wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	6U4M
BMRB ID	:	30658
Title	:	Solution structure of paxillin LIM4
Authors	:	Zhu, L.; Qin, J.
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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 (1)) were used in the production of this report:

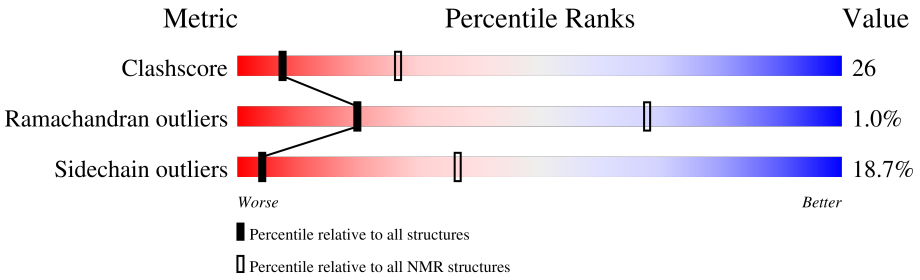
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 82%.

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	72	40% 33% 8% 8% 10%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 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:547-A:605 (59)	0.20	17

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1043 atoms, of which 516 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Paxillin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	65	1041	333	516	95	88	9	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	GLY	-	expression tag	UNP P49023
A	535	ALA	-	expression tag	UNP P49023
A	536	MET	-	expression tag	UNP P49023
A	537	ASP	-	expression tag	UNP P49023
A	538	PRO	-	expression tag	UNP P49023
A	539	GLU	-	expression tag	UNP P49023
A	540	PHE	-	expression tag	UNP P49023

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

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: Paxillin

Chain A: 40% 33% 8% 8% 10%

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

The representative model is number 17. Colouring as in section 4.1 above.

- Molecule 1: Paxillin

Chain A: 39% 36% 7% 8% 10%

5 Refinement protocol and experimental data overview (i)

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
X-PLOR NIH	structure calculation	
X-PLOR NIH	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	769
Number of shifts mapped to atoms	714
Number of unparsed shifts	0
Number of shifts with mapping errors	55
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	468	465	465	24±2
All	All	9400	9300	9300	487

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 26.

5 of 53 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:582:LEU:HD11	1:A:596:CYS:HA	0.68	1.65	20	20
1:A:598:ASN:ND2	1:A:598:ASN:H	0.63	1.91	17	2
1:A:561:ILE:HG21	1:A:573:PHE:CD2	0.63	2.28	7	9
1:A:561:ILE:HG21	1:A:573:PHE:CD1	0.61	2.30	4	9
1:A:564:MET:O	1:A:565:ALA:HB3	0.58	1.98	15	20

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	58/72 (81%)	45±1 (78±2%)	12±1 (21±2%)	1±1 (1±1%)	20	68
All	All	1160/1440 (81%)	906 (78%)	242 (21%)	12 (1%)	20	68

All 3 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	570	PRO	7
1	A	547	SER	4
1	A	585	GLY	1

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	53/63 (84%)	43±1 (81±2%)	10±1 (19±2%)	4	36
All	All	1060/1260 (84%)	862 (81%)	198 (19%)	4	36

5 of 15 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	547	SER	20
1	A	549	CYS	20
1	A	580	LYS	20
1	A	581	GLN	20
1	A	587	PHE	20

