



wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 19971
Title : Solution structure of the NDH-1 complex subunit CupS from *Thermosynechococcus elongatus*
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Deposited on : 2014-12-17

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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 : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

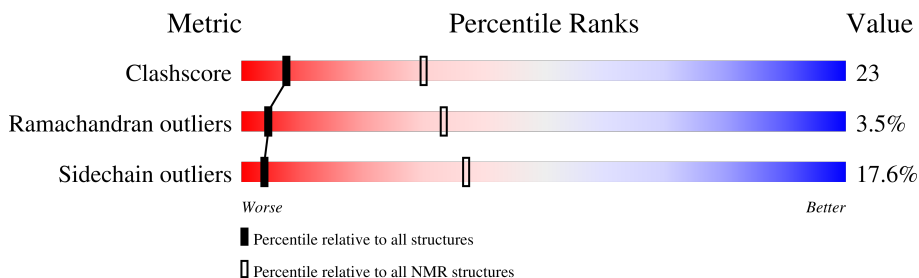
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	159	

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:3-A:45, A:54-A:129 (119)	0.63	1

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 6, 8, 9
2	3, 4, 5, 7, 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1932 atoms, of which 981 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NDH-1 complex sensory subunit CupS.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	129	1932	608	981	157	184	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	SER	-	expression tag	UNP Q8DMA1
A	151	ALA	-	expression tag	UNP Q8DMA1
A	152	TRP	-	expression tag	UNP Q8DMA1
A	153	SER	-	expression tag	UNP Q8DMA1
A	154	HIS	-	expression tag	UNP Q8DMA1
A	155	PRO	-	expression tag	UNP Q8DMA1
A	156	GLN	-	expression tag	UNP Q8DMA1
A	157	PHE	-	expression tag	UNP Q8DMA1
A	158	GLU	-	expression tag	UNP Q8DMA1
A	159	LYS	-	expression tag	UNP Q8DMA1

5 Refinement protocol and experimental data overview

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

Of the 40 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
NMRPipe	structure solution	any
NMRPipe	structure solution	any
CNS	structure solution	
TALOS	structure solution	
TALOS	structure solution	
TALOS	structure solution	
TALOS	structure solution	
ARIA	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	1866
Number of shifts mapped to atoms	1504
Number of unparsed shifts	0
Number of shifts with mapping errors	362
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.61±0.01	0±0/894 (0.0± 0.0%)	0.92±0.03	2±1/1227 (0.2± 0.1%)
All	All	0.61	0/8940 (0.0%)	0.92	24/12270 (0.2%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	124	HIS	CA-CB-CG	8.28	122.08	113.80	4	3
1	A	61	PRO	CA-C-N	6.39	127.82	119.84	7	8
1	A	61	PRO	C-N-CA	6.39	127.82	119.84	7	8
1	A	36	PHE	CA-CB-CG	6.13	119.93	113.80	9	3
1	A	25	ASN	CA-CB-CG	5.73	118.33	112.60	7	2

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	879	906	903	41±6
All	All	8790	9060	9030	414

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 23.

5 of 137 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:TYR:CG	1:A:82:LEU:HD21	0.89	2.03	6	1
1:A:42:ASN:ND2	1:A:127:ASP:HA	0.79	1.93	4	9
1:A:77:TYR:CD1	1:A:82:LEU:HD21	0.76	2.15	6	1
1:A:118:ALA:HB2	1:A:123:ILE:HG13	0.74	1.59	5	6
1:A:117:GLU:HA	1:A:122:ILE:HD13	0.70	1.63	2	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	118/159 (74%)	104±2 (88±2%)	10±1 (8±1%)	4±1 (3±1%)	4	33
All	All	1180/1590 (74%)	1043 (88%)	96 (8%)	41 (3%)	4	33

5 of 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	102	ASN	10
1	A	61	PRO	8
1	A	62	PRO	8
1	A	107	LYS	4
1	A	63	GLN	3

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	98/132 (74%)	81±3 (82±3%)	17±3 (18±3%)	4	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	980/1320 (74%)	808 (82%)	172 (18%)	4 37

5 of 35 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	21	VAL	10
1	A	25	ASN	10
1	A	27	VAL	10
1	A	68	LEU	10
1	A	82	LEU	10

