wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2L9L
BMRB ID	:	17477
Title	:	NMR Structure of the Mouse MFG-E8 C2 Domain
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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 (i)) were used in the production of this report:

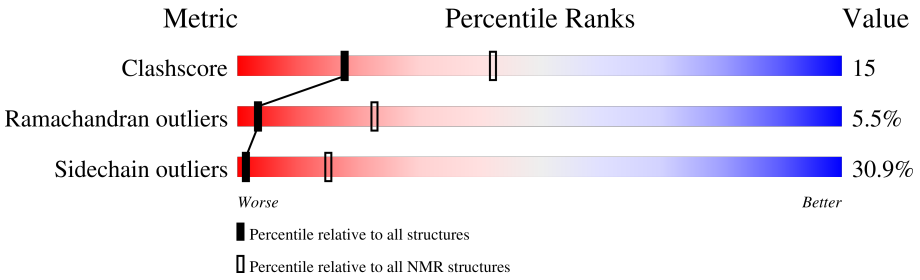
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 81%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	170	42% 37% 5% 13% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:1-A:23, A:34-A:104, A:111-A:158 (142)	1.04	7

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

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

The models can be grouped into 3 clusters and 10 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2379 atoms, of which 1068 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lactadherin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	164	2379	825	1068	238	243	5	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P21956
A	-4	LYS	-	expression tag	UNP P21956
A	-3	SER	-	expression tag	UNP P21956
A	-2	GLY	-	expression tag	UNP P21956
A	157	LEU	-	expression tag	UNP P21956
A	158	GLU	-	expression tag	UNP P21956
A	159	HIS	-	expression tag	UNP P21956
A	160	HIS	-	expression tag	UNP P21956
A	161	HIS	-	expression tag	UNP P21956
A	162	HIS	-	expression tag	UNP P21956
A	163	HIS	-	expression tag	UNP P21956
A	164	HIS	-	expression tag	UNP P21956

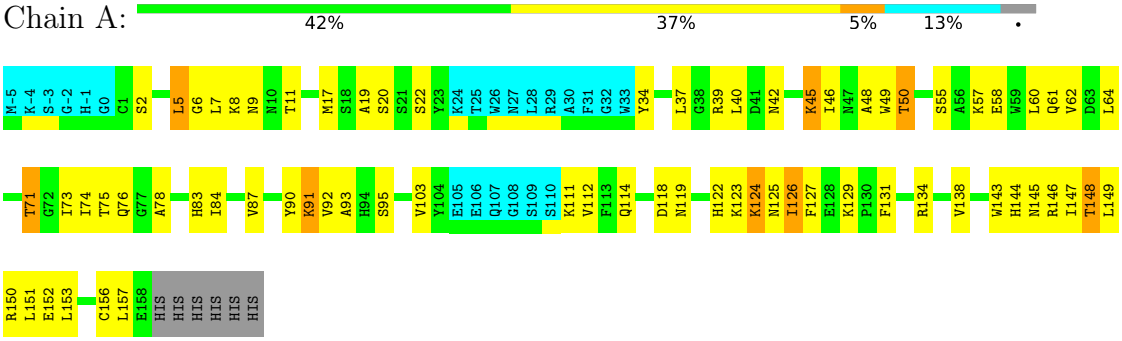
4 Residue-property plots (i)

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: Lactadherin

Chain A:

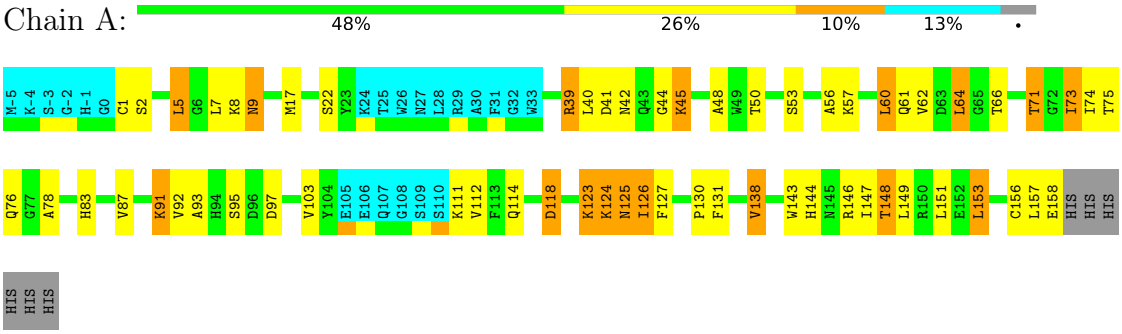


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 7. Colouring as in section 4.1 above.

• Molecule 1: Lactadherin

Chain A:



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	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	1706
Number of shifts mapped to atoms	1531
Number of unparsed shifts	0
Number of shifts with mapping errors	175
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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	1136	936	1108	34±4
All	All	22720	18720	22160	674

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 15.