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 82% for the well-defined parts and 80% 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 (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	769
Number of shifts mapped to atoms	714
Number of unparsed shifts	0
Number of shifts with mapping errors	55
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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 55) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	535	ALA	HA	4.112	0.03	1
1	A	535	ALA	HB1	1.265	0.03	1
1	A	535	ALA	HB2	1.265	0.03	1
1	A	535	ALA	HB3	1.265	0.03	1
1	A	535	ALA	C	177.592	0.50	1
1	A	535	ALA	CA	52.788	0.50	1
1	A	535	ALA	CB	18.966	0.50	1
1	A	536	MET	H	8.349	0.03	1
1	A	536	MET	HA	4.37	0.03	1
1	A	536	MET	HB2	1.95	0.03	2
1	A	536	MET	HB3	1.845	0.03	2
1	A	536	MET	HG2	2.427	0.03	2
1	A	536	MET	HG3	2.355	0.03	2
1	A	536	MET	C	175.441	0.50	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	536	MET	CA	54.718	0.50	1
1	A	536	MET	CB	32.15	0.50	1
1	A	536	MET	CG	32.27	0.50	1
1	A	536	MET	N	118.129	0.25	1
1	A	537	ASP	H	8.056	0.03	1
1	A	537	ASP	HA	4.718	0.03	1
1	A	537	ASP	HB2	2.634	0.03	2
1	A	537	ASP	HB3	2.461	0.03	2
1	A	537	ASP	CA	52.519	0.50	1
1	A	537	ASP	CB	40.591	0.50	1
1	A	537	ASP	N	123.081	0.25	1
1	A	538	PRO	HA	4.227	0.03	1
1	A	538	PRO	HB2	2.142	0.03	2
1	A	538	PRO	HG2	1.898	0.03	2
1	A	538	PRO	HG3	1.755	0.03	2
1	A	538	PRO	HD2	3.755	0.03	2
1	A	538	PRO	HD3	3.624	0.03	2
1	A	538	PRO	C	176.991	0.50	1
1	A	538	PRO	CA	63.553	0.50	1
1	A	538	PRO	CB	31.831	0.50	1
1	A	538	PRO	CG	27.156	0.50	1
1	A	538	PRO	CD	50.515	0.50	1
1	A	539	GLU	H	8.415	0.03	1
1	A	539	GLU	HA	3.991	0.03	1
1	A	539	GLU	HB2	1.932	0.03	2
1	A	539	GLU	HB3	1.746	0.03	2
1	A	539	GLU	HG2	2.048	0.03	2
1	A	539	GLU	HG3	1.943	0.03	2
1	A	539	GLU	C	176.251	0.50	1
1	A	539	GLU	CA	56.892	0.50	1
1	A	539	GLU	CB	29.582	0.50	1
1	A	539	GLU	CG	36.09	0.50	1
1	A	539	GLU	N	119.47	0.25	1
1	A	540	PHE	H	7.893	0.03	1
1	A	540	PHE	HA	4.443	0.03	1
1	A	540	PHE	HB2	2.898	0.03	2
1	A	540	PHE	HB3	2.848	0.03	2
1	A	540	PHE	C	175.303	0.50	1
1	A	540	PHE	CA	57.948	0.50	1
1	A	540	PHE	CB	39.638	0.50	1
1	A	540	PHE	N	119.35	0.25	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	71	-0.00 ± 0.19	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	67	0.30 ± 0.29	None needed (< 0.5 ppm)
$^{13}C'$	65	0.43 ± 0.18	None needed (< 0.5 ppm)
^{15}N	65	0.20 ± 0.51	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 82%, i.e. 660 atoms were assigned a chemical shift out of a possible 801. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	285/292 (98%)	117/118 (99%)	113/118 (96%)	55/56 (98%)
Sidechain	375/426 (88%)	248/275 (90%)	120/133 (90%)	7/18 (39%)
Aromatic	0/83 (0%)	0/42 (0%)	0/39 (0%)	0/2 (0%)
Overall	660/801 (82%)	365/435 (84%)	233/290 (80%)	62/76 (82%)

