wwPDB NMR Structure Validation Summary Report (i)

Oct 15, 2026 – 05:01 pm BST

PDB ID	:	31DM / pdb_000031dm
BMRB ID	:	53778
Title	:	Holo form of calmodulin-like domain of human alpha-actinin-4
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Deposited on	:	2026-05-27

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:

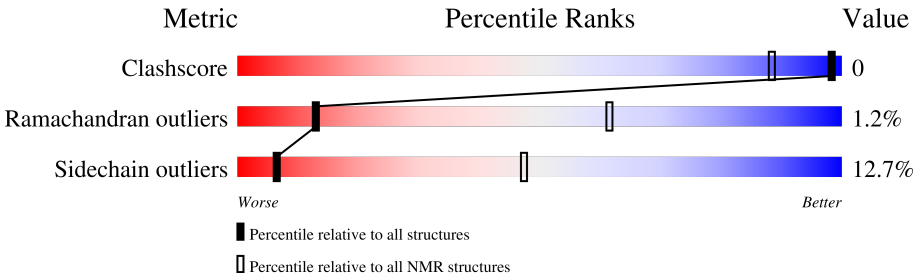
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.3.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 92%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	153	77% 8% 15%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:762-A:837 (76)	1.19	16
2	A:853-A:906 (54)	0.66	9

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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2310 atoms, of which 1115 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-actinin-4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	153	2309	745	1115	198	245	6	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	759	GLY	-	expression tag	UNP O43707
A	760	SER	-	expression tag	UNP O43707
A	761	SER	-	expression tag	UNP O43707

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	1	1	1

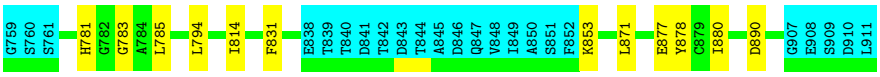
4 Residue-property plots (i)

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: Alpha-actinin-4

Chain A: 77% 8% 15%



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

The representative model is number 16. Colouring as in section 4.1 above.

- Molecule 1: Alpha-actinin-4

Chain A: 73% 12% 15%

5 Refinement protocol and experimental data overview (i)

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	**Classification**	**Version**
YASARA	refinement	14.7.17
ARTINA	structure calculation	
YASARA	structure calculation	14.7.17

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	1848
Number of shifts mapped to atoms	1847
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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: CA

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	0.83±0.04	1±1/1055 (0.1± 0.1%)	0.98±0.04	1±1/1425 (0.1± 0.1%)
All	All	0.83	14/21100 (0.1%)	0.98	25/28500 (0.1%)

5 of 11 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	779	LYS	N-CA	8.37	1.56	1.46	9	2
1	A	780	ASP	CA-C	6.87	1.61	1.52	12	3
1	A	832	ILE	CA-CB	6.82	1.62	1.54	8	1
1	A	781	HIS	ND1-CE1	6.73	1.39	1.32	15	1
1	A	779	LYS	CA-C	-6.04	1.44	1.52	1	1

5 of 13 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	832	ILE	CB-CA-C	-9.48	99.60	112.02	8	1
1	A	871	LEU	CA-C-N	-8.58	113.39	119.66	20	5
1	A	871	LEU	C-N-CA	-8.58	113.39	119.66	20	5
1	A	780	ASP	CA-CB-CG	7.38	119.98	112.60	15	1
1	A	778	ASP	N-CA-CB	6.94	119.20	110.45	2	1

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	1030	973	973	1±1
All	All	20620	19460	19460	14

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 0.

5 of 10 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:778:ASP:OD1	1:A:785:LEU:HD12	0.49	2.07	8	2
1:A:886:TYR:CE2	1:A:890:ASP:HB2	0.46	2.46	7	2
1:A:804:ASP:CG	1:A:805:ARG:N	0.45	2.74	18	3
1:A:882:ARG:HD3	1:A:903:THR:HG22	0.45	1.88	9	1
1:A:765:GLU:H	1:A:765:GLU:CD	0.43	2.20	19	1

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	130/153 (85%)	124±1 (95±1%)	4±1 (3±1%)	2±1 (1±1%)	13	61
All	All	2600/3060 (85%)	2481 (95%)	88 (3%)	31 (1%)	13	61