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 i

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping i

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	1866
Number of shifts mapped to atoms	1504
Number of unparsed shifts	0
Number of shifts with mapping errors	362
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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 362) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	130	ILE	H	10.381	0.004	1
1	A	130	ILE	HA	4.108	0.005	1
1	A	130	ILE	HB	1.261	0.005	1
1	A	130	ILE	HD11	0.233	0.002	1
1	A	130	ILE	HD12	0.233	0.002	1
1	A	130	ILE	HD13	0.233	0.002	1
1	A	130	ILE	HG12	0.522	0.002	2
1	A	130	ILE	HG13	1.27	0.003	2
1	A	130	ILE	HG21	0.696	0.005	1
1	A	130	ILE	HG22	0.696	0.005	1
1	A	130	ILE	HG23	0.696	0.005	1
1	A	130	ILE	C	174.461	0.0	1
1	A	130	ILE	CA	62.651	0.074	1
1	A	130	ILE	CB	38.126	0.048	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	130	ILE	CD1	13.724	0.044	1
1	A	130	ILE	CG1	26.365	0.031	1
1	A	130	ILE	CG2	18.894	0.044	1
1	A	130	ILE	N	131.606	0.047	1
1	A	131	LEU	H	7.808	0.007	1
1	A	131	LEU	HA	4.542	0.004	1
1	A	131	LEU	HB2	1.474	0.008	2
1	A	131	LEU	HB3	1.475	0.008	2
1	A	131	LEU	HD11	0.794	0.008	2
1	A	131	LEU	HD12	0.794	0.008	2
1	A	131	LEU	HD13	0.794	0.008	2
1	A	131	LEU	HD21	0.808	0.003	2
1	A	131	LEU	HD22	0.808	0.003	2
1	A	131	LEU	HD23	0.808	0.003	2
1	A	131	LEU	HG	1.569	0.006	1
1	A	131	LEU	C	176.911	0.0	1
1	A	131	LEU	CA	53.828	0.03	1
1	A	131	LEU	CB	44.673	0.048	1
1	A	131	LEU	CD1	23.687	0.056	2
1	A	131	LEU	CD2	23.884	0.001	2
1	A	131	LEU	CG	26.239	0.002	1
1	A	131	LEU	N	121.996	0.047	1
1	A	132	MET	H	7.936	0.006	1
1	A	132	MET	HA	3.925	0.002	1
1	A	132	MET	HB2	1.645	0.002	2
1	A	132	MET	HB3	1.609	0.006	2
1	A	132	MET	HG2	1.904	0.001	2
1	A	132	MET	HG3	1.855	0.001	2
1	A	132	MET	CA	55.996	0.062	1
1	A	132	MET	CB	31.419	0.017	1
1	A	132	MET	CG	31.899	0.002	1
1	A	132	MET	N	119.785	0.026	1
1	A	133	GLY	H	8.129	0.002	1
1	A	133	GLY	HA2	3.841	0.001	2
1	A	133	GLY	HA3	3.841	0.001	2
1	A	133	GLY	C	173.744	0.0	1
1	A	133	GLY	CA	45.125	0.055	1
1	A	133	GLY	N	108.379	0.057	1
1	A	134	LEU	H	8.06	0.006	1
1	A	134	LEU	HA	4.287	0.003	1
1	A	134	LEU	HB2	1.502	0.002	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	134	LEU	HB3	1.563	0.003	2
1	A	134	LEU	HD11	0.842	0.004	2
1	A	134	LEU	HD12	0.842	0.004	2
1	A	134	LEU	HD13	0.842	0.004	2
1	A	134	LEU	HD21	0.788	0.004	2
1	A	134	LEU	HD22	0.788	0.004	2
1	A	134	LEU	HD23	0.788	0.004	2
1	A	134	LEU	HG	1.552	0.001	1
1	A	134	LEU	C	176.638	0.0	1
1	A	134	LEU	CA	54.93	0.075	1
1	A	134	LEU	CB	42.674	0.038	1
1	A	134	LEU	CD1	25.014	0.041	2
1	A	134	LEU	CD2	23.473	0.007	2
1	A	134	LEU	CG	27.032	0.042	1
1	A	134	LEU	N	121.379	0.061	1
1	A	135	ASP	H	8.312	0.006	1
1	A	135	ASP	HA	4.813	0.001	1
1	A	135	ASP	HB2	2.671	0.002	2
1	A	135	ASP	HB3	2.508	0.003	2
1	A	135	ASP	CA	51.902	0.064	1
1	A	135	ASP	CB	41.613	0.031	1
1	A	135	ASP	N	122.414	0.035	1
1	A	136	PRO	HA	4.259	0.002	1
1	A	136	PRO	HB2	2.236	0.004	2
1	A	136	PRO	HB3	1.9	0.003	2
1	A	136	PRO	HD2	3.814	0.004	1
1	A	136	PRO	HD3	3.814	0.004	1
1	A	136	PRO	HG2	1.955	0.006	1
1	A	136	PRO	HG3	1.955	0.006	1
1	A	136	PRO	C	176.933	0.0	1
1	A	136	PRO	CA	64.063	0.05	1
1	A	136	PRO	CB	32.112	0.032	1
1	A	136	PRO	CD	50.984	0.093	1
1	A	136	PRO	CG	27.309	0.068	1
1	A	137	ALA	H	8.343	0.003	1
1	A	137	ALA	HA	4.172	0.002	1
1	A	137	ALA	HB1	1.268	0.002	1
1	A	137	ALA	HB2	1.268	0.002	1
1	A	137	ALA	HB3	1.268	0.002	1
1	A	137	ALA	C	177.938	0.0	1
1	A	137	ALA	CA	53.03	0.031	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	137	ALA	CB	18.737	0.062	1
1	A	137	ALA	N	121.178	0.022	1
1	A	138	HIS	H	7.841	0.004	1
1	A	138	HIS	HA	4.566	0.003	1
1	A	138	HIS	HB2	3.128	0.006	2
1	A	138	HIS	HB3	2.983	0.006	2
1	A	138	HIS	C	175.404	0.0	1
1	A	138	HIS	CA	56.252	0.062	1
1	A	138	HIS	CB	30.972	0.059	1
1	A	138	HIS	N	117.273	0.109	1
1	A	139	SER	H	7.977	0.006	1
1	A	139	SER	HA	4.347	0.005	1
1	A	139	SER	HB2	3.726	0.001	2
1	A	139	SER	HB3	3.726	0.001	2
1	A	139	SER	C	174.169	0.0	1
1	A	139	SER	CA	58.681	0.043	1
1	A	139	SER	CB	63.855	0.085	1
1	A	139	SER	N	115.934	0.029	1
1	A	140	PHE	H	8.217	0.005	1
1	A	140	PHE	HA	4.558	0.004	1
1	A	140	PHE	HB2	3.141	0.007	2
1	A	140	PHE	HB3	3.024	0.015	2
1	A	140	PHE	HD1	7.233	0.004	3
1	A	140	PHE	HD2	7.233	0.004	3
1	A	140	PHE	C	175.476	0.0	1
1	A	140	PHE	CA	58.002	0.075	1
1	A	140	PHE	CB	39.124	0.072	1
1	A	140	PHE	CD1	131.813	0.001	3
1	A	140	PHE	CD2	131.813	0.001	3
1	A	140	PHE	N	121.295	0.015	1
1	A	141	GLN	H	8.094	0.004	1
1	A	141	GLN	HA	4.279	0.002	1
1	A	141	GLN	HB2	2.044	0.002	2
1	A	141	GLN	HB3	1.924	0.002	2
1	A	141	GLN	HE21	7.467	0.005	1
1	A	141	GLN	HE22	6.82	0.001	1
1	A	141	GLN	HG2	2.275	0.003	2
1	A	141	GLN	HG3	2.275	0.003	2
1	A	141	GLN	C	175.652	0.0	1
1	A	141	GLN	CA	55.898	0.023	1
1	A	141	GLN	CB	29.677	0.025	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	141	GLN	CD	180.381	0.002	1
1	A	141	GLN	CG	33.884	0.089	1
1	A	141	GLN	N	121.005	0.021	1
1	A	141	GLN	NE2	112.205	0.001	1
1	A	142	GLU	H	8.407	0.004	1
1	A	142	GLU	HA	4.272	0.002	1
1	A	142	GLU	HB2	2.061	0.006	2
1	A	142	GLU	HB3	1.95	0.006	2
1	A	142	GLU	HG2	2.255	0.008	2
1	A	142	GLU	HG3	2.255	0.008	2
1	A	142	GLU	C	176.569	0.0	1
1	A	142	GLU	CA	56.929	0.025	1
1	A	142	GLU	CB	30.321	0.028	1
1	A	142	GLU	CG	36.481	0.008	1
1	A	142	GLU	N	122.091	0.017	1
1	A	143	THR	H	8.135	0.005	1
1	A	143	THR	HA	4.33	0.004	1
1	A	143	THR	HB	4.212	0.003	1
1	A	143	THR	HG21	1.183	0.003	1
1	A	143	THR	HG22	1.183	0.003	1
1	A	143	THR	HG23	1.183	0.003	1
1	A	143	THR	C	174.131	0.0	1
1	A	143	THR	CA	61.908	0.021	1
1	A	143	THR	CB	69.791	0.053	1
1	A	143	THR	CG2	21.481	0.053	1
1	A	143	THR	N	114.211	0.022	1
1	A	144	ASN	H	8.455	0.007	1
1	A	144	ASN	HA	4.691	0.001	1
1	A	144	ASN	HB2	2.792	0.002	2
1	A	144	ASN	HB3	2.726	0.004	2
1	A	144	ASN	HD21	7.561	0.007	1
1	A	144	ASN	HD22	6.868	0.006	1
1	A	144	ASN	C	174.485	0.0	1
1	A	144	ASN	CA	53.27	0.05	1
1	A	144	ASN	CB	38.856	0.074	1
1	A	144	ASN	CG	177.138	0.0	1
1	A	144	ASN	N	120.943	0.066	1
1	A	144	ASN	ND2	112.698	0.004	1
1	A	145	ILE	H	8.002	0.004	1
1	A	145	ILE	HA	4.397	0.001	1
1	A	145	ILE	HB	1.806	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	145	ILE	HD11	0.829	0.002	1
1	A	145	ILE	HD12	0.829	0.002	1
1	A	145	ILE	HD13	0.829	0.002	1
1	A	145	ILE	HG12	1.458	0.002	2
1	A	145	ILE	HG13	1.114	0.004	2
1	A	145	ILE	HG21	0.84	0.006	1