7.1.4 Statistically unusual chemical shifts (i)

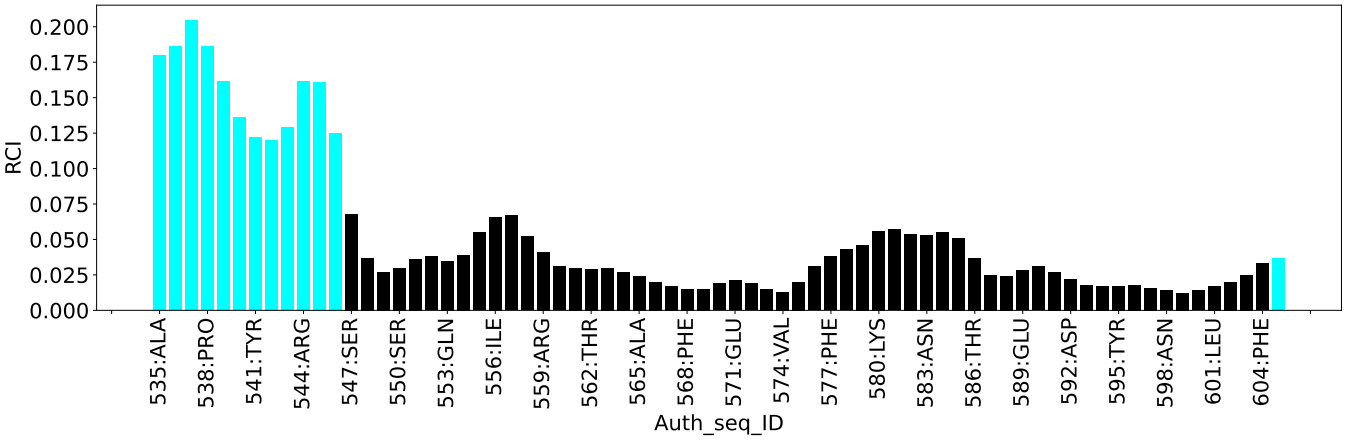
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	603	LEU	HB3	-0.48	-0.26 – 3.31	-5.6
1	A	590	GLN	HB3	0.57	0.71 – 3.33	-5.5

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
535:ALA
538:PRO
541:TYR
544:ARG
547:SER
550:SER
553:GLN
556:ILE
559:ARG
562:THR
565:ALA
568:PHE
571:GLU
574:VAL
577:PHE
580:LYS
583:ASN
586:THR
589:GLU
592:ASP
595:TYR
598:ASN
601:LEU
604:PHE
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	3149
Intra-residue (|i-j|=0)	754
Sequential (|i-j|=1)	1006
Medium range (|i-j|>1 and |i-j|<5)	541
Long range (|i-j|≥5)	848
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	120
Number of restraints per residue	43.7
Number of long range restraints per residue[1]	11.8

[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 (i)

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 (i)

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)	108.7	0.2
0.2-0.5 (Medium)	156.7	0.5
>0.5 (Large)	35.4	1.87

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)

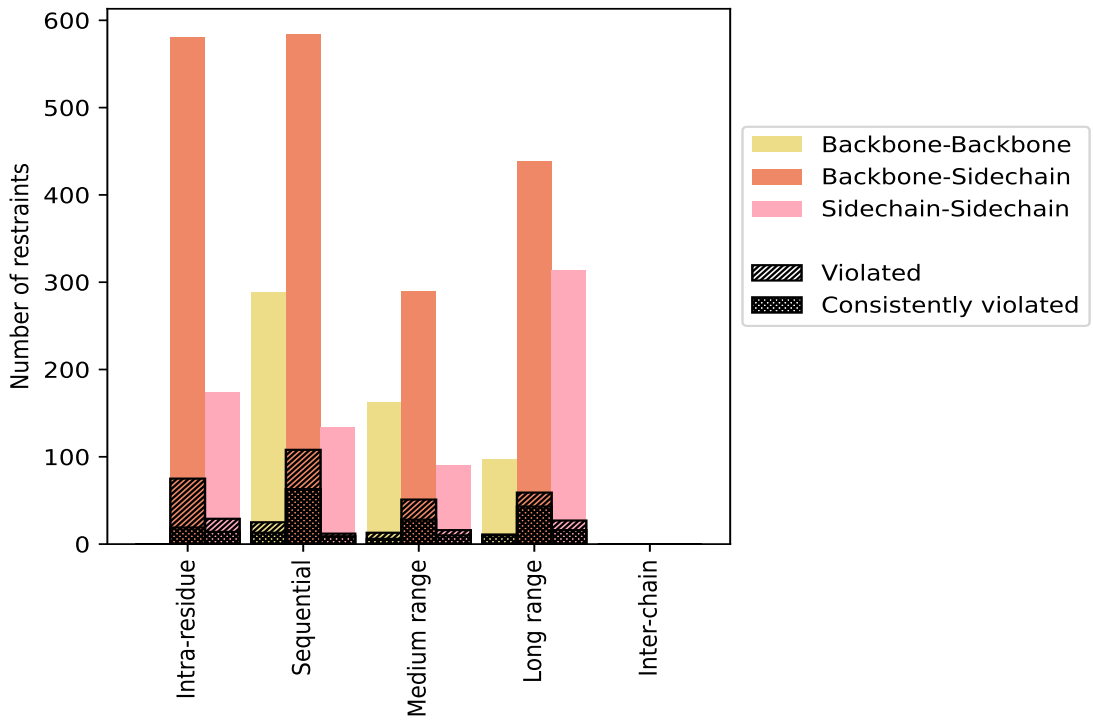
9.1 Summary of distance violations (i)