All 5 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	783	GLY	18
1	A	804	ASP	6
1	A	801	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	906	TYR	2
1	A	891	ALA	2

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	108/127 (85%)	94±2 (87±2%)	14±2 (13±2%)	6 47
All	All	2160/2540 (85%)	1886 (87%)	274 (13%)	6 47

5 of 51 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	814	ILE	20
1	A	831	PHE	19
1	A	880	ILE	17
1	A	785	LEU	14
1	A	794	LEU	13

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)

Of 1 ligands modelled in this entry, 1 is 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 92% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *flya*

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	1848
Number of shifts mapped to atoms	1847
Number of unparsed shifts	0
Number of shifts with mapping errors	1
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. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	759	GLY	H	8.588	0.010	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
$^{13}C_{\alpha}$	153	-0.24 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	142	0.16 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	152	-0.23 ± 0.18	None needed (< 0.5 ppm)
^{15}N	146	0.13 ± 0.24	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 92%, i.e. 1605 atoms were assigned a chemical shift out of a possible 1739. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	644/645 (100%)	262/262 (100%)	259/260 (100%)	123/123 (100%)
Sidechain	834/928 (90%)	571/599 (95%)	251/291 (86%)	12/38 (32%)
Aromatic	127/166 (77%)	79/82 (96%)	45/81 (56%)	3/3 (100%)
Overall	1605/1739 (92%)	912/943 (97%)	555/632 (88%)	138/164 (84%)

7.1.4 Statistically unusual chemical shifts (i)

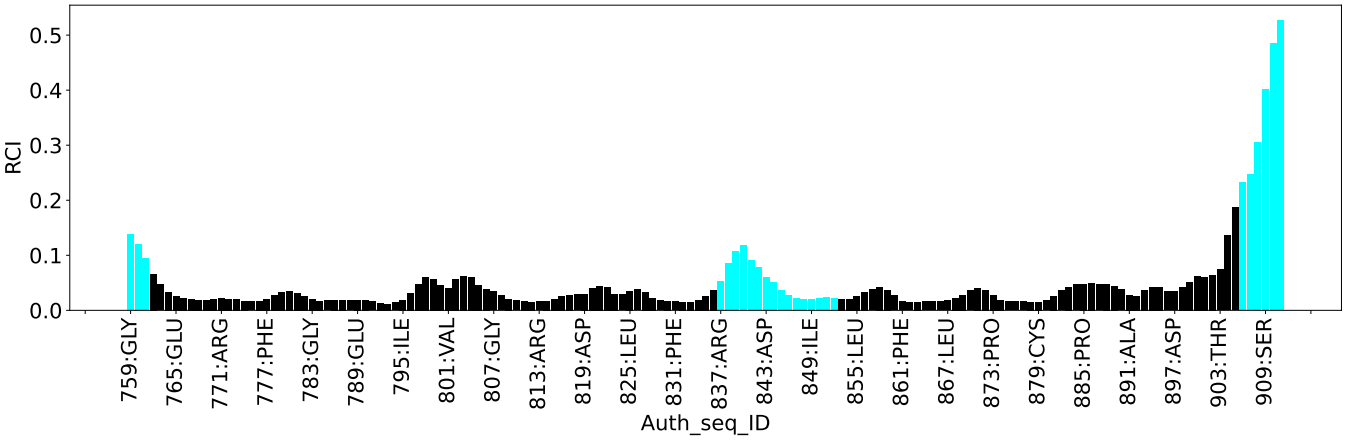
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	901	PHE	HD1	1.79	5.51 – 8.60	-17.1
1	A	835	MET	CE	27.65	8.39 – 25.85	6.0
1	A	810	GLU	HB2	0.83	1.00 – 3.05	-5.8
1	A	774	PHE	HE2	8.71	5.54 – 8.63	5.2
1	A	908	GLU	HB3	3.09	0.95 – 3.05	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:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
759:GLY
765:GLU
771:ARG
777:PHE
783:GLY
789:GLU
795:ILE
801:VAL
807:GLY
813:ARG
819:ASP
825:LEU
831:PHE
837:ARG
843:ASP
849:ILE
855:LEU
861:PHE
867:LEU
873:PRO
879:CYS
885:PRO
891:ALA
897:ASP
903:THR
909:SER
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	1924
Intra-residue (|i-j|=0)	582
Sequential (|i-j|=1)	520
Medium range (|i-j|>1 and |i-j|<5)	424
Long range (|i-j|≥5)	393
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	12.5
Number of long range restraints per residue[1]	2.6