5 of 287 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:HD22	1:A:40:LEU:HD23	0.97	1.35	17	1
1:A:92:VAL:HG22	1:A:138:VAL:HG13	0.89	1.41	18	2
1:A:75:THR:HG23	1:A:149:LEU:HD23	0.87	1.47	12	1
1:A:48:ALA:HB3	1:A:78:ALA:HB2	0.87	1.45	10	17
1:A:92:VAL:HG13	1:A:138:VAL:HG22	0.85	1.49	18	1

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	141/170 (83%)	105±4 (74±3%)	28±3 (20±2%)	8±3 (6±2%)	3 23
All	All	2820/3400 (83%)	2098 (74%)	566 (20%)	156 (6%)	3 23

5 of 39 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	45	LYS	19
1	A	147	ILE	13
1	A	124	LYS	9
1	A	118	ASP	7
1	A	81	PHE	6

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	124/147 (84%)	86±4 (69±4%)	38±4 (31±4%)	1 15
All	All	2480/2940 (84%)	1714 (69%)	766 (31%)	1 15

5 of 100 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	45	LYS	20
1	A	50	THR	20
1	A	148	THR	20
1	A	157	LEU	20
1	A	5	LEU	19

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 monosaccharides 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 81% for the well-defined parts and 76% 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	1706
Number of shifts mapped to atoms	1531
Number of unparsed shifts	0
Number of shifts with mapping errors	175
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 175) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	-3	SER	HB2	3.73	0.020	2
1	A	-1	HIS	HB2	3.044	0.020	2
1	A	1	CYS	HB2	3.211	0.020	2
1	A	2	SER	HB2	3.547	0.020	2
1	A	3	GLU	HB2	2.226	0.020	2
1	A	3	GLU	HG2	1.922	0.020	2
1	A	4	PRO	HB2	2.168	0.020	2
1	A	4	PRO	HG2	1.903	0.020	2
1	A	4	PRO	HD2	3.621	0.020	2
1	A	5	LEU	HB2	1.507	0.020	2
1	A	7	LEU	HB2	2.375	0.020	2
1	A	8	LYS	HB2	1.871	0.020	2
1	A	9	ASN	HB2	3.153	0.020	2
1	A	10	ASN	HB2	2.91	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	ILE	HG12	1.252	0.020	2
1	A	13	PRO	HB2	2.236	0.020	2
1	A	13	PRO	HG2	1.953	0.020	2
1	A	13	PRO	HD2	3.724	0.020	2
1	A	14	ASP	HB2	2.349	0.020	2
1	A	15	SER	HB2	3.91	0.020	2
1	A	16	GLN	HB2	1.808	0.020	2
1	A	16	GLN	HG2	2.407	0.020	2
1	A	17	MET	HB2	1.818	0.020	2
1	A	17	MET	HG2	2.058	0.020	2
1	A	18	SER	HB2	3.922	0.020	2
1	A	20	SER	HB2	2.865	0.020	2
1	A	21	SER	HB2	4.104	0.020	2
1	A	22	SER	HB2	3.684	0.020	2
1	A	23	TYR	HB2	2.526	0.020	2
1	A	24	LYS	HB2	1.748	0.020	2
1	A	24	LYS	HG2	1.571	0.020	2
1	A	24	LYS	HD2	1.65	0.020	2
1	A	24	LYS	HE2	2.53	0.020	2
1	A	31	PHE	HB2	3.272	0.020	2
1	A	33	TRP	HB2	3.013	0.020	2
1	A	35	PRO	HB2	2.142	0.020	2
1	A	35	PRO	HG2	1.616	0.020	2
1	A	36	HIS	HB2	3.698	0.020	2
1	A	37	LEU	HB2	1.703	0.020	2
1	A	39	ARG	HB2	1.558	0.020	2
1	A	39	ARG	HG2	1.147	0.020	2
1	A	39	ARG	HD2	2.949	0.020	2
1	A	40	LEU	HB2	1.494	0.020	2
1	A	41	ASP	HB2	3.042	0.020	2
1	A	42	ASN	HB2	3.342	0.020	2
1	A	43	GLN	HB2	2.143	0.020	2
1	A	43	GLN	HG2	2.434	0.020	2
1	A	45	LYS	HB2	1.766	0.020	2
1	A	45	LYS	HG2	1.308	0.020	2
1	A	45	LYS	HD2	1.567	0.020	2
1	A	46	ILE	HG12	0.982	0.020	2
1	A	47	ASN	HB2	2.335	0.020	2
1	A	49	TRP	HB2	3.18	0.020	2
1	A	52	GLN	HB2	1.875	0.020	2
1	A	52	GLN	HG2	2.302	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	SER	HB2	3.822	0.020	2
1	A	54	ASN	HB2	2.503	0.020	2
1	A	55	SER	HB2	3.841	0.020	2
1	A	57	LYS	HB2	1.984	0.020	2
1	A	57	LYS	HG2	1.297	0.020	2
1	A	57	LYS	HD2	1.565	0.020	2
1	A	57	LYS	HE2	3.171	0.020	2
1	A	58	GLU	HB2	1.669	0.020	2
1	A	58	GLU	HG2	2.015	0.020	2
1	A	59	TRP	HB2	3.438	0.020	2
1	A	60	LEU	HB2	1.131	0.020	2
1	A	61	GLN	HB2	1.911	0.020	2
1	A	61	GLN	HG2	2.315	0.020	2
1	A	63	ASP	HB2	2.599	0.020	2
1	A	64	LEU	HB2	2.273	0.020	2
1	A	67	GLN	HB2	1.86	0.020	2
1	A	67	GLN	HG2	2.147	0.020	2
1	A	68	ARG	HB2	1.545	0.020	2
1	A	68	ARG	HG2	1.708	0.020	2
1	A	68	ARG	HD2	3.22	0.020	2
1	A	69	GLN	HB2	1.651	0.020	2
1	A	69	GLN	HG2	1.811	0.020	2