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)	754	23.9	104	13.8	3.3	33	4.4	1.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	580	18.4	75	12.9	2.4	19	3.3	0.6
Sidechain-Sidechain	174	5.5	29	16.7	0.9	14	8.0	0.4
Sequential (|i-j|=1)	1006	31.9	145	14.4	4.6	85	8.4	2.7
Backbone-Backbone	288	9.1	25	8.7	0.8	13	4.5	0.4
Backbone-Sidechain	584	18.5	108	18.5	3.4	63	10.8	2.0
Sidechain-Sidechain	134	4.3	12	9.0	0.4	9	6.7	0.3
Medium range (|i-j|>1 & |i-j|<5)	541	17.2	80	14.8	2.5	44	8.1	1.4
Backbone-Backbone	162	5.1	13	8.0	0.4	6	3.7	0.2
Backbone-Sidechain	289	9.2	51	17.6	1.6	28	9.7	0.9
Sidechain-Sidechain	90	2.9	16	17.8	0.5	10	11.1	0.3
Long range (|i-j|≥5)	848	26.9	97	11.4	3.1	69	8.1	2.2
Backbone-Backbone	97	3.1	11	11.3	0.3	10	10.3	0.3
Backbone-Sidechain	438	13.9	59	13.5	1.9	43	9.8	1.4
Sidechain-Sidechain	313	9.9	27	8.6	0.9	16	5.1	0.5
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	3149	100.0	426	13.5	13.5	231	7.3	7.3
Backbone-Backbone	547	17.4	49	9.0	1.6	29	5.3	0.9
Backbone-Sidechain	1891	60.1	293	15.5	9.3	153	8.1	4.9
Sidechain-Sidechain	711	22.6	84	11.8	2.7	49	6.9	1.6

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	54	100	57	82	0	293	0.31	1.83	0.23	0.25
2	50	105	61	83	0	299	0.33	1.8	0.27	0.26
3	51	111	56	82	0	300	0.31	1.81	0.23	0.26
4	60	112	57	79	0	308	0.29	1.58	0.2	0.24
5	50	109	60	81	0	300	0.3	1.83	0.23	0.25
6	48	109	55	81	0	293	0.31	1.8	0.23	0.26
7	58	108	62	79	0	307	0.31	1.81	0.23	0.25
8	52	102	58	81	0	293	0.31	1.8	0.23	0.26
9	54	105	57	78	0	294	0.31	1.82	0.23	0.25
10	54	102	61	83	0	300	0.33	1.8	0.26	0.26
11	59	111	66	82	0	318	0.32	1.79	0.26	0.26