[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)	0.9	0.19
0.2-0.5 (Medium)	1.0	0.5
>0.5 (Large)	3.5	1.5

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)

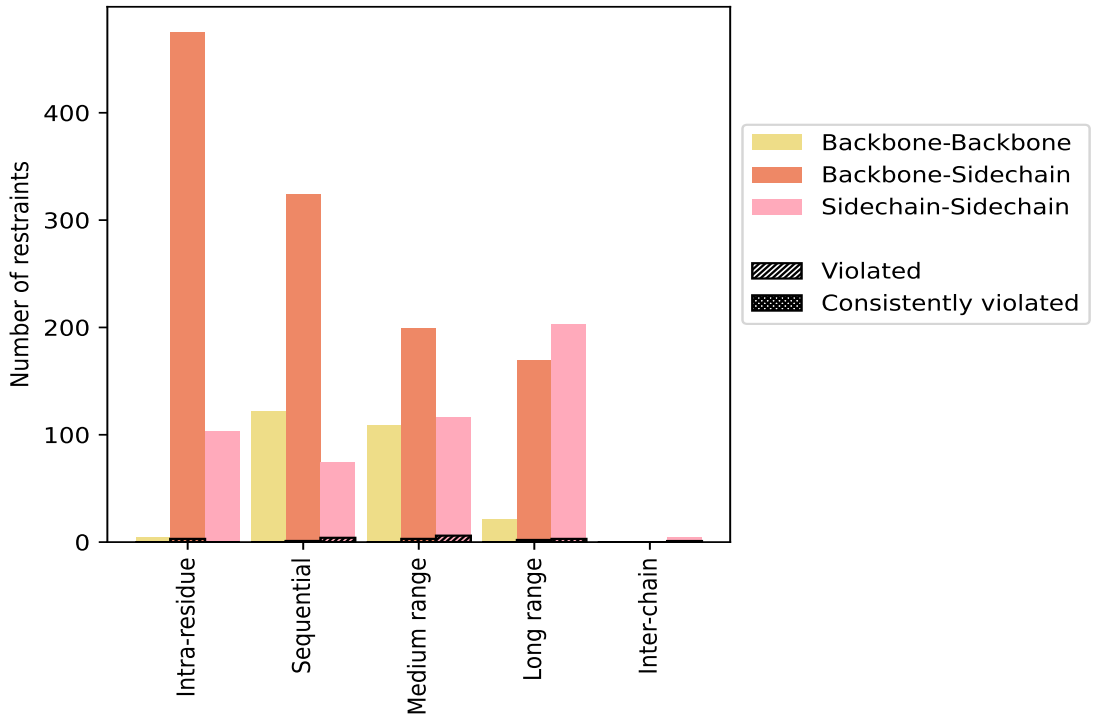
9.1 Summary of distance violations (i)