1	A	145	ILE	HG22	0.84	0.006	1
1	A	145	ILE	HG23	0.84	0.006	1
1	A	145	ILE	CA	58.861	0.066	1
1	A	145	ILE	CB	38.719	0.048	1
1	A	145	ILE	CD1	12.648	0.067	1
1	A	145	ILE	CG1	26.932	0.065	1
1	A	145	ILE	CG2	17.246	0.082	1
1	A	145	ILE	N	122.46	0.074	1
1	A	146	PRO	HA	4.357	0.003	1
1	A	146	PRO	HB2	2.189	0.005	2
1	A	146	PRO	HB3	1.805	0.006	2
1	A	146	PRO	HD2	3.814	0.003	2
1	A	146	PRO	HD3	3.618	0.003	2
1	A	146	PRO	HG2	1.95	0.004	2
1	A	146	PRO	HG3	1.95	0.004	2
1	A	146	PRO	C	176.356	0.0	1
1	A	146	PRO	CA	63.362	0.025	1
1	A	146	PRO	CB	31.866	0.017	1
1	A	146	PRO	CD	50.973	0.052	1
1	A	146	PRO	CG	27.314	0.042	1
1	A	147	TYR	H	8.007	0.005	1
1	A	147	TYR	HA	4.488	0.004	1
1	A	147	TYR	HB2	2.968	0.008	2
1	A	147	TYR	HB3	2.969	0.008	2
1	A	147	TYR	HD1	7.072	0.006	3
1	A	147	TYR	HD2	7.072	0.006	3
1	A	147	TYR	HE1	6.795	0.006	3
1	A	147	TYR	HE2	6.795	0.006	3
1	A	147	TYR	C	175.324	0.0	1
1	A	147	TYR	CA	57.902	0.055	1
1	A	147	TYR	CB	38.816	0.073	1
1	A	147	TYR	CD1	133.201	0.022	3
1	A	147	TYR	CD2	133.201	0.022	3
1	A	147	TYR	CE1	118.216	0.028	3
1	A	147	TYR	CE2	118.216	0.028	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	TYR	N	120.291	0.019	1
1	A	148	LYS	H	8.042	0.004	1
1	A	148	LYS	HA	4.268	0.005	1
1	A	148	LYS	HB2	1.727	0.005	2
1	A	148	LYS	HB3	1.632	0.006	2
1	A	148	LYS	HD2	1.621	0.002	1
1	A	148	LYS	HD3	1.621	0.002	1
1	A	148	LYS	HE2	2.937	0.002	2
1	A	148	LYS	HE3	2.937	0.002	2
1	A	148	LYS	HG2	1.28	0.003	2
1	A	148	LYS	HG3	1.317	0.008	2
1	A	148	LYS	C	175.846	0.0	1
1	A	148	LYS	CA	55.986	0.047	1
1	A	148	LYS	CB	33.378	0.019	1
1	A	148	LYS	CD	29.113	0.053	1
1	A	148	LYS	CE	42.209	0.021	1
1	A	148	LYS	CG	24.636	0.019	1
1	A	148	LYS	N	123.461	0.017	1
1	A	149	VAL	H	8.069	0.004	1
1	A	149	VAL	HA	4.022	0.002	1
1	A	149	VAL	HB	2.012	0.002	1
1	A	149	VAL	HG11	0.894	0.004	2
1	A	149	VAL	HG12	0.894	0.004	2
1	A	149	VAL	HG13	0.894	0.004	2
1	A	149	VAL	HG21	0.914	0.007	2
1	A	149	VAL	HG22	0.914	0.007	2
1	A	149	VAL	HG23	0.914	0.007	2
1	A	149	VAL	C	176.103	0.0	1
1	A	149	VAL	CA	62.446	0.039	1
1	A	149	VAL	CB	32.756	0.049	1
1	A	149	VAL	CG1	20.893	0.033	2
1	A	149	VAL	CG2	20.441	0.0	2
1	A	149	VAL	N	121.671	0.032	1
1	A	150	SER	H	8.31	0.007	1
1	A	150	SER	HA	4.336	0.0	1
1	A	150	SER	HB2	3.718	0.0	1
1	A	150	SER	HB3	3.718	0.0	1
1	A	150	SER	C	174.259	0.0	1
1	A	150	SER	CA	58.184	0.064	1
1	A	150	SER	CB	63.956	0.022	1
1	A	150	SER	N	119.318	0.038	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	151	ALA	H	8.24	0.008	1
1	A	151	ALA	HA	4.212	0.003	1
1	A	151	ALA	HB1	1.228	0.003	1
1	A	151	ALA	HB2	1.228	0.003	1
1	A	151	ALA	HB3	1.228	0.003	1
1	A	151	ALA	C	177.197	0.0	1
1	A	151	ALA	CA	52.853	0.042	1
1	A	151	ALA	CB	19.099	0.026	1
1	A	151	ALA	N	125.7	0.018	1
1	A	152	TRP	H	7.934	0.005	1
1	A	152	TRP	HA	4.603	0.001	1
1	A	152	TRP	HB2	3.251	0.001	2
1	A	152	TRP	HB3	3.175	0.002	2
1	A	152	TRP	HE1	10.095	0.001	1
1	A	152	TRP	HH2	7.154	0.003	1
1	A	152	TRP	HZ2	7.429	0.004	1
1	A	152	TRP	HZ3	7.06	0.004	1
1	A	152	TRP	C	177.93	0.0	1
1	A	152	TRP	CA	57.27	0.031	1
1	A	152	TRP	CB	29.709	0.024	1
1	A	152	TRP	CH2	124.453	0.033	1
1	A	152	TRP	CZ2	114.499	0.063	1
1	A	152	TRP	CZ3	121.876	0.016	1
1	A	152	TRP	N	119.068	0.018	1
1	A	152	TRP	NE1	129.244	0.022	1
1	A	153	SER	H	7.824	0.012	1
1	A	153	SER	HA	4.318	0.001	1
1	A	153	SER	HB2	3.671	0.018	2
1	A	153	SER	HB3	3.64	0.001	2
1	A	153	SER	C	173.204	0.0	1
1	A	153	SER	CA	57.952	0.058	1
1	A	153	SER	CB	63.892	0.083	1
1	A	153	SER	N	116.976	0.034	1
1	A	154	HIS	H	8.04	0.004	1
1	A	154	HIS	HA	4.696	0.001	1
1	A	154	HIS	HB2	3.034	0.002	2
1	A	154	HIS	HB3	2.945	0.001	2
1	A	154	HIS	CA	54.713	0.043	1
1	A	154	HIS	CB	30.737	0.044	1
1	A	154	HIS	N	122.653	0.026	1
1	A	155	PRO	HA	4.324	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	155	PRO	HB2	2.2	0.006	2
1	A	155	PRO	HB3	1.763	0.006	2
1	A	155	PRO	HD2	3.685	0.006	2
1	A	155	PRO	HD3	3.362	0.006	2
1	A	155	PRO	HG2	1.943	0.004	2
1	A	155	PRO	HG3	1.944	0.003	2
1	A	155	PRO	C	176.829	0.0	1
1	A	155	PRO	CA	63.611	0.046	1
1	A	155	PRO	CB	32.106	0.102	1
1	A	155	PRO	CD	50.658	0.035	1
1	A	155	PRO	CG	27.481	0.045	1
1	A	156	GLN	H	8.714	0.005	1
1	A	156	GLN	HA	4.245	0.002	1
1	A	156	GLN	HB2	1.95	0.003	2
1	A	156	GLN	HB3	1.869	0.002	2
1	A	156	GLN	HE21	6.801	0.002	1
1	A	156	GLN	HE22	7.412	0.004	1
1	A	156	GLN	HG2	2.186	0.002	2
1	A	156	GLN	HG3	2.186	0.002	2
1	A	156	GLN	C	175.595	0.0	1
1	A	156	GLN	CA	55.898	0.025	1
1	A	156	GLN	CB	29.416	0.013	1
1	A	156	GLN	CD	180.437	0.006	1
1	A	156	GLN	CG	33.75	0.041	1
1	A	156	GLN	N	120.311	0.034	1
1	A	156	GLN	NE2	112.38	0.03	1
1	A	157	PHE	H	8.129	0.004	1
1	A	157	PHE	HA	4.658	0.002	1
1	A	157	PHE	HB2	2.984	0.005	2
1	A	157	PHE	HB3	3.192	0.004	2
1	A	157	PHE	C	175.397	0.0	1
1	A	157	PHE	CA	57.421	0.056	1
1	A	157	PHE	CB	39.784	0.041	1
1	A	157	PHE	N	120.408	0.015	1
1	A	158	GLU	H	8.268	0.004	1
1	A	158	GLU	HA	4.247	0.002	1
1	A	158	GLU	HB2	2.025	0.006	2
1	A	158	GLU	HB3	1.884	0.005	2
1	A	158	GLU	HG2	2.202	0.005	2
1	A	158	GLU	HG3	2.202	0.005	2
1	A	158	GLU	C	175.102	0.0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	158	GLU	CA	56.603	0.03	1
1	A	158	GLU	CB	30.552	0.029	1
1	A	158	GLU	CG	36.354	0.04	1
1	A	158	GLU	N	122.621	0.008	1
1	A	159	LYS	H	7.869	0.004	1
1	A	159	LYS	HA	4.12	0.003	1
1	A	159	LYS	HB2	1.804	0.006	2
1	A	159	LYS	HB3	1.701	0.006	2
1	A	159	LYS	HD2	1.664	0.005	1
1	A	159	LYS	HD3	1.664	0.005	1
1	A	159	LYS	HE2	2.981	0.004	1
1	A	159	LYS	HE3	2.981	0.004	1
1	A	159	LYS	HG2	1.379	0.002	2
1	A	159	LYS	HG3	1.379	0.002	2
1	A	159	LYS	CA	57.755	0.034	1
1	A	159	LYS	CB	33.828	0.082	1
1	A	159	LYS	CD	29.299	0.054	1
1	A	159	LYS	CE	42.295	0.027	1
1	A	159	LYS	CG	24.711	0.006	1
1	A	159	LYS	N	127.136	0.009	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
$^{13}\text{C}_\alpha$	157	-0.30 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	147	0.08 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	136	0.06 ± 0.16	None needed (< 0.5 ppm)
^{15}N	142	0.47 ± 0.44	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1413 atoms were assigned a chemical shift out of a possible 1564. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	568/587 (97%)	235/238 (99%)	223/238 (94%)	110/111 (99%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	827/905 (91%)	562/600 (94%)	255/284 (90%)	10/21 (48%)
Aromatic	18/72 (25%)	9/35 (26%)	9/31 (29%)	0/6 (0%)
Overall	1413/1564 (90%)	806/873 (92%)	487/553 (88%)	120/138 (87%)