1	A	74	ILE	HG12	1.278	0.020	2
1	A	76	GLN	HB2	1.814	0.020	2
1	A	76	GLN	HG2	2.294	0.020	2
1	A	79	ARG	HB2	1.595	0.020	2
1	A	79	ARG	HG2	1.286	0.020	2
1	A	79	ARG	HD2	2.941	0.020	2
1	A	80	ASP	HB2	2.45	0.020	2
1	A	81	PHE	HB2	3.274	0.020	2
1	A	83	HIS	HB2	3.213	0.020	2
1	A	84	ILE	HG12	1.638	0.020	2
1	A	85	GLN	HB2	1.864	0.020	2
1	A	85	GLN	HG2	2.156	0.020	2
1	A	86	TYR	HB2	3.455	0.020	2
1	A	89	SER	HB2	3.528	0.020	2
1	A	90	TYR	HB2	3.056	0.020	2
1	A	91	LYS	HB2	1.762	0.020	2
1	A	91	LYS	HD2	1.64	0.020	2
1	A	91	LYS	HE2	3.078	0.020	2
1	A	94	HIS	HB2	3.105	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	95	SER	HB2	3.698	0.020	2
1	A	96	ASP	HB2	2.63	0.020	2
1	A	97	ASP	HB2	2.74	0.020	2
1	A	100	GLN	HB2	1.86	0.020	2
1	A	100	GLN	HG2	2.232	0.020	2
1	A	101	TRP	HB2	2.694	0.020	2
1	A	104	TYR	HB2	2.472	0.020	2
1	A	105	GLU	HB2	1.526	0.020	2
1	A	105	GLU	HG2	2.157	0.020	2
1	A	106	GLU	HB2	1.938	0.020	2
1	A	106	GLU	HG2	2.314	0.020	2
1	A	107	GLN	HB2	2.009	0.020	2
1	A	107	GLN	HG2	2.252	0.020	2
1	A	109	SER	HB2	3.7	0.020	2
1	A	110	SER	HB2	3.633	0.020	2
1	A	111	LYS	HB2	1.781	0.020	2
1	A	111	LYS	HG2	1.283	0.020	2
1	A	111	LYS	HD2	1.227	0.020	2
1	A	113	PHE	HB2	2.253	0.020	2
1	A	114	GLN	HB2	2.07	0.020	2
1	A	114	GLN	HG2	2.392	0.020	2
1	A	116	ASN	HB2	2.957	0.020	2
1	A	117	LEU	HB2	1.514	0.020	2
1	A	118	ASP	HB2	2.831	0.020	2
1	A	119	ASN	HB2	2.43	0.020	2
1	A	120	ASN	HB2	2.668	0.020	2
1	A	121	SER	HB2	3.697	0.020	2
1	A	122	HIS	HB2	3.003	0.020	2
1	A	123	LYS	HB2	1.791	0.020	2
1	A	123	LYS	HG2	1.276	0.020	2
1	A	123	LYS	HD2	1.666	0.020	2
1	A	123	LYS	HE2	2.885	0.020	2
1	A	124	LYS	HB2	1.728	0.020	2
1	A	124	LYS	HG2	1.453	0.020	2
1	A	124	LYS	HE2	2.685	0.020	2
1	A	125	ASN	HB2	2.307	0.020	2
1	A	126	ILE	HG12	1.229	0.020	2
1	A	127	PHE	HB2	3.199	0.020	2
1	A	128	GLU	HB2	2.091	0.020	2
1	A	128	GLU	HG2	2.454	0.020	2
1	A	129	LYS	HB2	1.925	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	129	LYS	HG2	1.435	0.020	2
1	A	129	LYS	HD2	1.74	0.020	2
1	A	129	LYS	HE2	3.0	0.020	2
1	A	130	PRO	HB2	2.165	0.020	2
1	A	130	PRO	HG2	1.947	0.020	2
1	A	130	PRO	HD2	3.593	0.020	2
1	A	131	PHE	HB2	2.839	0.020	2
1	A	132	MET	HB2	1.926	0.020	2
1	A	132	MET	HG2	2.425	0.020	2
1	A	134	ARG	HG2	1.42	0.020	2
1	A	134	ARG	HD2	2.808	0.020	2
1	A	135	TYR	HB2	2.805	0.020	2
1	A	137	ARG	HB2	1.172	0.020	2
1	A	137	ARG	HG2	1.049	0.020	2
1	A	139	LEU	HB2	1.459	0.020	2
1	A	140	PRO	HB2	1.999	0.020	2
1	A	140	PRO	HG2	1.875	0.020	2
1	A	140	PRO	HD2	3.071	0.020	2
1	A	142	SER	HB2	3.553	0.020	2
1	A	143	TRP	HB2	3.276	0.020	2
1	A	144	HIS	HB2	3.814	0.020	2
1	A	145	ASN	HB2	3.427	0.020	2
1	A	146	ARG	HB2	1.054	0.020	2
1	A	146	ARG	HG2	0.84	0.020	2
1	A	146	ARG	HD2	2.259	0.020	2
1	A	147	ILE	HG12	-0.001	0.020	2
1	A	149	LEU	HB2	1.712	0.020	2
1	A	150	ARG	HB2	1.949	0.020	2
1	A	150	ARG	HG2	1.625	0.020	2
1	A	151	LEU	HB2	1.715	0.020	2
1	A	152	GLU	HB2	1.731	0.020	2
1	A	152	GLU	HG2	2.059	0.020	2
1	A	153	LEU	HB2	1.537	0.020	2
1	A	154	LEU	HB2	1.071	0.020	2
1	A	156	CYS	HB2	3.197	0.020	2
1	A	157	LEU	HB2	1.404	0.020	2
1	A	158	GLU	HB2	1.788	0.020	2
1	A	158	GLU	HG2	2.049	0.020	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	156	2.90 ± 0.21	Should be applied
$^{13}C_{\beta}$	142	2.45 ± 0.17	Should be applied
$^{13}C'$	148	3.28 ± 0.13	Should be applied
^{15}N	149	0.38 ± 0.36	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 81%, i.e. 1581 atoms were assigned a chemical shift out of a possible 1948. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	699/710 (98%)	287/289 (99%)	276/284 (97%)	136/137 (99%)
Sidechain	859/1061 (81%)	597/687 (87%)	255/325 (78%)	7/49 (14%)
Aromatic	23/177 (13%)	20/88 (23%)	0/80 (0%)	3/9 (33%)
Overall	1581/1948 (81%)	904/1064 (85%)	531/689 (77%)	146/195 (75%)

