wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2AVG
BMRB ID	:	6015
Title	:	NMR structure of cC1 domain from Human Cardiac Myosin Binding Protein C
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Deposited on	:	2005-08-30

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:

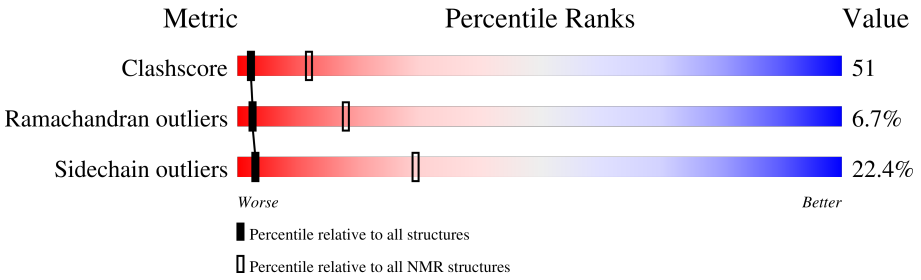
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

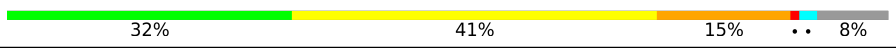
The overall completeness of chemical shifts assignment is 79%.

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	120	

2 Ensemble composition and analysis (i)

This entry contains 29 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:2-A:108 (107)	0.54	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, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 24, 25, 26, 28, 29
2	23, 27

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1706 atoms, of which 845 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Myosin-binding protein C, cardiac-type.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	110	1706	550	845	146	161	4	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q14896
A	-9	HIS	-	expression tag	UNP Q14896
A	-8	HIS	-	expression tag	UNP Q14896
A	-7	HIS	-	expression tag	UNP Q14896
A	-6	HIS	-	expression tag	UNP Q14896
A	-5	HIS	-	expression tag	UNP Q14896
A	-4	HIS	-	expression tag	UNP Q14896
A	-3	SER	-	expression tag	UNP Q14896
A	-2	SER	-	expression tag	UNP Q14896
A	-1	MET	-	expression tag	UNP Q14896
A	86	GLY	SER	SEE REMARK 999	UNP Q14896

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: Myosin-binding protein C, cardiac-type

Chain A: 32% 41% 15% • • 8%

MET HIS HIS HIS HIS HIS HIS SER SER MET D1 D2 P3 I4 G5 L6 F7 R10 P11 Q12 D13 T17 V18 S21 I22 T23 F24 S25 A26 G30 A31 S32 L33 L34 K35 P36 P37 V38 V39 K40 W41 F42 K43 G44 K45 W46 V47 D48 L49 K52 V53 G54 Q55 H56 L57

Q58 L59 H60 D61 S62 Y63 D64 R65 K68 V69 Y70 L71 F72 E73 L74 H75 I76 T77 Q80 P81 A82 F83 T84 G85 G86 Y87 R88 C89 E90 V91 S92 T93 K94 D95 K96 S100 N101 F102 N103 L104 T105 V106 A109 M110

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

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: Myosin-binding protein C, cardiac-type

Chain A: 36% 35% 18% • • 8%

MET HIS HIS HIS HIS HIS HIS SER SER MET D1 I4 G5 L6 F7 P11 Q12 D13 G14 E15 V16 T17 V18 S21 I22 S25 A26 A29 G30 A31 S32 L33 L34 K35 P36 P37 V38 V39 K40 W41 F42 K43 G44 K45 W46 V47 D48 L49 K52 V53 G54 Q55 H56 L57

Q58 L59 H60 D61 S62 R65 K68 V69 Y70 L71 F72 E73 L74 H75 I76 T77 Q80 P81 A82 F83 T84 G85 G86 Y87 V91 S92 T93 K94 D95 K96 N101 F102 N103 L104 T105 V106 H107 E108 A109 M110

5 Refinement protocol and experimental data overview (i)

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

Of the 40 calculated structures, 29 were deposited, based on the following criterion: *no NOE violation > 0.5 A.*

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

Software name	Classification	Version
ARIA	structure solution	1.2
ARIA	refinement	1.2