7.1.4 Statistically unusual chemical shifts [i](#)

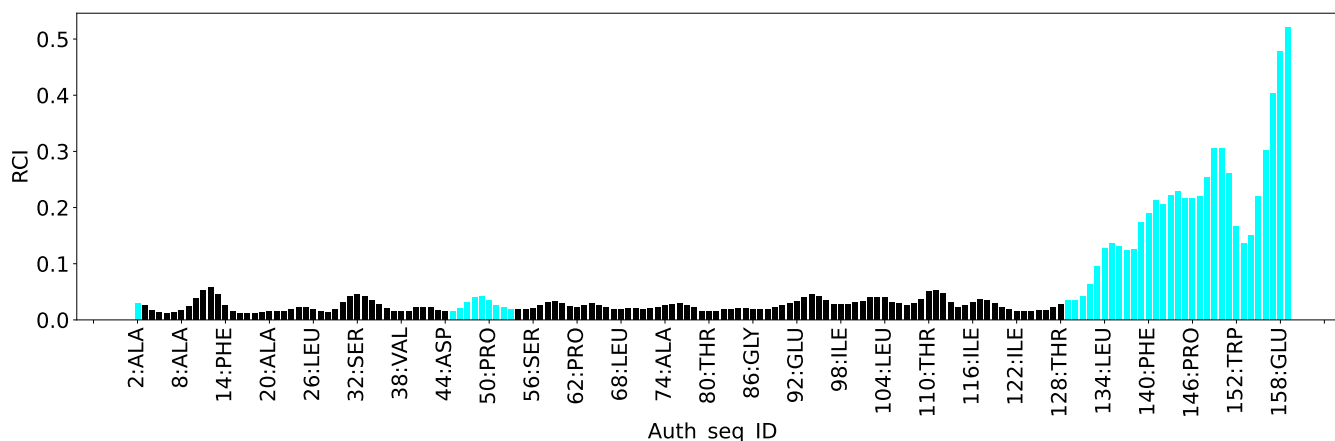
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	37	THR	HG1	6.10	0.08 – 2.19	23.5
1	A	11	THR	HG1	5.95	0.08 – 2.19	22.8
1	A	79	ALA	H	11.65	5.31 – 11.08	6.0
1	A	105	GLU	HB3	0.87	0.95 – 3.05	-5.4
1	A	121	GLY	HA3	5.76	2.08 – 5.71	5.1

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	2089
Intra-residue ($ i-j =0$)	929
Sequential ($ i-j =1$)	449
Medium range ($ i-j >1$ and $ i-j <5$)	283
Long range ($ i-j \geq 5$)	428
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	221
Number of unmapped restraints	0
Number of restraints per residue	14.5
Number of long range restraints per residue ¹	2.7

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	54.6	0.2
0.2-0.5 (Medium)	72.3	0.5
>0.5 (Large)	154.3	3.71

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)	19.9	9.2
10.0-20.0 (Medium)	0.2	12.71
>20.0 (Large)	None	None