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.

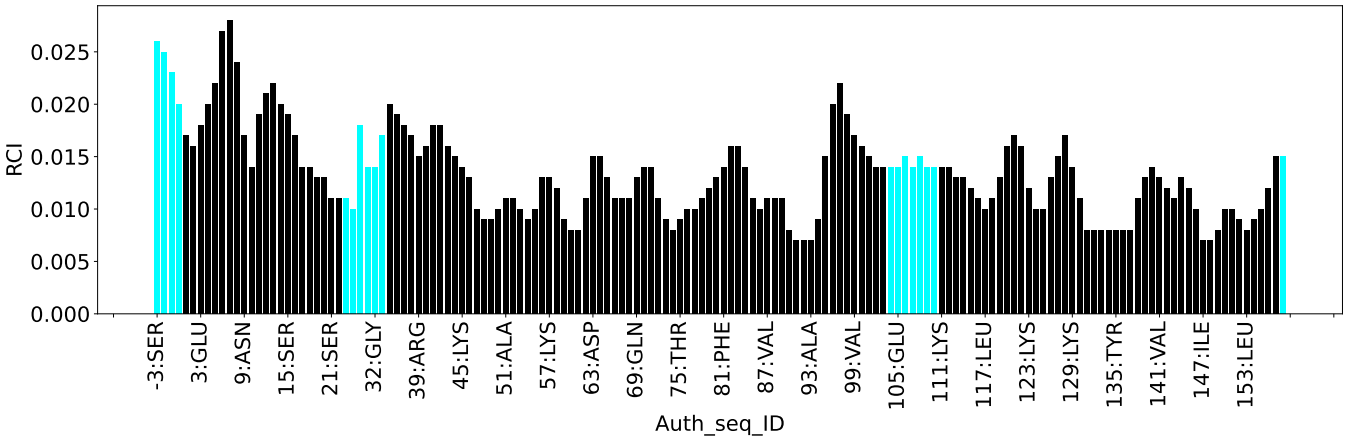
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	46	ILE	HG21	-0.90	-0.56 – 2.11	-6.3
1	A	46	ILE	HG22	-0.90	-0.56 – 2.11	-6.3
1	A	46	ILE	HG23	-0.90	-0.56 – 2.11	-6.3
1	A	98	GLY	HA3	2.02	2.08 – 5.71	-5.2
1	A	24	LYS	HE3	1.89	1.92 – 3.89	-5.2

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	2099
Intra-residue (|i-j|=0)	400
Sequential (|i-j|=1)	640
Medium range (|i-j|>1 and |i-j|<5)	180
Long range (|i-j|≥5)	676
Inter-chain	0
Hydrogen bond restraints	198
Disulfide bond restraints	5
Total dihedral-angle restraints	0
Number of unmapped restraints	688
Number of restraints per residue	12.3
Number of long range restraints per residue[1]	5.2

[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)	57.5	0.2
0.2-0.5 (Medium)	90.1	0.5
>0.5 (Large)	73.2	2.71