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	1151
Number of shifts mapped to atoms	1151
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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	0.87±0.04	1±1/862 (0.1± 0.1%)	0.80±0.02	0±0/1169 (0.0± 0.0%)
All	All	0.87	20/24998 (0.1%)	0.80	2/33901 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.6±0.6
All	All	0	18

5 of 8 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	83	PHE	CE1-CZ	8.26	1.53	1.37	5	6
1	A	87	TYR	CE2-CZ	-7.70	1.28	1.38	21	3
1	A	83	PHE	CE2-CZ	-7.21	1.23	1.37	5	4
1	A	70	TYR	CE2-CZ	-6.97	1.29	1.38	20	2
1	A	70	TYR	CE1-CZ	6.72	1.47	1.38	20	2

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	84	THR	CA-CB-CG2	-7.42	102.01	112.40	14	1
1	A	84	THR	CA-C-N	-5.41	105.38	116.20	14	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the

ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	44	GLY	Mainchain,Peptide	15
1	A	70	TYR	Sidechain	1
1	A	63	TYR	Sidechain	1
1	A	85	GLY	Peptide	1

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	839	827	823	85±10
All	All	24331	23983	23867	2460

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 51.

5 of 598 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:GLY:HA2	1:A:86:GLY:H	1.01	1.12	29	10
1:A:4:ILE:HB	1:A:96:LYS:HD3	0.99	1.27	4	3
1:A:94:LYS:HD3	1:A:95:ASP:H	0.99	1.18	4	23
1:A:33:LEU:HD22	1:A:93:THR:HA	0.99	1.34	23	3
1:A:41:TRP:HB3	1:A:49:LEU:HD13	0.96	1.33	27	28

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	107/120 (89%)	89±2 (83±2%)	11±2 (10±2%)	7±1 (7±1%)	2 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3103/3480 (89%)	2576 (83%)	320 (10%)	207 (7%)	2 18

5 of 14 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	13	ASP	29
1	A	46	TRP	29
1	A	53	VAL	29
1	A	94	LYS	29
1	A	84	THR	22

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	92/104 (88%)	71±2 (78±2%)	21±2 (22±2%)	3 29
All	All	2668/3016 (88%)	2071 (78%)	597 (22%)	3 29

5 of 53 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	7	PHE	29
1	A	40	LYS	29
1	A	57	LEU	29
1	A	58	GLN	29
1	A	59	LEU	29

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 (i)

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 78% 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	1151
Number of shifts mapped to atoms	1151
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	108	-0.52 ± 0.09	Should be applied
$^{13}C_{\beta}$	99	-0.45 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	99	-3.22 ± 0.34	Should be applied
^{15}N	102	-1.32 ± 0.33	Should be applied

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 79%, i.e. 1143 atoms were assigned a chemical shift out of a possible 1439. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	522/534 (98%)	216/218 (99%)	205/214 (96%)	101/102 (99%)
Sidechain	577/752 (77%)	382/490 (78%)	190/236 (81%)	5/26 (19%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	44/153 (29%)	24/75 (32%)	18/68 (26%)	2/10 (20%)
Overall	1143/1439 (79%)	622/783 (79%)	413/518 (80%)	108/138 (78%)