9 Distance violation analysis i

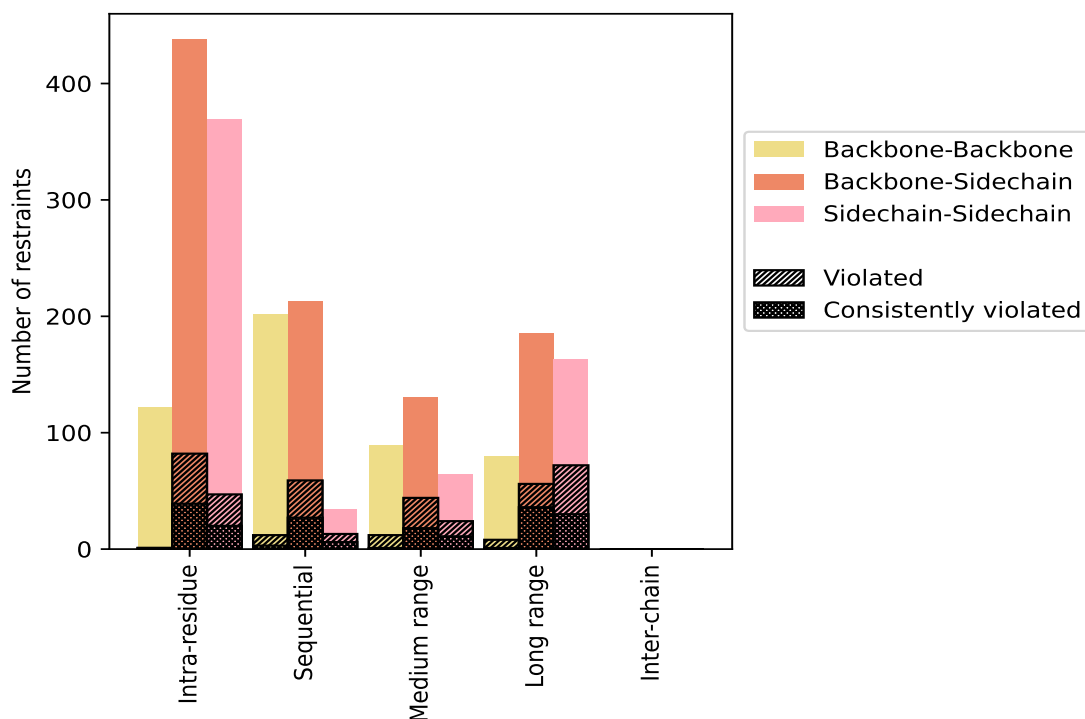
9.1 Summary of distance violations i

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	929	44.5	130	14.0	6.2	60	6.5	2.9
Backbone-Backbone	122	5.8	1	0.8	0.0	1	0.8	0.0
Backbone-Sidechain	438	21.0	82	18.7	3.9	39	8.9	1.9
Sidechain-Sidechain	369	17.7	47	12.7	2.2	20	5.4	1.0
Sequential ($i-j =1$)	449	21.5	84	18.7	4.0	36	8.0	1.7
Backbone-Backbone	202	9.7	12	5.9	0.6	3	1.5	0.1
Backbone-Sidechain	213	10.2	59	27.7	2.8	27	12.7	1.3
Sidechain-Sidechain	34	1.6	13	38.2	0.6	6	17.6	0.3
Medium range ($i-j >1$ & $i-j <5$)	283	13.5	80	28.3	3.8	30	10.6	1.4
Backbone-Backbone	89	4.3	12	13.5	0.6	1	1.1	0.0
Backbone-Sidechain	130	6.2	44	33.8	2.1	18	13.8	0.9
Sidechain-Sidechain	64	3.1	24	37.5	1.1	11	17.2	0.5
Long range ($i-j \geq 5$)	428	20.5	136	31.8	6.5	67	15.7	3.2
Backbone-Backbone	80	3.8	8	10.0	0.4	1	1.2	0.0
Backbone-Sidechain	185	8.9	56	30.3	2.7	36	19.5	1.7
Sidechain-Sidechain	163	7.8	72	44.2	3.4	30	18.4	1.4
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	2089	100.0	430	20.6	20.6	193	9.2	9.2
Backbone-Backbone	493	23.6	33	6.7	1.6	6	1.2	0.3
Backbone-Sidechain	966	46.2	241	24.9	11.5	120	12.4	5.7
Sidechain-Sidechain	630	30.2	156	24.8	7.5	67	10.6	3.2

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

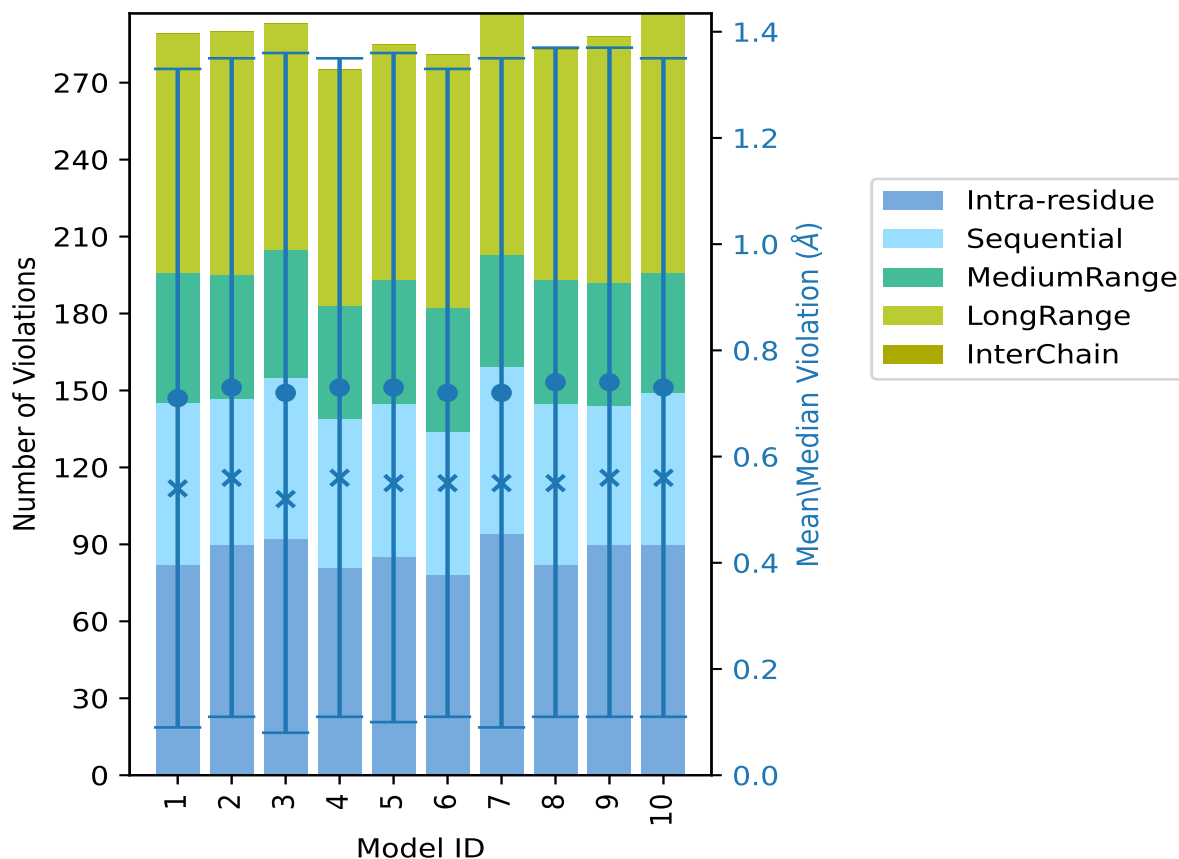
9.2 Distance violation statistics for each model [i](#)

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	63	51	93	0	289	0.71	3.57	0.62	0.54
2	90	57	48	95	0	290	0.73	3.2	0.62	0.56
3	92	63	50	88	0	293	0.72	3.71	0.64	0.52
4	81	58	44	92	0	275	0.73	2.7	0.62	0.56
5	85	60	48	92	0	285	0.73	3.57	0.63	0.55
6	78	56	48	99	0	281	0.72	2.71	0.61	0.55
7	94	65	44	94	0	297	0.72	3.25	0.63	0.55
8	82	63	48	90	0	283	0.74	2.9	0.63	0.55
9	90	54	48	96	0	288	0.74	3.19	0.63	0.56
10	90	59	47	101	0	297	0.73	3.17	0.62	0.56

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, 1659(IR:799, SQ:365, MR:203, LR:292, 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	%
22	9	11	20	0	62	1	10.0
8	8	13	8	0	37	2	20.0
12	6	3	7	0	28	3	30.0

