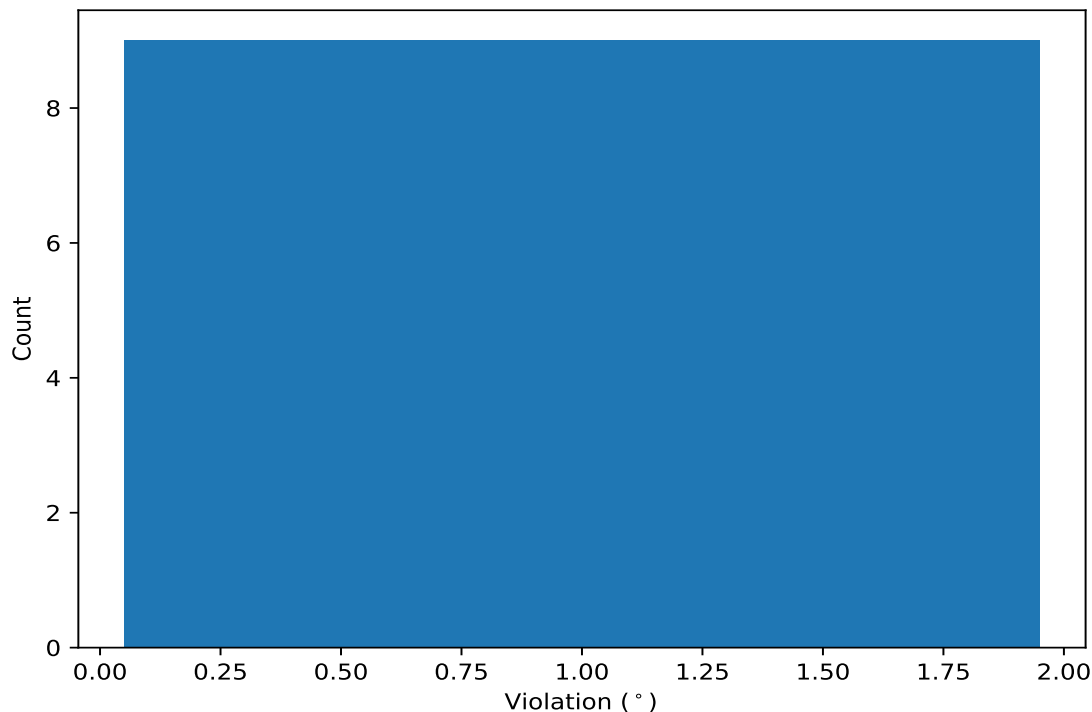
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,11)	1:232:A:PRO:N	1:232:A:PRO:CA	1:232:A:PRO:C	1:233:A:VAL:N	2	1.21	0.17	1.21
(1,97)	1:232:B:PRO:N	1:232:B:PRO:CA	1:232:B:PRO:C	1:233:B:VAL:N	2	1.19	0.17	1.19
(1,51)	1:258:A:ALA:C	1:259:A:LEU:N	1:259:A:LEU:CA	1:259:A:LEU:C	2	1.03	0.02	1.03

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

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

10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its 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 (°)
(1,11)	1:232:A:PRO:N	1:232:A:PRO:CA	1:232:A:PRO:C	1:233:A:VAL:N	3	1.38
(1,97)	1:232:B:PRO:N	1:232:B:PRO:CA	1:232:B:PRO:C	1:233:B:VAL:N	3	1.36
(1,32)	1:247:A:GLN:C	1:248:A:ARG:N	1:248:A:ARG:CA	1:248:A:ARG:C	1	1.29
(1,137)	1:258:B:ALA:C	1:259:B:LEU:N	1:259:B:LEU:CA	1:259:B:LEU:C	6	1.11
(1,118)	1:247:B:GLN:C	1:248:B:ARG:N	1:248:B:ARG:CA	1:248:B:ARG:C	1	1.11
(1,51)	1:258:A:ALA:C	1:259:A:LEU:N	1:259:A:LEU:CA	1:259:A:LEU:C	6	1.05
(1,11)	1:232:A:PRO:N	1:232:A:PRO:CA	1:232:A:PRO:C	1:233:A:VAL:N	7	1.04
(1,97)	1:232:B:PRO:N	1:232:B:PRO:CA	1:232:B:PRO:C	1:233:B:VAL:N	7	1.02
(1,51)	1:258:A:ALA:C	1:259:A:LEU:N	1:259:A:LEU:CA	1:259:A:LEU:C	3	1.01