7.1.4 Statistically unusual chemical shifts (i)

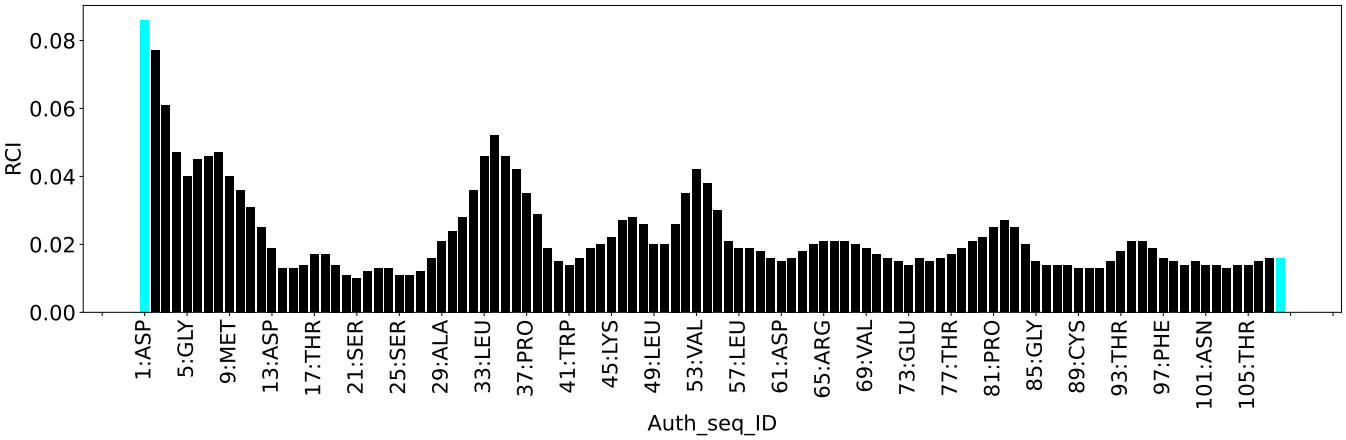
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	43	LYS	CE	31.57	37.57 – 46.21	-11.9
1	A	74	LEU	HB3	-0.84	-0.26 – 3.31	-6.6
1	A	87	TYR	HB3	0.70	0.93 – 4.76	-5.6

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 (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	17898
Intra-residue (|i-j|=0)	7067
Sequential (|i-j|=1)	4364
Medium range (|i-j|>1 and |i-j|<5)	1525
Long range (|i-j|≥5)	4942
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	149.2
Number of long range restraints per residue[1]	41.2

[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 (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)	127.1	0.2
0.2-0.5 (Medium)	166.1	0.5
>0.5 (Large)	126.0	3.43

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)

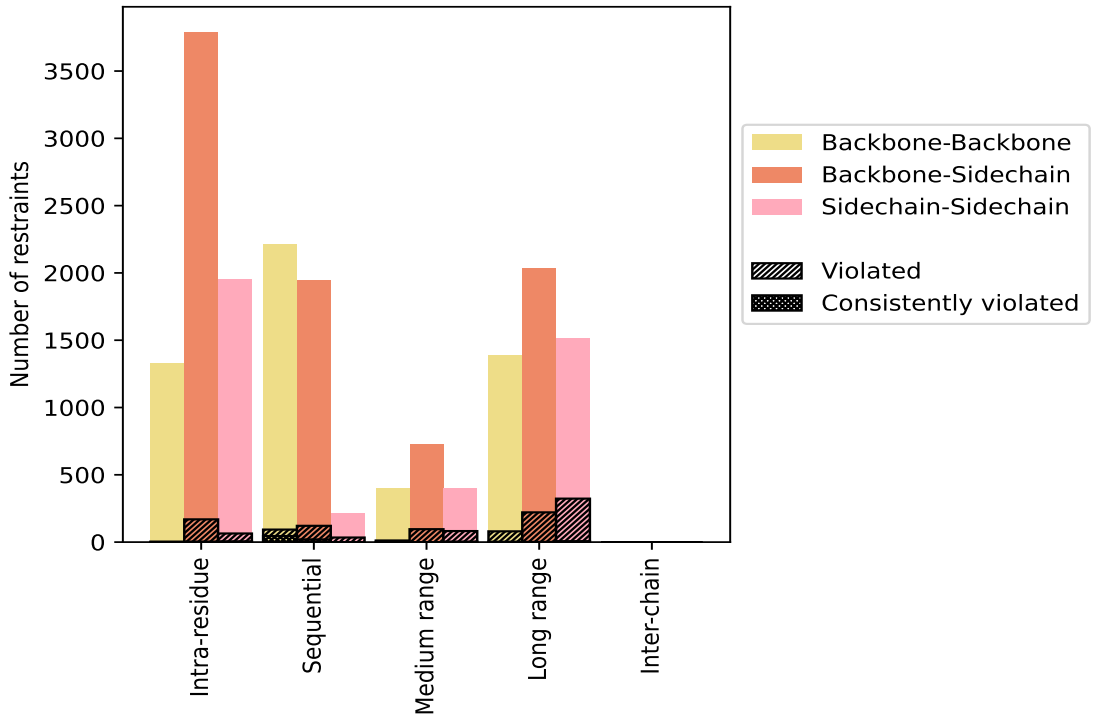
9.1 Summary of distance violations (i)