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)	582	30.2	3	0.5	0.2	0	0.0	0.0
Backbone-Backbone	4	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	475	24.7	3	0.6	0.2	0	0.0	0.0
Sidechain-Sidechain	103	5.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	520	27.0	5	1.0	0.3	1	0.2	0.1
Backbone-Backbone	122	6.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	324	16.8	1	0.3	0.1	1	0.3	0.1
Sidechain-Sidechain	74	3.8	4	5.4	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	424	22.0	9	2.1	0.5	0	0.0	0.0
Backbone-Backbone	109	5.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	199	10.3	3	1.5	0.2	0	0.0	0.0
Sidechain-Sidechain	116	6.0	6	5.2	0.3	0	0.0	0.0
Long range (|i-j|≥5)	393	20.4	5	1.3	0.3	0	0.0	0.0
Backbone-Backbone	21	1.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	169	8.8	2	1.2	0.1	0	0.0	0.0
Sidechain-Sidechain	203	10.6	3	1.5	0.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1924	100.0	23	1.2	1.2	1	0.1	0.1
Backbone-Backbone	256	13.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1168	60.7	9	0.8	0.5	1	0.1	0.1
Sidechain-Sidechain	500	26.0	14	2.8	0.7	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations (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	2	3	1	0	0	6	0.62	1.12	0.39	0.53
2	0	2	3	0	0	5	0.7	1.14	0.3	0.65
3	0	1	4	0	0	5	0.96	1.14	0.26	1.08
4	2	3	1	3	0	9	0.49	1.13	0.39	0.22
5	0	2	3	1	0	6	0.67	1.15	0.41	0.72
6	0	4	4	0	1	9	0.76	1.5	0.54	0.88
7	0	3	2	0	0	5	0.7	1.09	0.42	0.97
8	1	3	4	0	0	8	0.56	1.14	0.34	0.52
9	0	2	2	0	0	4	0.7	0.97	0.27	0.78
10	0	2	3	1	0	6	0.56	1.13	0.41	0.47

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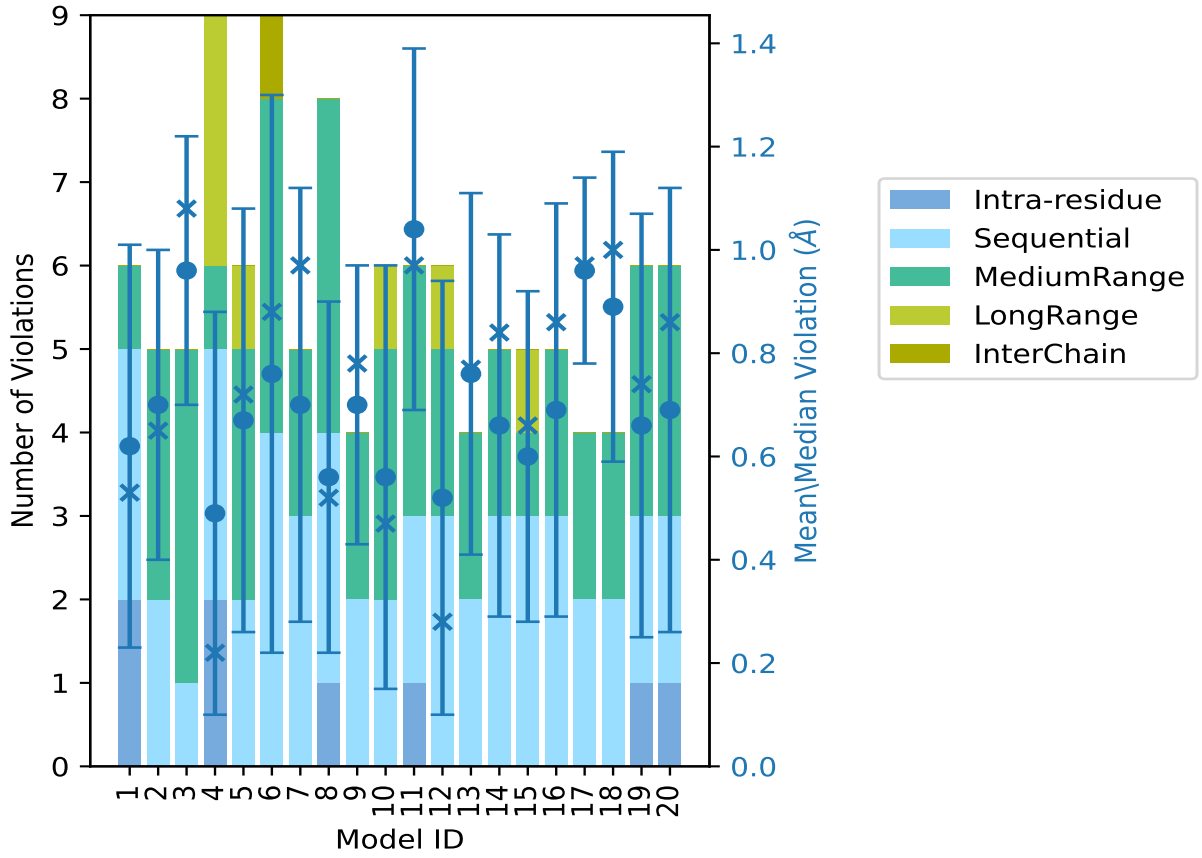
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	1	2	3	0	0	6	1.04	1.48	0.35	0.97
12	0	3	2	1	0	6	0.52	1.15	0.42	0.28
13	0	2	2	0	0	4	0.76	1.14	0.35	0.77
14	0	3	2	0	0	5	0.66	1.12	0.37	0.84
15	0	3	1	1	0	5	0.6	0.95	0.32	0.66
16	0	3	2	0	0	5	0.69	1.14	0.4	0.86
17	0	2	2	0	0	4	0.96	1.14	0.18	0.97
18	0	2	2	0	0	4	0.89	1.14	0.3	1.0
19	1	2	3	0	0	6	0.66	1.13	0.41	0.74
20	1	2	3	0	0	6	0.69	1.09	0.43	0.86