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

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

9 Distance violation analysis (i)

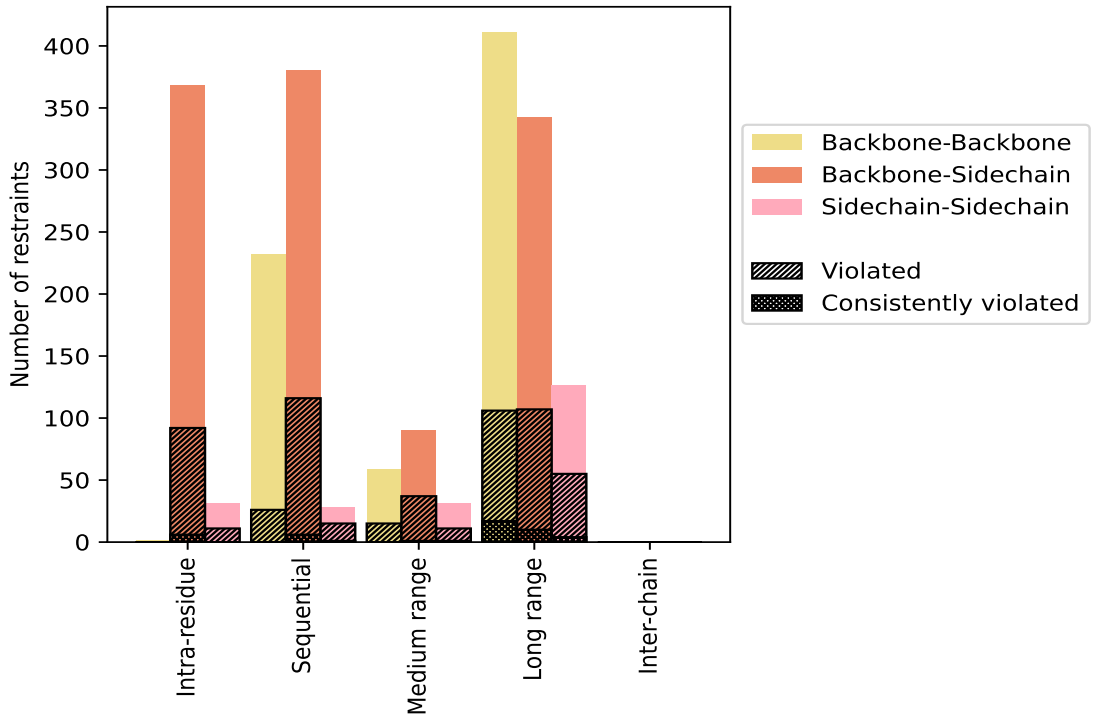
9.1 Summary of distance violations (i)

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)	400	19.1	103	25.8	4.9	6	1.5	0.3
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	368	17.5	92	25.0	4.4	6	1.6	0.3
Sidechain-Sidechain	31	1.5	11	35.5	0.5	0	0.0	0.0
Sequential (|i-j|=1)	640	30.5	157	24.5	7.5	7	1.1	0.3
Backbone-Backbone	232	11.1	26	11.2	1.2	0	0.0	0.0
Backbone-Sidechain	380	18.1	116	30.5	5.5	6	1.6	0.3
Sidechain-Sidechain	28	1.3	15	53.6	0.7	1	3.6	0.0
Medium range (|i-j|>1 & |i-j|<5)	180	8.6	63	35.0	3.0	2	1.1	0.1
Backbone-Backbone	59	2.8	15	25.4	0.7	0	0.0	0.0
Backbone-Sidechain	90	4.3	37	41.1	1.8	1	1.1	0.0
Sidechain-Sidechain	31	1.5	11	35.5	0.5	1	3.2	0.0
Long range (|i-j|≥5)	676	32.2	177	26.2	8.4	14	2.1	0.7
Backbone-Backbone	213	10.1	19	8.9	0.9	0	0.0	0.0
Backbone-Sidechain	342	16.3	107	31.3	5.1	10	2.9	0.5
Sidechain-Sidechain	121	5.8	51	42.1	2.4	4	3.3	0.2
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	198	9.4	87	43.9	4.1	17	8.6	0.8
Disulfide bond	5	0.2	4	80.0	0.2	0	0.0	0.0
Total	2099	100.0	591	28.2	28.2	46	2.2	2.2
Backbone-Backbone	703	33.5	147	20.9	7.0	17	2.4	0.8
Backbone-Sidechain	1180	56.2	352	29.8	16.8	23	1.9	1.1
Sidechain-Sidechain	216	10.3	92	42.6	4.4	6	2.8	0.3

[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



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	36	48	18	105	0	207	0.47	2.05	0.4	0.33
2	38	53	25	100	0	216	0.51	2.11	0.4	0.38
3	35	47	12	94	0	188	0.48	1.93	0.37	0.39
4	31	50	21	97	0	199	0.54	2.26	0.45	0.36
5	36	47	17	108	0	208	0.47	2.3	0.39	0.34
6	38	63	24	125	0	250	0.49	2.48	0.41	0.33
7	38	56	21	117	0	232	0.48	1.89	0.39	0.34
8	40	54	22	98	0	214	0.48	1.95	0.42	0.32
9	38	59	18	106	0	221	0.47	2.34	0.36	0.37
10	43	60	13	102	0	218	0.45	2.65	0.39	0.31
11	40	63	15	106	0	224	0.46	1.95	0.36	0.35