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)	7067	39.5	236	3.3	1.3	11	0.2	0.1
Backbone-Backbone	1328	7.4	3	0.2	0.0	1	0.1	0.0
Backbone-Sidechain	3788	21.2	169	4.5	0.9	4	0.1	0.0
Sidechain-Sidechain	1951	10.9	64	3.3	0.4	6	0.3	0.0
Sequential (|i-j|=1)	4364	24.4	248	5.7	1.4	65	1.5	0.4
Backbone-Backbone	2211	12.4	93	4.2	0.5	45	2.0	0.3
Backbone-Sidechain	1942	10.9	121	6.2	0.7	20	1.0	0.1
Sidechain-Sidechain	211	1.2	34	16.1	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	1525	8.5	190	12.5	1.1	6	0.4	0.0
Backbone-Backbone	401	2.2	12	3.0	0.1	2	0.5	0.0
Backbone-Sidechain	727	4.1	96	13.2	0.5	0	0.0	0.0
Sidechain-Sidechain	397	2.2	82	20.7	0.5	4	1.0	0.0
Long range (|i-j|≥5)	4942	27.6	624	12.6	3.5	12	0.2	0.1
Backbone-Backbone	1389	7.8	80	5.8	0.4	3	0.2	0.0
Backbone-Sidechain	2037	11.4	221	10.8	1.2	2	0.1	0.0
Sidechain-Sidechain	1516	8.5	323	21.3	1.8	7	0.5	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	17898	100.0	1298	7.3	7.3	94	0.5	0.5
Backbone-Backbone	5329	29.8	188	3.5	1.1	51	1.0	0.3
Backbone-Sidechain	8494	47.5	607	7.1	3.4	26	0.3	0.1
Sidechain-Sidechain	4075	22.8	503	12.3	2.8	17	0.4	0.1

[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	89	115	35	215	0	454	0.51	2.47	0.39	0.35
2	67	125	31	127	0	350	0.42	2.53	0.35	0.3
3	63	141	54	136	0	394	0.41	2.14	0.38	0.28
4	60	117	38	182	0	397	0.46	2.57	0.38	0.3
5	73	143	44	162	0	422	0.52	2.7	0.45	0.33
6	55	140	54	129	0	378	0.45	2.11	0.42	0.29
7	95	155	59	144	0	453	0.4	2.59	0.37	0.26
8	52	141	33	199	0	425	0.48	2.6	0.41	0.31
9	64	139	89	150	0	442	0.51	1.71	0.41	0.35
10	83	155	52	171	0	461	0.44	2.67	0.35	0.31
11	63	129	64	155	0	411	0.42	2.65	0.38	0.28