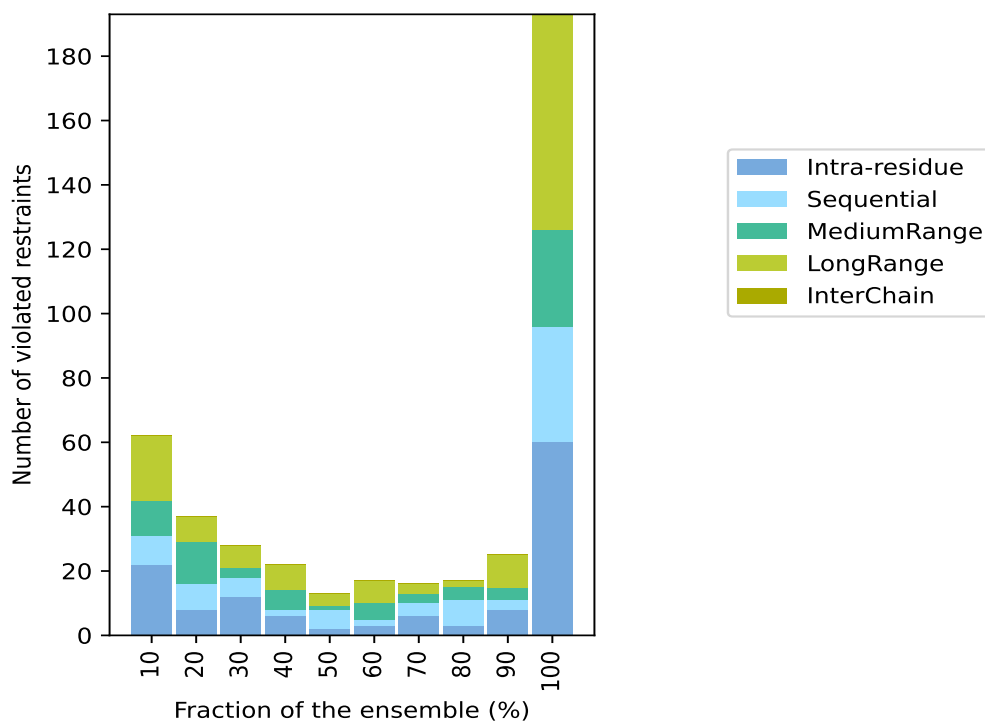
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
6	2	6	8	0	22	4	40.0
2	6	1	4	0	13	5	50.0
3	2	5	7	0	17	6	60.0
6	4	3	3	0	16	7	70.0
3	8	4	2	0	17	8	80.0
8	3	4	10	0	25	9	90.0
60	36	30	67	0	193	10	100.0

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 [i](#)

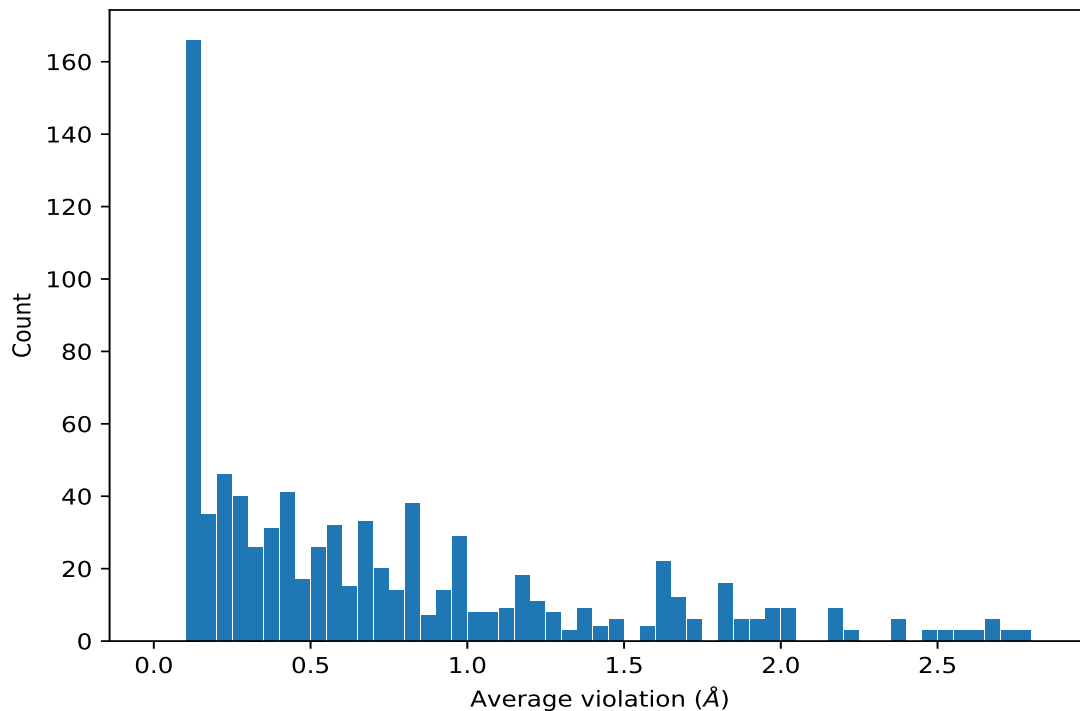


9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	10	2.79	0.74	2.87
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	10	2.79	0.74	2.87
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	10	2.79	0.74	2.87
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	10	2.71	0.03	2.71
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	10	2.71	0.03	2.71
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	10	2.71	0.03	2.71
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	10	2.69	0.03	2.68
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	10	2.69	0.03	2.68
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	10	2.69	0.03	2.68
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	10	2.68	0.25	2.62
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	10	2.68	0.25	2.62
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	10	2.68	0.25	2.62
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	10	2.61	0.1	2.64
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	10	2.61	0.1	2.64
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	10	2.61	0.1	2.64

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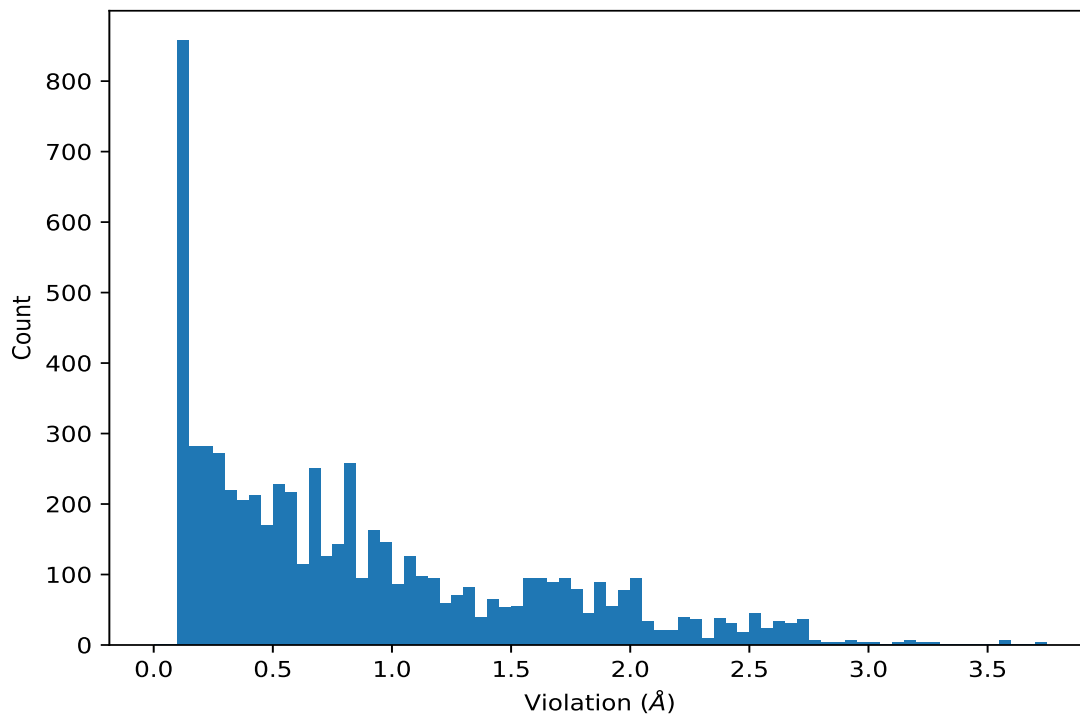
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	10	2.59	0.09	2.56
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	10	2.59	0.09	2.56
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	10	2.59	0.09	2.56
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	10	2.51	0.04	2.51
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	10	2.51	0.04	2.51
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	10	2.51	0.04	2.51
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	10	2.45	0.05	2.46
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	10	2.45	0.05	2.46
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	10	2.45	0.05	2.46
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	10	2.39	0.19	2.39
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	10	2.39	0.19	2.39
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	10	2.39	0.19	2.39
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	10	2.37	0.04	2.38