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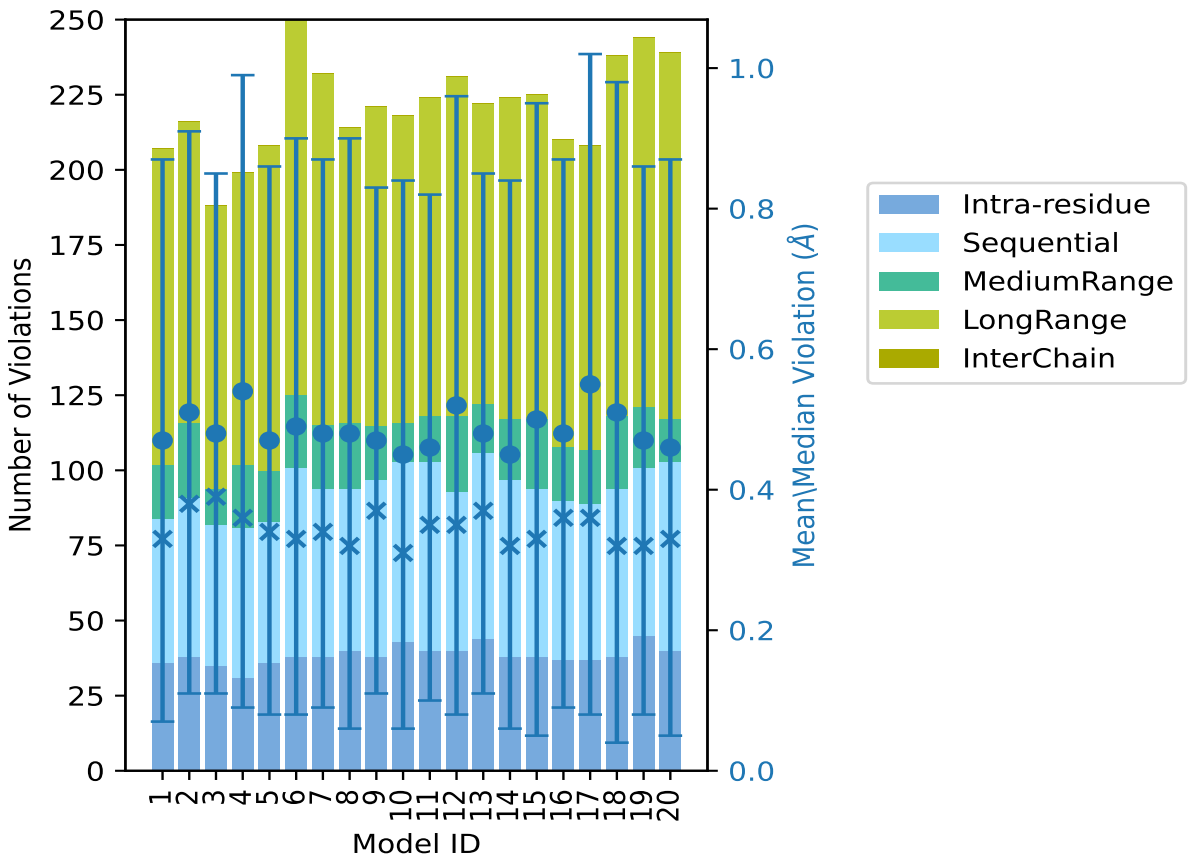
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	40	53	25	113	0	231	0.52	2.09	0.44	0.35
13	44	62	16	100	0	222	0.48	2.15	0.37	0.37
14	38	59	20	107	0	224	0.45	2.0	0.39	0.32
15	38	56	23	108	0	225	0.5	2.71	0.45	0.33
16	37	53	18	102	0	210	0.48	2.12	0.39	0.36
17	37	52	18	101	0	208	0.55	2.6	0.47	0.36
18	38	56	24	120	0	238	0.51	2.51	0.47	0.32
19	45	56	20	123	0	244	0.47	1.94	0.39	0.32
20	40	63	14	122	0	239	0.46	2.37	0.41	0.33