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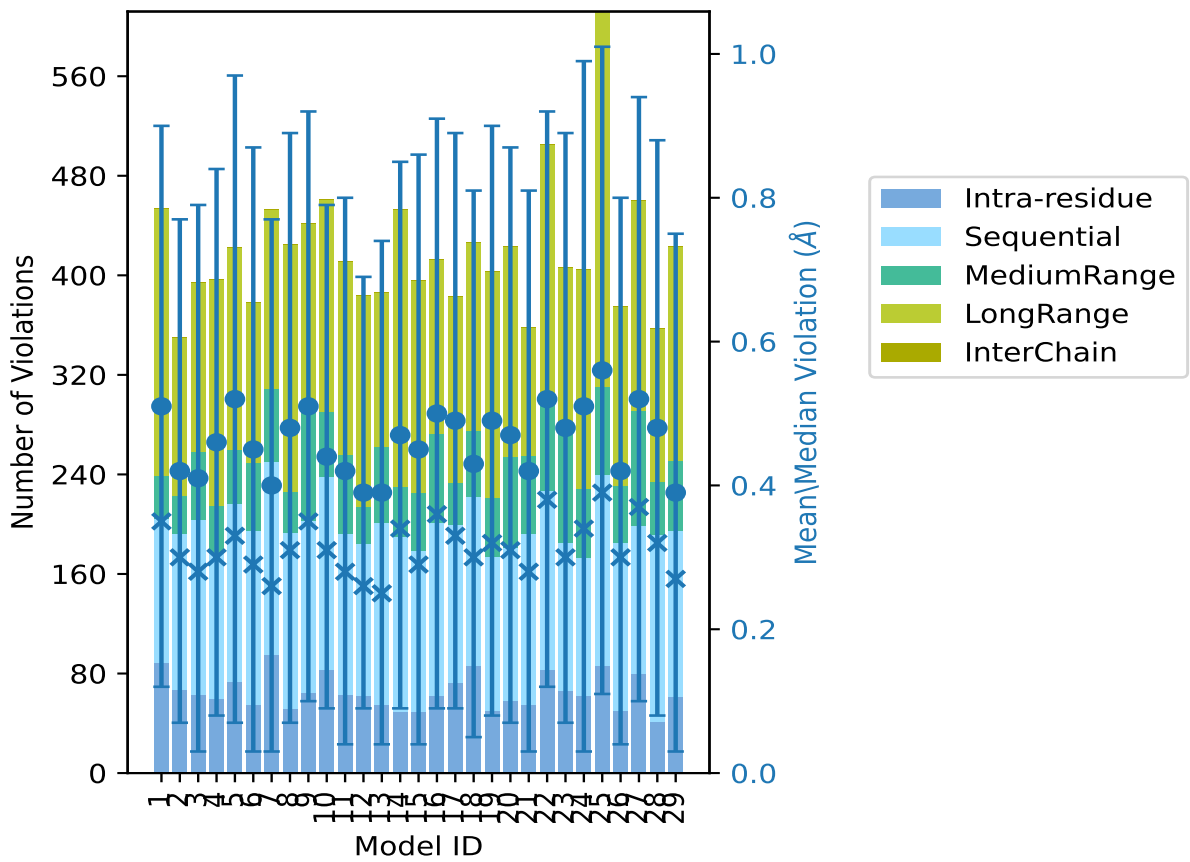
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	62	122	30	170	0	384	0.39	1.84	0.3	0.26
13	55	146	61	124	0	386	0.39	3.01	0.35	0.25
14	49	141	40	223	0	453	0.47	3.11	0.38	0.34
15	49	130	46	171	0	396	0.45	2.69	0.41	0.29
16	62	139	72	140	0	413	0.5	1.91	0.41	0.36
17	73	127	33	150	0	383	0.49	1.84	0.4	0.33
18	86	136	53	151	0	426	0.43	2.56	0.38	0.3
19	50	124	47	182	0	403	0.49	2.34	0.41	0.32
20	58	123	73	169	0	423	0.47	2.56	0.4	0.31
21	55	137	63	103	0	358	0.42	2.54	0.39	0.28
22	83	144	78	200	0	505	0.52	1.97	0.4	0.38
23	66	119	88	133	0	406	0.48	1.91	0.41	0.3
24	62	111	56	176	0	405	0.51	3.43	0.48	0.34
25	86	154	70	302	0	612	0.56	2.34	0.45	0.39
26	50	135	46	144	0	375	0.42	2.64	0.38	0.3
27	80	119	92	169	0	460	0.52	1.88	0.42	0.37
28	41	151	42	123	0	357	0.48	1.8	0.4	0.32
29	61	134	56	172	0	423	0.39	2.97	0.36	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, 16600(IR:6831, SQ:4116, MR:1335, LR:4318, 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]	%
29	35	32	175	0	271	1	3.4
66	23	23	98	0	210	2	6.9
4	4	13	44	0	65	3	10.3
25	7	19	15	0	66	4	13.8
21	4	7	12	0	44	5	17.2
13	3	8	32	0	56	6	20.7