[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

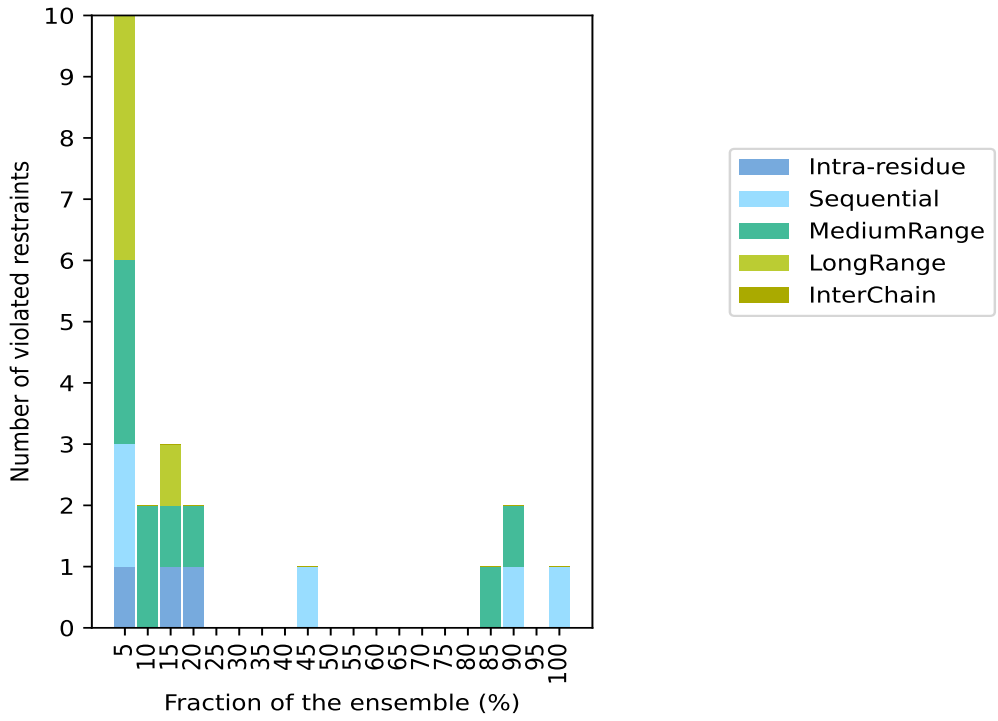
9.3 Distance violation statistics for the ensemble (i)

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, 1897(IR:579, SQ:515, MR:415, LR:388, 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]	%
1	2	3	4	0	10	1	5.0
0	0	2	0	0	2	2	10.0
1	0	1	1	0	3	3	15.0
1	0	1	0	0	2	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	1	0	0	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	1	0	0	1	17	85.0
0	1	1	0	0	2	18	90.0
0	0	0	0	0	0	19	95.0
0	1	0	0	0	1	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