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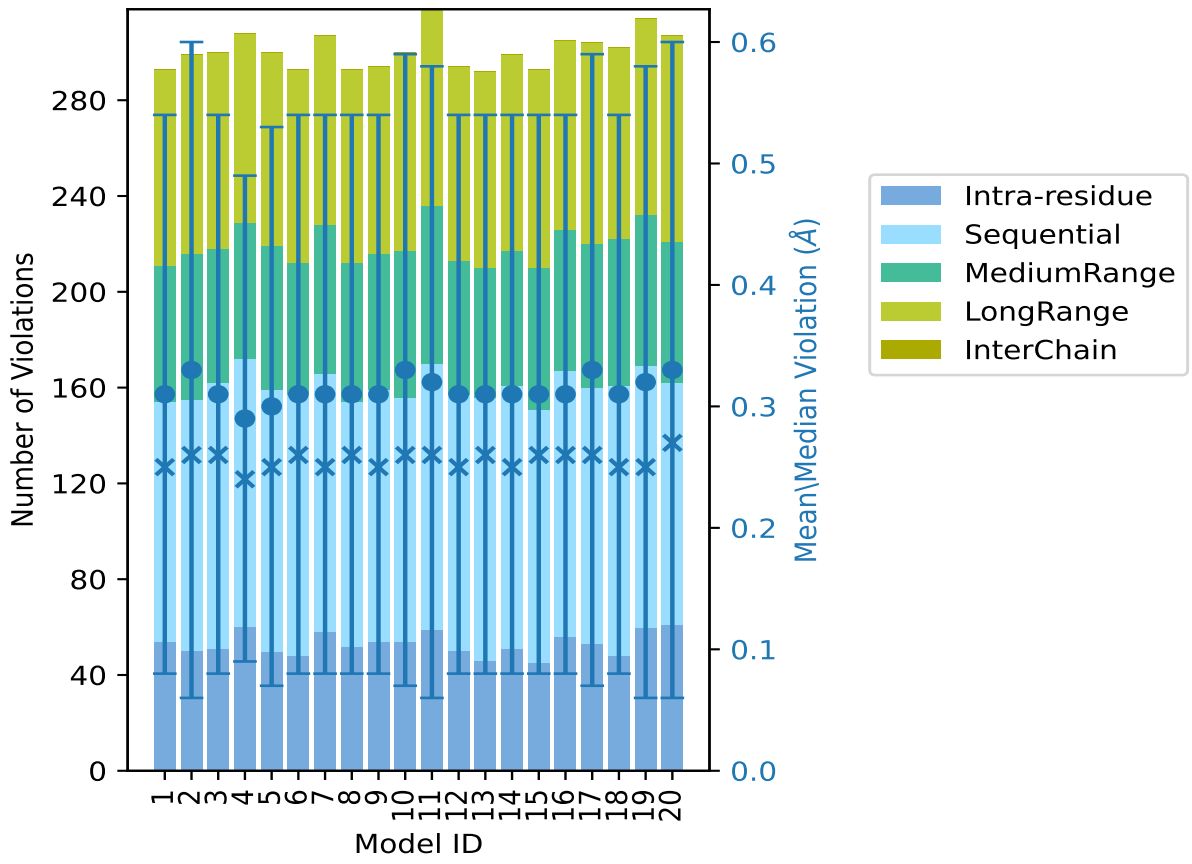
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	50	107	56	81	0	294	0.31	1.87	0.23	0.25
13	46	110	54	82	0	292	0.31	1.78	0.23	0.26
14	51	110	56	82	0	299	0.31	1.82	0.23	0.25
15	45	106	59	83	0	293	0.31	1.87	0.23	0.26
16	56	111	59	79	0	305	0.31	1.84	0.23	0.26
17	53	107	60	84	0	304	0.33	1.79	0.26	0.26
18	48	113	61	80	0	302	0.31	1.87	0.23	0.25
19	60	109	63	82	0	314	0.32	1.79	0.26	0.25
20	61	101	59	86	0	307	0.33	1.79	0.27	0.27