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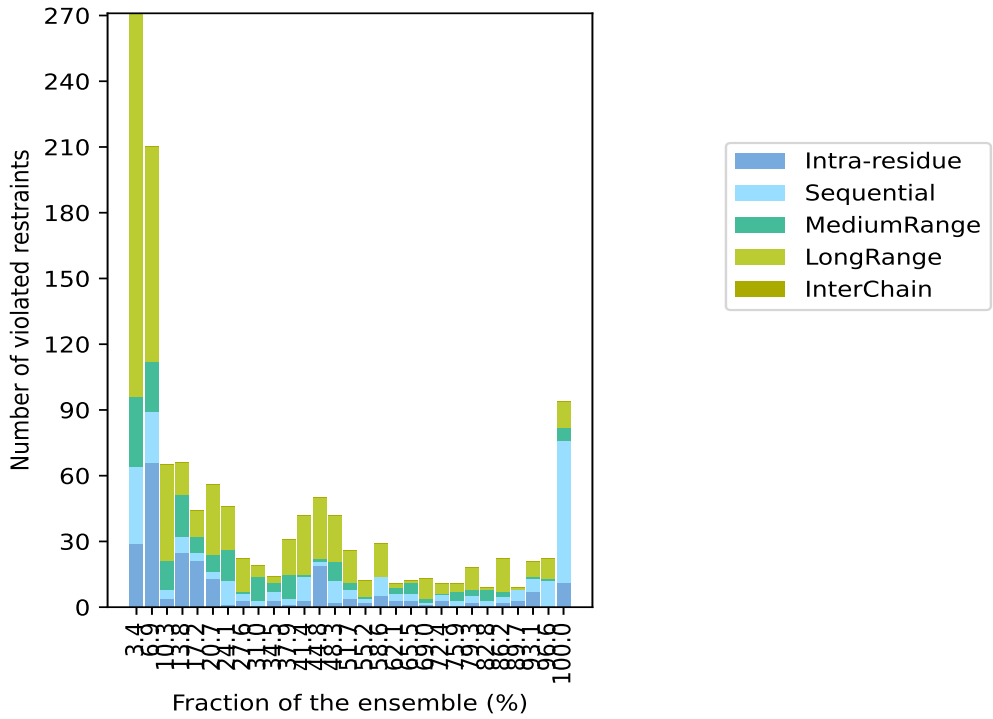
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	11	14	20	0	46	7	24.1
3	3	1	15	0	22	8	27.6
0	3	11	5	0	19	9	31.0
3	4	4	3	0	14	10	34.5
1	3	11	16	0	31	11	37.9
3	11	1	27	0	42	12	41.4
19	2	1	28	0	50	13	44.8
2	10	9	21	0	42	14	48.3
4	4	3	15	0	26	15	51.7
2	2	1	7	0	12	16	55.2
5	9	0	15	0	29	17	58.6
3	3	3	2	0	11	18	62.1
3	3	5	1	0	12	19	65.5
1	1	2	9	0	13	20	69.0
3	3	0	5	0	11	21	72.4
0	3	4	4	0	11	22	75.9
2	3	3	10	0	18	23	79.3
0	3	5	1	0	9	24	82.8
2	3	2	15	0	22	25	86.2
3	5	0	1	0	9	26	89.7
7	6	1	7	0	21	27	93.1
0	12	1	9	0	22	28	96.6
11	65	6	12	0	94	29	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