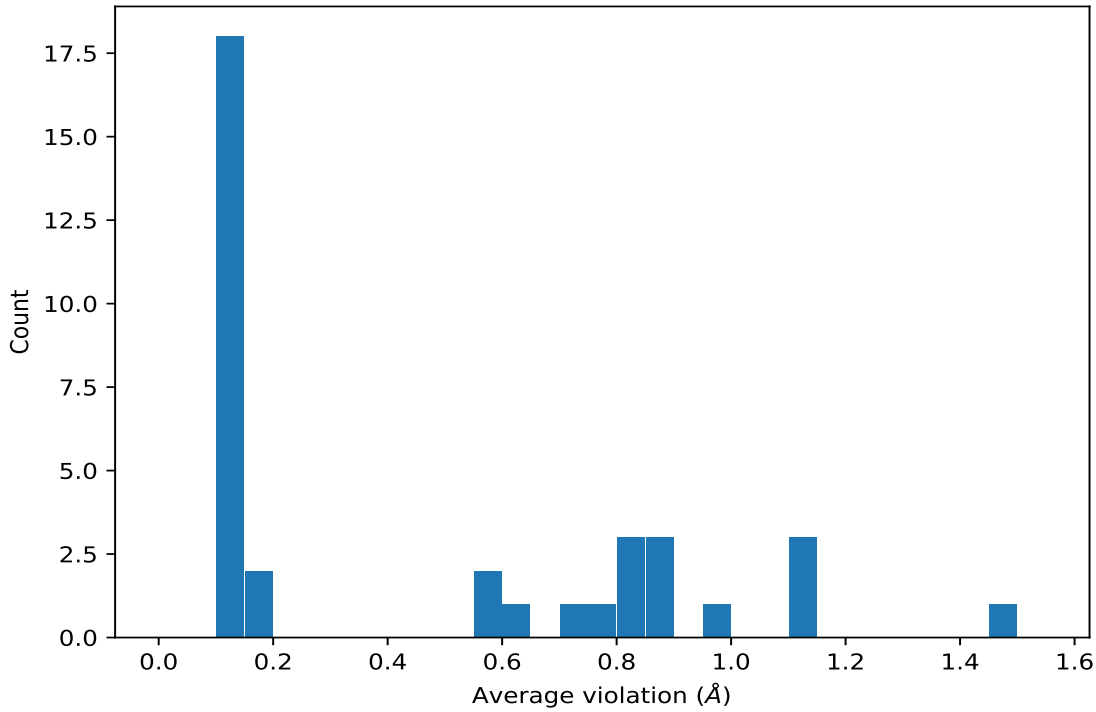
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