[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



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

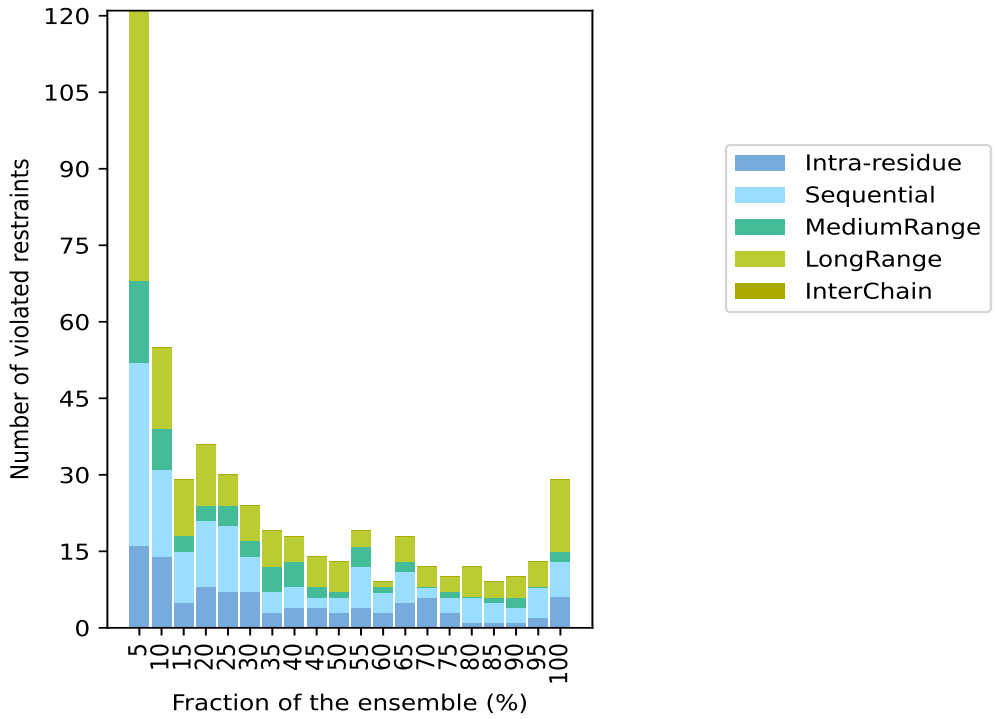
9.3 Distance violation statistics for the ensemble (i)

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, 1396(IR:297, SQ:483, MR:117, LR:499, 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]	%
16	36	16	53	0	121	1	5.0
14	17	8	16	0	55	2	10.0
5	10	3	11	0	29	3	15.0
8	13	3	12	0	36	4	20.0
7	13	4	6	0	30	5	25.0
7	7	3	7	0	24	6	30.0
3	4	5	7	0	19	7	35.0
4	4	5	5	0	18	8	40.0
4	2	2	6	0	14	9	45.0
3	3	1	6	0	13	10	50.0
4	8	4	3	0	19	11	55.0
3	4	1	1	0	9	12	60.0
5	6	2	5	0	18	13	65.0
6	2	0	4	0	12	14	70.0
3	3	1	3	0	10	15	75.0
1	5	0	6	0	12	16	80.0
1	4	1	3	0	9	17	85.0
1	3	2	4	0	10	18	90.0
2	6	0	5	0	13	19	95.0
6	7	2	14	0	29	20	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

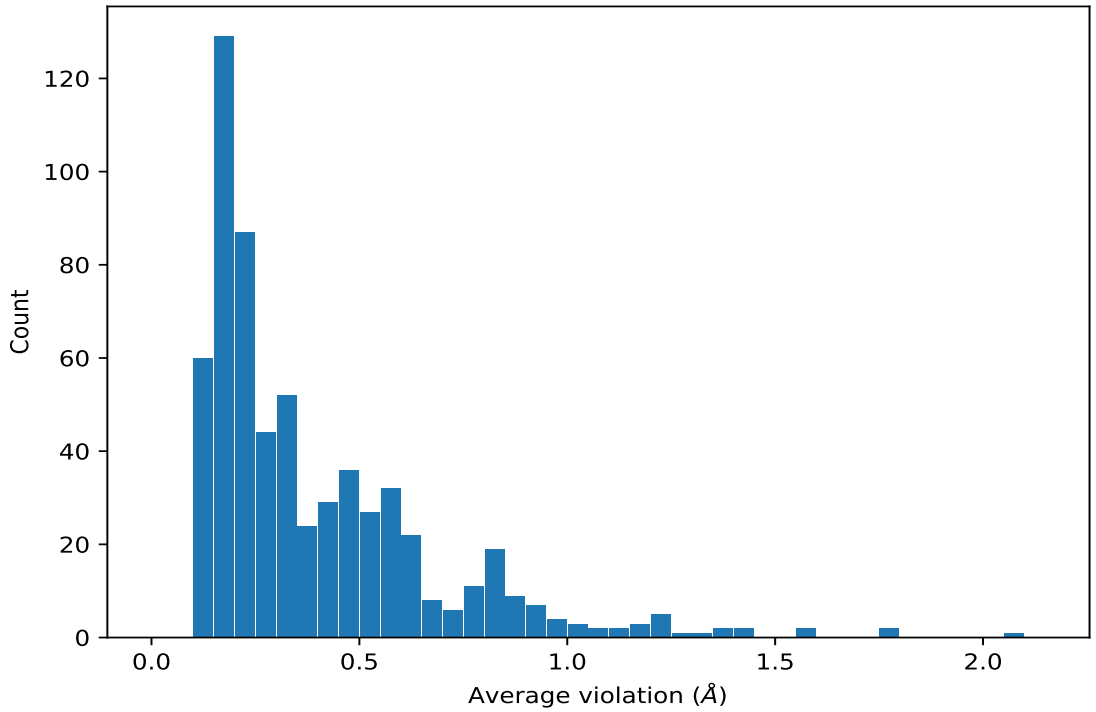
9.3.1 Bar graph : Distance violation statistics for the ensemble



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.