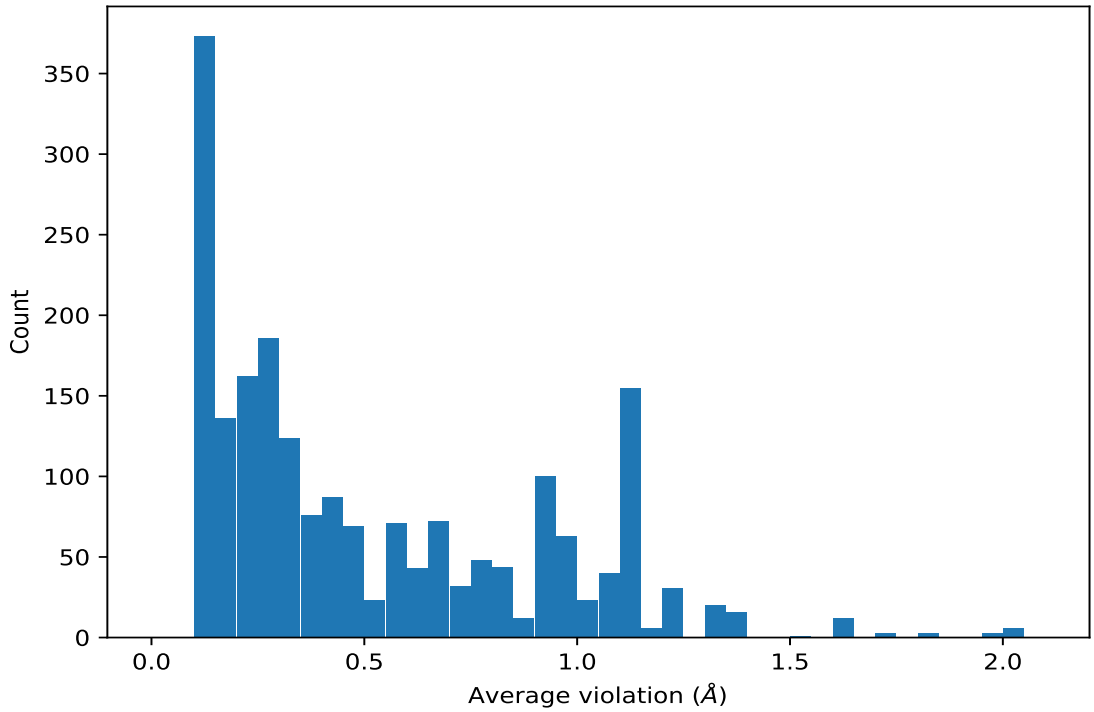
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

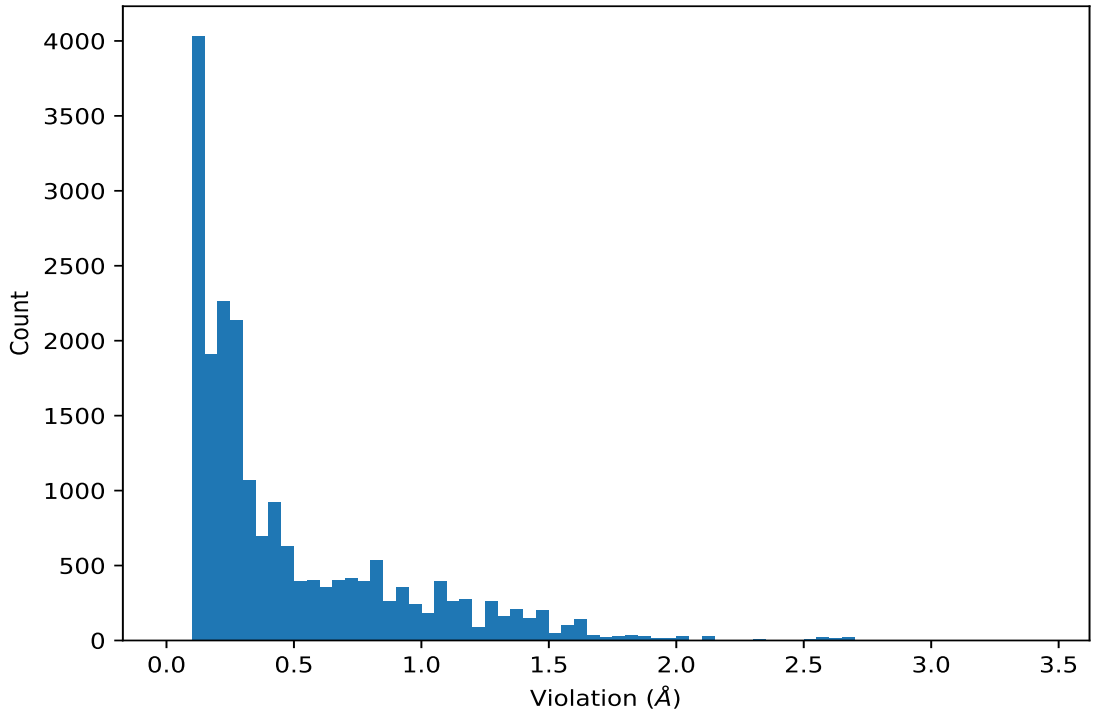
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,389)	1:A:41:TRP:HE1	1:A:71:LEU:HD11	29	1.74	0.13	1.74
(3,389)	1:A:41:TRP:HE1	1:A:71:LEU:HD12	29	1.74	0.13	1.74
(3,389)	1:A:41:TRP:HE1	1:A:71:LEU:HD13	29	1.74	0.13	1.74
(1,3867)	1:A:49:LEU:HB2	1:A:52:LYS:HB2	29	1.21	0.32	1.33
(1,5282)	1:A:37:PRO:HD2	1:A:31:ALA:HB1	29	1.03	0.29	1.07
(1,5282)	1:A:37:PRO:HD2	1:A:31:ALA:HB2	29	1.03	0.29	1.07
(1,5282)	1:A:37:PRO:HD2	1:A:31:ALA:HB3	29	1.03	0.29	1.07
(1,5247)	1:A:83:PHE:HA	1:A:44:GLY:HA2	29	0.98	0.47	0.99
(1,7917)	1:A:57:LEU:HG	1:A:49:LEU:HB2	29	0.95	0.25	1.03
(3,262)	1:A:97:PHE:H	1:A:96:LYS:HB2	29	0.93	0.15	0.94
(1,6549)	1:A:49:LEU:HB2	1:A:52:LYS:HB2	29	0.91	0.32	1.03
(3,476)	1:A:47:VAL:H	1:A:46:TRP:HB3	29	0.78	0.09	0.8
(1,4006)	1:A:46:TRP:HD1	1:A:46:TRP:HB2	29	0.78	0.18	0.83
(3,212)	1:A:62:SER:H	1:A:61:ASP:HB3	29	0.72	0.19	0.8