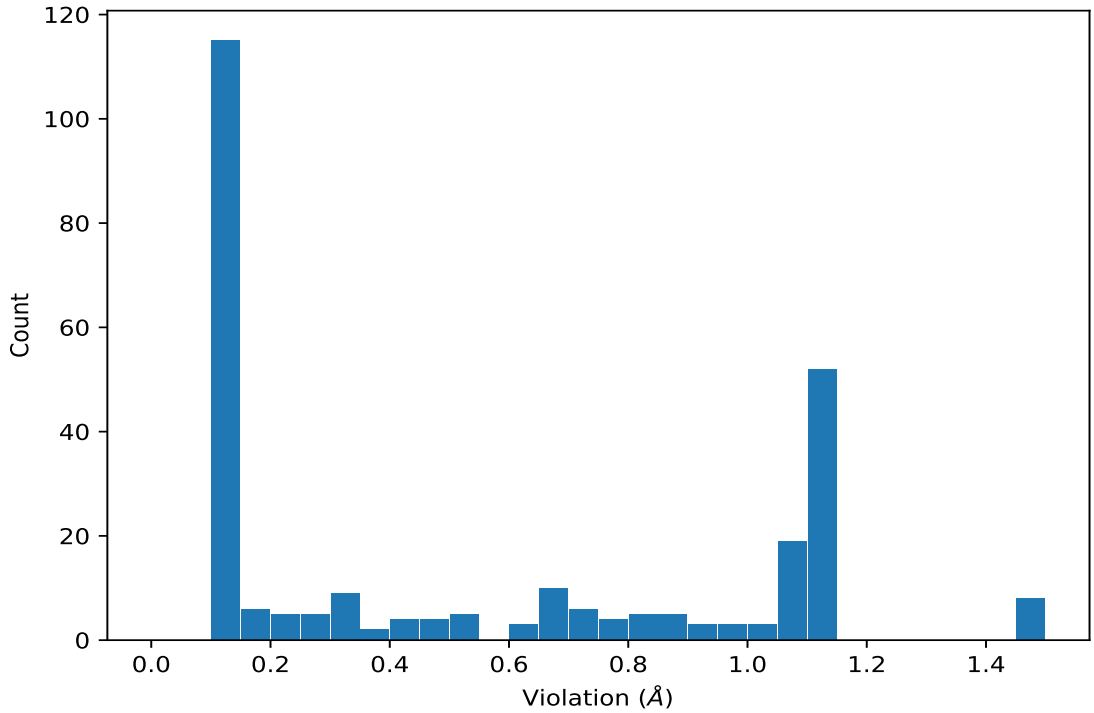
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1376)	1:766:A:GLN:HE21	1:767:A:MET:HA	20	0.99	0.1	1.0
(1,943)	1:809:A:ALA:HB1	1:812:A:ASN:HD21	18	1.13	0.02	1.14
(1,943)	1:809:A:ALA:HB2	1:812:A:ASN:HD21	18	1.13	0.02	1.14
(1,943)	1:809:A:ALA:HB3	1:812:A:ASN:HD21	18	1.13	0.02	1.14
(1,920)	1:779:A:LYS:HD2	1:780:A:ASP:HB2	18	0.55	0.22	0.55
(1,920)	1:779:A:LYS:HD3	1:780:A:ASP:HB2	18	0.55	0.22	0.55
(1,1369)	1:871:A:LEU:HG	1:875:A:GLN:HE21	17	0.72	0.29	0.76
(1,965)	1:780:A:ASP:HB3	1:781:A:HIS:HB2	9	0.18	0.08	0.15
(1,484)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	4	0.8	0.67	0.81
(1,484)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	4	0.8	0.67	0.81
(1,484)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	4	0.8	0.67	0.81
(1,1064)	1:821:A:ASN:HA	1:821:A:ASN:HD21	4	0.19	0.08	0.16
(1,1312)	1:875:A:GLN:HA	1:875:A:GLN:HE21	3	0.75	0.0	0.75
(1,744)	1:847:A:GLN:HE21	1:851:A:SER:HA	3	0.61	0.34	0.5
(1,1798)	1:863:A:THR:HG21	1:892:A:VAL:HG11	3	0.14	0.0	0.14

[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)
(1,1404)	1:763:A:SER:H	1:766:A:GLN:HE21	6	1.5
(1,1404)	1:763:A:SER:H	1:766:A:GLN:HE21	11	1.48
(1,484)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	11	1.48
(1,484)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	11	1.48
(1,484)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	11	1.48
(1,484)	1:762:A:ILE:HG21	1:766:A:GLN:HE21	6	1.46
(1,484)	1:762:A:ILE:HG22	1:766:A:GLN:HE21	6	1.46
(1,484)	1:762:A:ILE:HG23	1:766:A:GLN:HE21	6	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:809:A:ALA:HB1	1:812:A:ASN:HD21	5	1.15
(1,943)	1:809:A:ALA:HB2	1:812:A:ASN:HD21	5	1.15
(1,943)	1:809:A:ALA:HB3	1:812:A:ASN:HD21	5	1.15
(1,943)	1:809:A:ALA:HB1	1:812:A:ASN:HD21	12	1.15
(1,943)	1:809:A:ALA:HB2	1:812:A:ASN:HD21	12	1.15
(1,943)	1:809:A:ALA:HB3	1:812:A:ASN:HD21	12	1.15
(1,1376)	1:766:A:GLN:HE21	1:767:A:MET:HA	5	1.14
(1,1369)	1:871:A:LEU:HG	1:875:A:GLN:HE21	18	1.14
(1,943)	1:809:A:ALA:HB1	1:812:A:ASN:HD21	2	1.14
(1,943)	1:809:A:ALA:HB2	1:812:A:ASN:HD21	2	1.14
(1,943)	1:809:A:ALA:HB3	1:812:A:ASN:HD21	2	1.14
(1,943)	1:809:A:ALA:HB1	1:812:A:ASN:HD21	3	1.14

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found