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

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

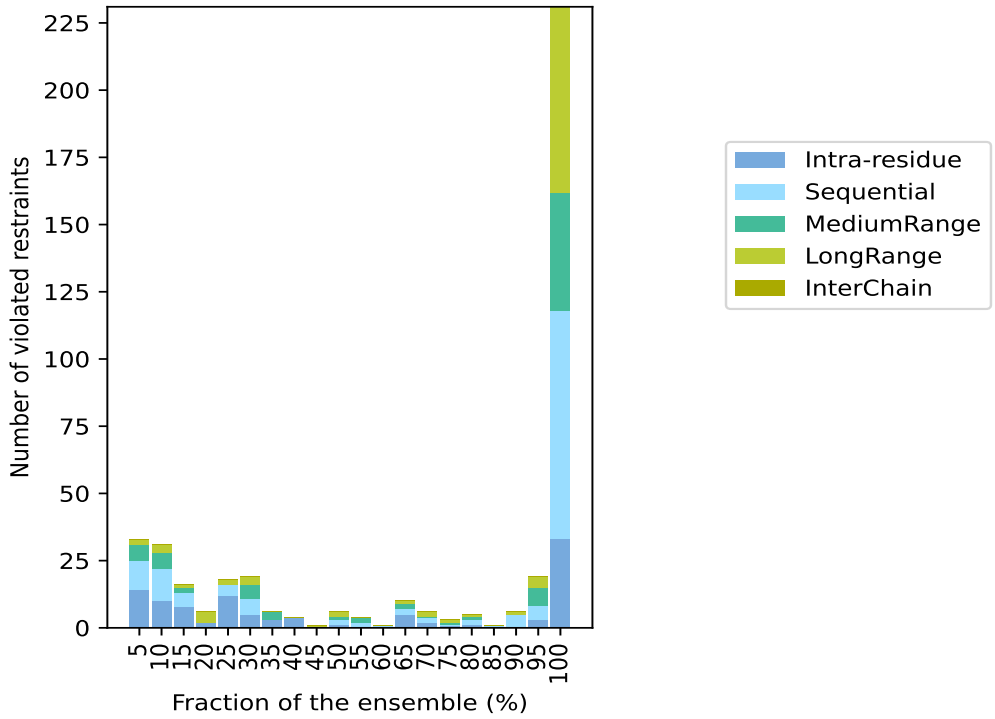
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2723(IR:650, SQ:861, MR:461, LR:751, 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]	%
14	11	6	2	0	33	1	5.0
10	12	6	3	0	31	2	10.0
8	5	2	1	0	16	3	15.0
2	0	0	4	0	6	4	20.0
12	4	0	2	0	18	5	25.0
5	6	5	3	0	19	6	30.0
3	0	3	0	0	6	7	35.0
4	0	0	0	0	4	8	40.0
0	0	0	1	0	1	9	45.0
1	2	1	2	0	6	10	50.0
0	2	2	0	0	4	11	55.0
0	1	0	0	0	1	12	60.0
5	2	2	1	0	10	13	65.0
2	2	0	2	0	6	14	70.0
1	0	1	1	0	3	15	75.0
1	2	1	1	0	5	16	80.0
0	1	0	0	0	1	17	85.0
0	5	0	1	0	6	18	90.0
3	5	7	4	0	19	19	95.0
33	85	44	69	0	231	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