[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)
(1,1068)	1:A:52:LYS:HE2	1:A:47:VAL:HG21	24	3.43
(1,1068)	1:A:52:LYS:HE2	1:A:47:VAL:HG22	24	3.43
(1,1068)	1:A:52:LYS:HE2	1:A:47:VAL:HG23	24	3.43
(1,6431)	1:A:52:LYS:HE2	1:A:47:VAL:HG21	24	3.13
(1,6431)	1:A:52:LYS:HE2	1:A:47:VAL:HG22	24	3.13
(1,6431)	1:A:52:LYS:HE2	1:A:47:VAL:HG23	24	3.13
(1,1068)	1:A:52:LYS:HE2	1:A:47:VAL:HG21	14	3.11
(1,1068)	1:A:52:LYS:HE2	1:A:47:VAL:HG22	14	3.11
(1,1068)	1:A:52:LYS:HE2	1:A:47:VAL:HG23	14	3.11
(1,6533)	1:A:52:LYS:HD3	1:A:48:ASP:HB2	13	3.01
(1,1068)	1:A:52:LYS:HE2	1:A:47:VAL:HG21	29	2.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:A:52:LYS:HE2	1:A:47:VAL:HG22	29	2.97
(1,1068)	1:A:52:LYS:HE2	1:A:47:VAL:HG23	29	2.97
(1,6431)	1:A:52:LYS:HE2	1:A:47:VAL:HG21	14	2.81
(1,6431)	1:A:52:LYS:HE2	1:A:47:VAL:HG22	14	2.81
(1,6431)	1:A:52:LYS:HE2	1:A:47:VAL:HG23	14	2.81
(2,523)	1:A:45:LYS:HG2	1:A:47:VAL:HG11	5	2.7
(2,523)	1:A:45:LYS:HG2	1:A:47:VAL:HG12	5	2.7
(2,523)	1:A:45:LYS:HG2	1:A:47:VAL:HG13	5	2.7
(2,286)	1:A:45:LYS:HG2	1:A:47:VAL:HG11	5	2.7
(2,286)	1:A:45:LYS:HG2	1:A:47:VAL:HG12	5	2.7
(2,286)	1:A:45:LYS:HG2	1:A:47:VAL:HG13	5	2.7
(2,523)	1:A:45:LYS:HG2	1:A:47:VAL:HG11	15	2.69
(2,523)	1:A:45:LYS:HG2	1:A:47:VAL:HG12	15	2.69
(2,523)	1:A:45:LYS:HG2	1:A:47:VAL:HG13	15	2.69
(2,523)	1:A:45:LYS:HG2	1:A:47:VAL:HG11	24	2.69

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found