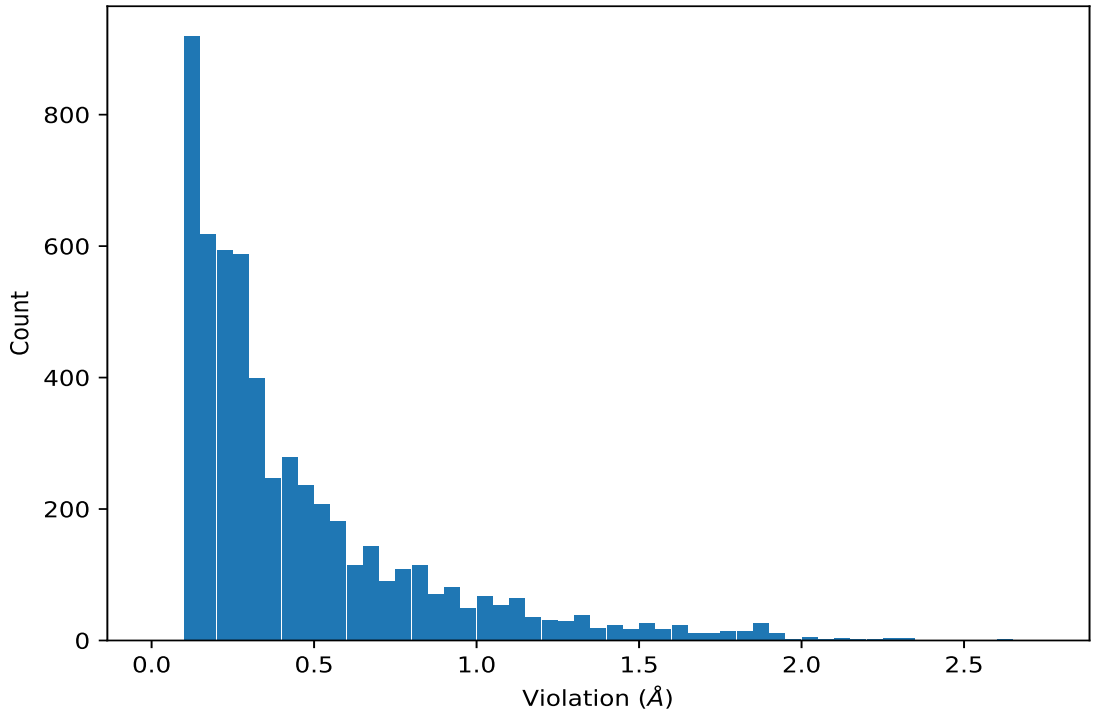
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1570)	1:A:79:ARG:H	1:A:85:GLN:HB3	20	1.78	0.18	1.88
(1,1454)	1:A:58:GLU:H	1:A:147:ILE:HG13	20	1.77	0.36	1.85
(1,1284)	1:A:14:ASP:HA	1:A:17:MET:HB3	20	1.24	0.5	1.28
(1,1469)	1:A:61:GLN:HB3	1:A:137:ARG:HB3	20	1.2	0.41	1.06
(1,1791)	1:A:122:HIS:H	1:A:123:LYS:HB3	20	1.11	0.26	1.11
(1,1357)	1:A:37:LEU:HB3	1:A:49:TRP:H	20	1.03	0.43	1.0
(1,1664)	1:A:91:LYS:HA	1:A:113:PHE:HB3	20	0.97	0.41	0.9
(1,1607)	1:A:85:GLN:HB3	1:A:148:THR:HG21	20	0.94	0.18	0.96
(1,1607)	1:A:85:GLN:HB3	1:A:148:THR:HG22	20	0.94	0.18	0.96
(1,1607)	1:A:85:GLN:HB3	1:A:148:THR:HG23	20	0.94	0.18	0.96
(1,1887)	1:A:157:LEU:H	1:A:157:LEU:HB3	20	0.89	0.1	0.9
(1,1885)	1:A:156:CYS:HB3	1:A:157:LEU:HB3	20	0.8	0.37	0.68

[1]Number of violated models, [2]Standard 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)
(1,1731)	1:A:105:GLU:HG3	1:A:110:SER:HB3	15	2.71
(1,1514)	1:A:68:ARG:HD3	1:A:157:LEU:HB3	10	2.65
(1,1514)	1:A:68:ARG:HD3	1:A:157:LEU:HB3	17	2.6
(1,1731)	1:A:105:GLU:HG3	1:A:110:SER:HB3	18	2.51
(1,1514)	1:A:68:ARG:HD3	1:A:157:LEU:HB3	6	2.48
(1,1377)	1:A:39:ARG:HD3	1:A:42:ASN:HB3	20	2.37
(1,1514)	1:A:68:ARG:HD3	1:A:157:LEU:HB3	9	2.34
(1,1731)	1:A:105:GLU:HG3	1:A:110:SER:HB3	10	2.31
(1,1514)	1:A:68:ARG:HD3	1:A:157:LEU:HB3	18	2.31
(1,1514)	1:A:68:ARG:HD3	1:A:157:LEU:HB3	5	2.3

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value