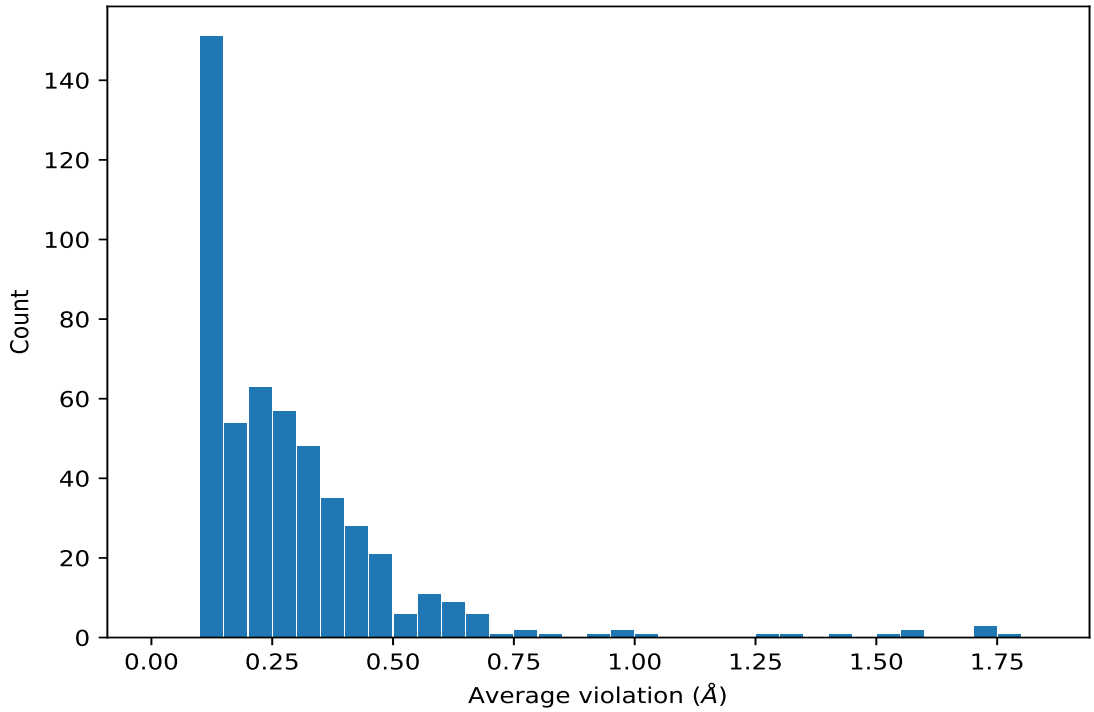
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

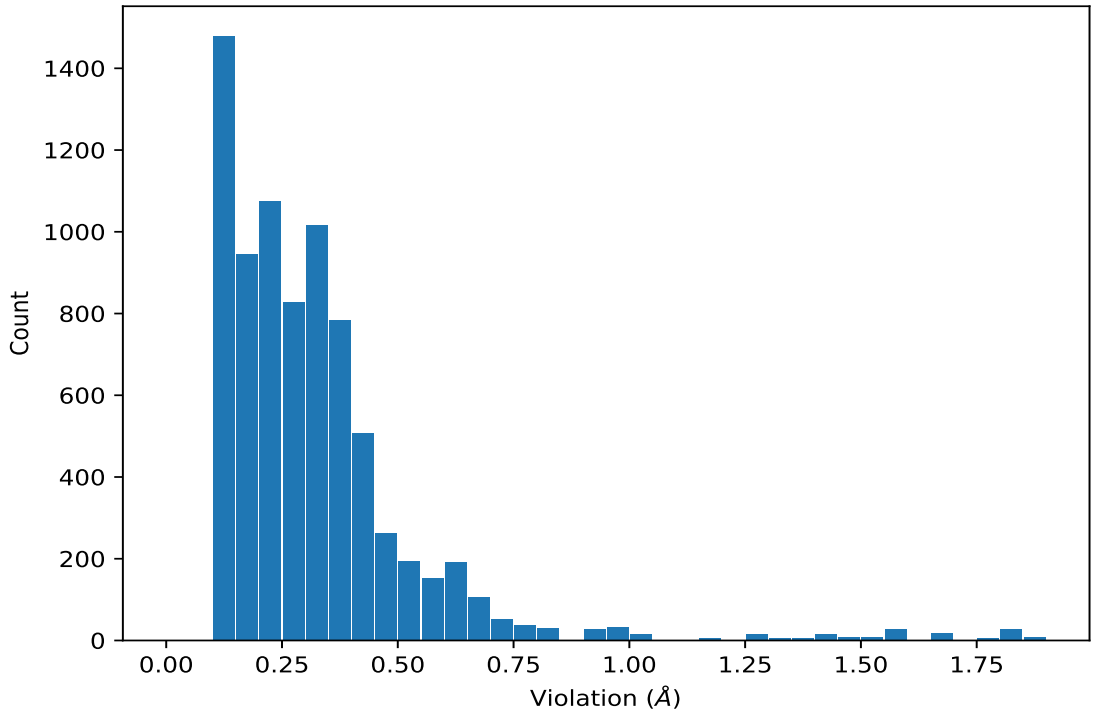
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	20	1.72	0.25	1.81
(2,167)	1:A:548:LEU:HD12	1:A:553:GLN:HE22	20	1.72	0.25	1.81
(2,167)	1:A:548:LEU:HD13	1:A:553:GLN:HE22	20	1.72	0.25	1.81
(2,286)	1:A:551:GLY:HA2	1:A:572:HIS:HB2	20	1.58	0.01	1.58
(2,285)	1:A:551:GLY:HA2	1:A:572:HIS:HB3	20	1.44	0.02	1.44
(2,288)	1:A:551:GLY:H	1:A:572:HIS:HB2	20	1.26	0.02	1.26
(2,287)	1:A:551:GLY:H	1:A:572:HIS:HB3	20	1.0	0.03	1.0
(2,303)	1:A:552:CYS:H	1:A:569:HIS:HB3	20	0.98	0.01	0.98
(2,619)	1:A:565:ALA:H	1:A:566:LYS:HB3	20	0.96	0.03	0.95
(2,849)	1:A:575:CYS:HB2	1:A:580:LYS:H	20	0.92	0.01	0.92
(2,304)	1:A:552:CYS:H	1:A:569:HIS:HB2	20	0.81	0.01	0.81
(2,431)	1:A:558:GLY:H	1:A:570:PRO:HG2	20	0.79	0.02	0.78