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)
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	3	3.71
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	3	3.71
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	3	3.71
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	1	3.57
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	1	3.57
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	1	3.57
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	5	3.57
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	5	3.57
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	5	3.57
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	7	3.25
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	7	3.25
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	7	3.25
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	2	3.2
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	2	3.2
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	2	3.2
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	9	3.19
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	9	3.19
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	9	3.19
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	10	3.17
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	10	3.17
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	10	3.17
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	3	3.1
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	3	3.1
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	3	3.1
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	7	3.01
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	7	3.01
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	7	3.01
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	9	2.99

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

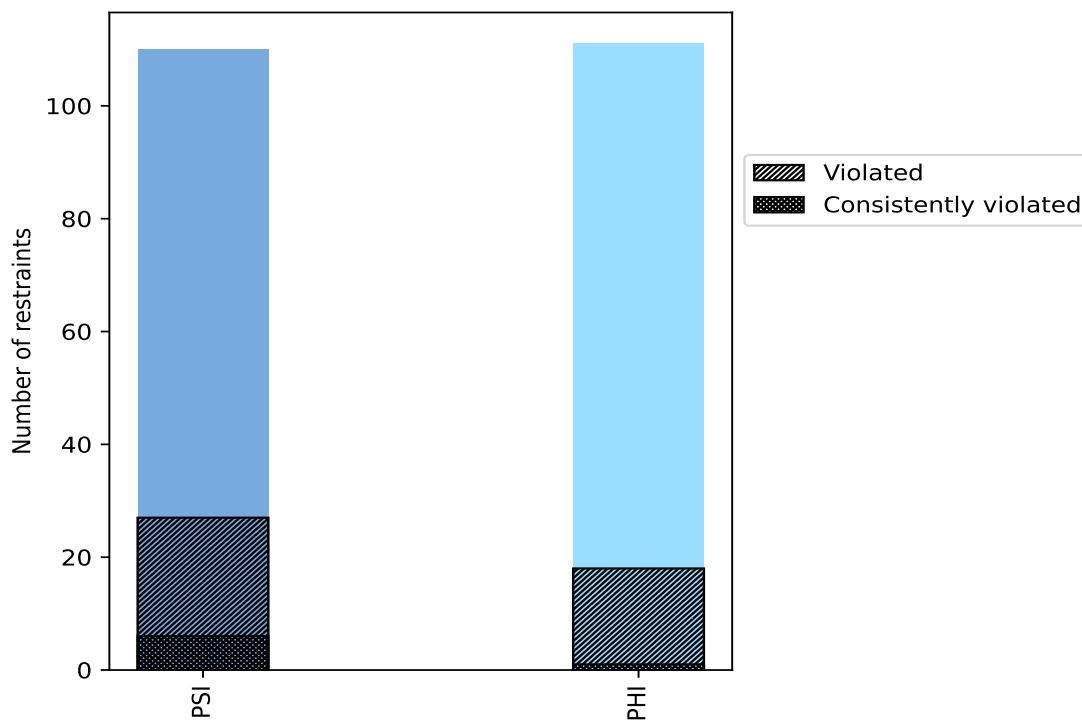
10.1 Summary of dihedral-angle violations [i](#)

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	110	49.8	27	24.5	12.2	6	5.5	2.7
PHI	111	50.2	18	16.2	8.1	1	0.9	0.5
Total	221	100.0	45	20.4	20.4	7	3.2	3.2

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](#)



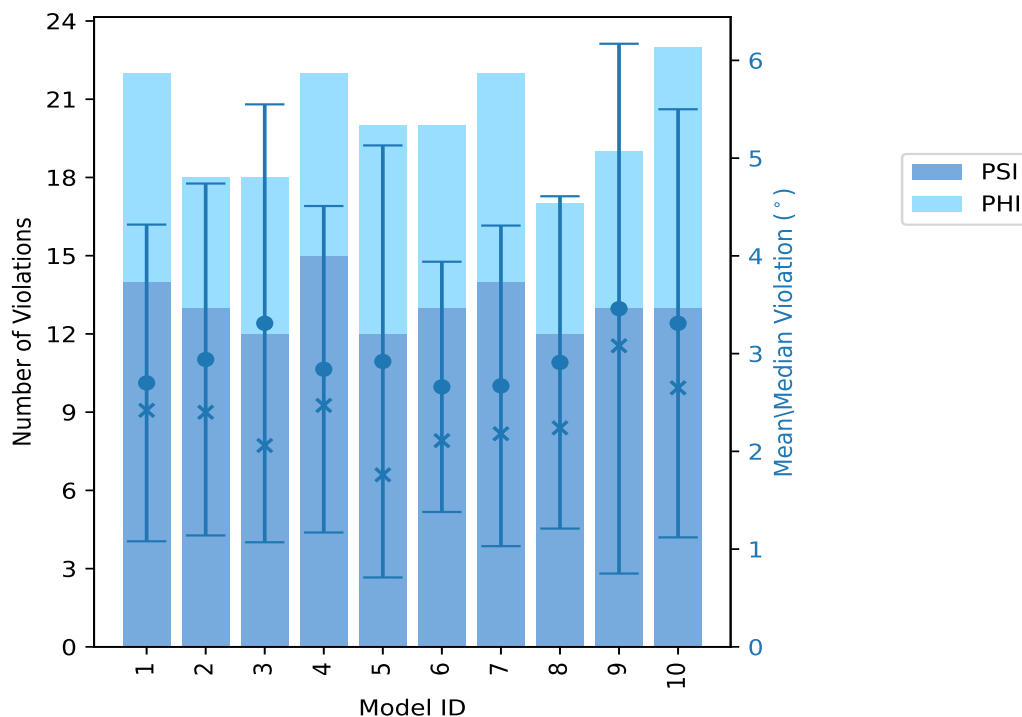
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	14	8	22	2.7	8.24	1.62	2.42
2	13	5	18	2.94	8.99	1.8	2.4
3	12	6	18	3.31	8.67	2.24	2.06
4	15	7	22	2.84	7.37	1.67	2.47
5	12	8	20	2.92	9.2	2.21	1.76
6	13	7	20	2.66	6.29	1.28	2.11
7	14	8	22	2.67	7.97	1.64	2.18
8	12	5	17	2.91	7.67	1.7	2.24
9	13	6	19	3.46	12.71	2.71	3.08
10	13	10	23	3.31	11.1	2.19	2.65