[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)
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	12	1.87
(2,167)	1:A:548:LEU:HD12	1:A:553:GLN:HE22	12	1.87
(2,167)	1:A:548:LEU:HD13	1:A:553:GLN:HE22	12	1.87
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	15	1.87
(2,167)	1:A:548:LEU:HD12	1:A:553:GLN:HE22	15	1.87
(2,167)	1:A:548:LEU:HD13	1:A:553:GLN:HE22	15	1.87
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	18	1.87
(2,167)	1:A:548:LEU:HD12	1:A:553:GLN:HE22	18	1.87
(2,167)	1:A:548:LEU:HD13	1:A:553:GLN:HE22	18	1.87
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	16	1.84
(2,167)	1:A:548:LEU:HD12	1:A:553:GLN:HE22	16	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,167)	1:A:548:LEU:HD13	1:A:553:GLN:HE22	16	1.84
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	1	1.83
(2,167)	1:A:548:LEU:HD12	1:A:553:GLN:HE22	1	1.83
(2,167)	1:A:548:LEU:HD13	1:A:553:GLN:HE22	1	1.83
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	5	1.83
(2,167)	1:A:548:LEU:HD12	1:A:553:GLN:HE22	5	1.83
(2,167)	1:A:548:LEU:HD13	1:A:553:GLN:HE22	5	1.83
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	9	1.82
(2,167)	1:A:548:LEU:HD12	1:A:553:GLN:HE22	9	1.82
(2,167)	1:A:548:LEU:HD13	1:A:553:GLN:HE22	9	1.82
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	14	1.82
(2,167)	1:A:548:LEU:HD12	1:A:553:GLN:HE22	14	1.82
(2,167)	1:A:548:LEU:HD13	1:A:553:GLN:HE22	14	1.82
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	3	1.81
(2,167)	1:A:548:LEU:HD12	1:A:553:GLN:HE22	3	1.81
(2,167)	1:A:548:LEU:HD13	1:A:553:GLN:HE22	3	1.81
(2,167)	1:A:548:LEU:HD11	1:A:553:GLN:HE22	7	1.81

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found