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

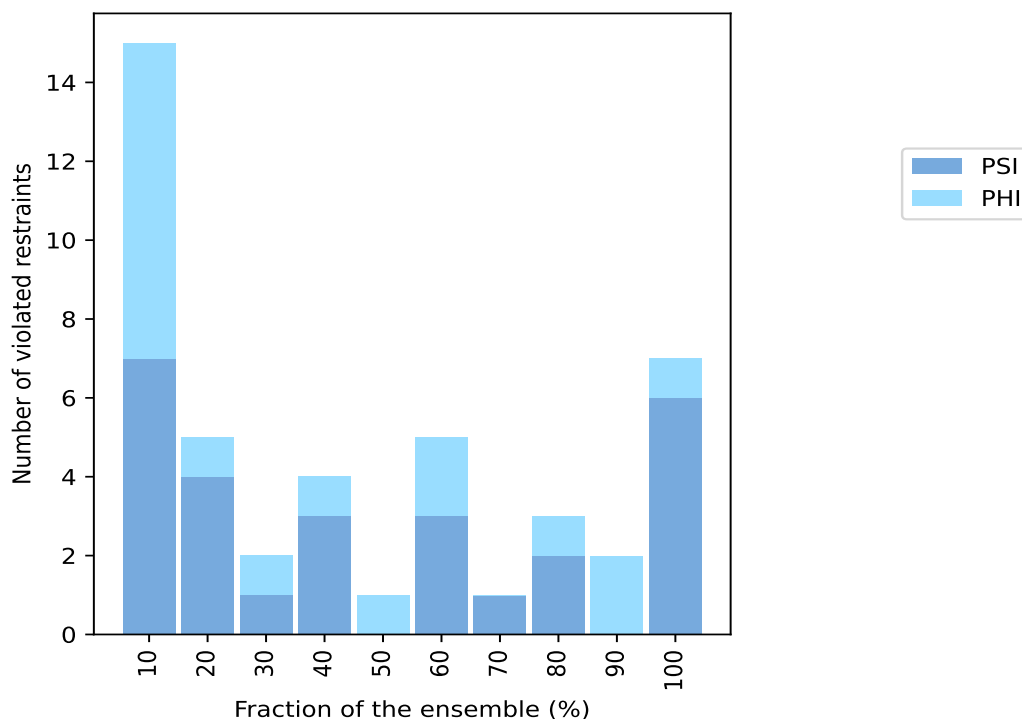
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
7	8	15	1	10.0
4	1	5	2	20.0
1	1	2	3	30.0
3	1	4	4	40.0
0	1	1	5	50.0
3	2	5	6	60.0
1	0	1	7	70.0
2	1	3	8	80.0
0	2	2	9	90.0
6	1	7	10	100.0

¹ Number of models with violations

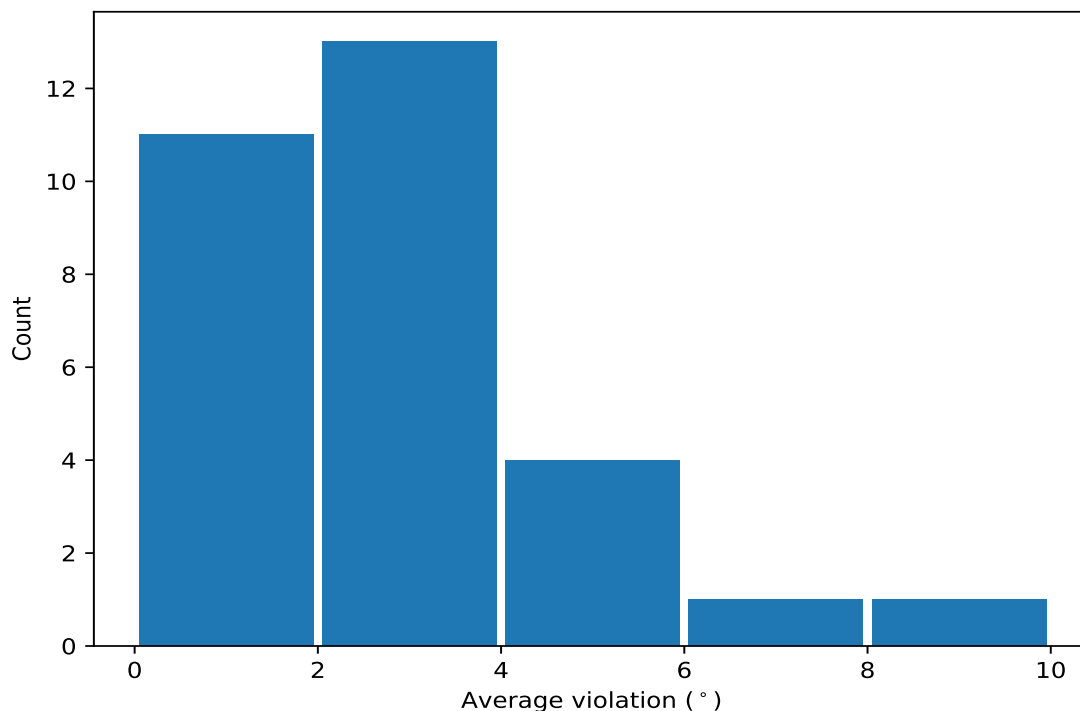
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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 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.

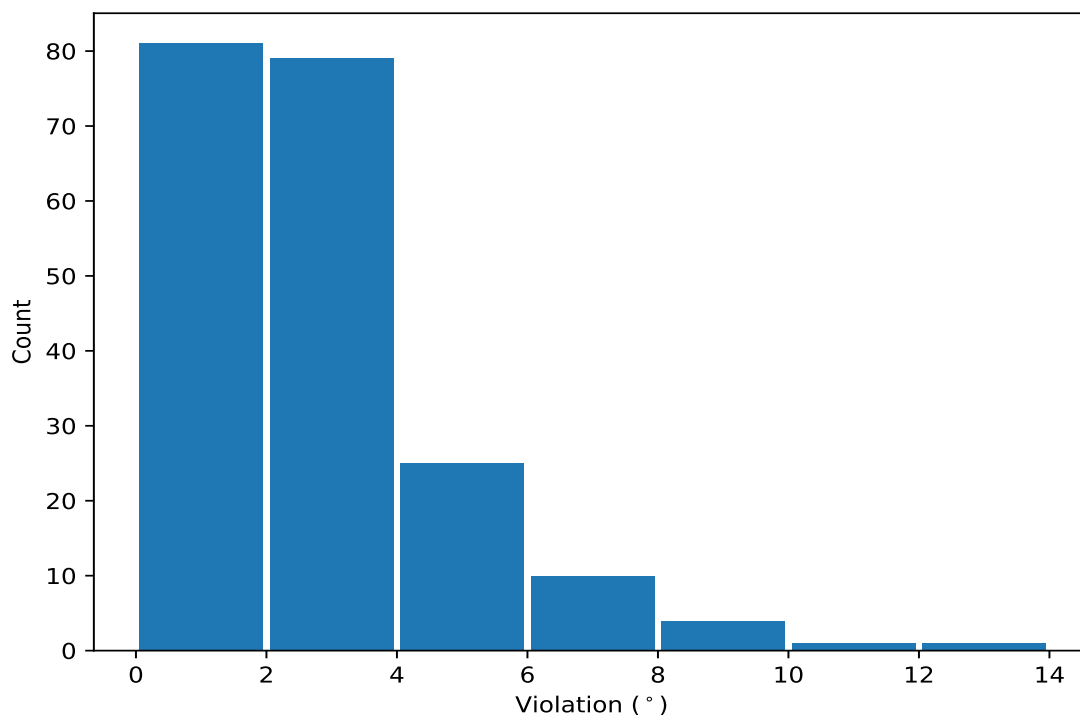
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	10	8.28	1.82	8.1
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	10	5.23	2.28	4.94
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	10	4.48	1.41	5.0
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	10	4.1	0.97	4.03
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	10	3.49	0.5	3.34
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	10	2.98	0.71	3.06
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	10	2.11	0.44	2.26
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	9	4.24	1.46	4.19
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	9	3.0	0.95	3.14
(1,102)	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	1:63:A:GLN:N	8	2.57	0.88	2.6

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	9	12.71
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	10	11.1
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	5	9.2
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	2	8.99
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	3	8.67
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	1	8.24
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	7	7.97
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	8	7.67
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	4	7.37
(1,92)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:VAL:N	9	6.71