wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2XV9
BMRB ID	:	6333
Title	:	The solution structure of ABA-1A saturated with oleic acid
Authors	:	Smith, B.O.; Kennedy, M.W.; Cooper, A.; Meenan, N.A.G.; Bromek, K.
Deposited on	:	2010-10-25

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:

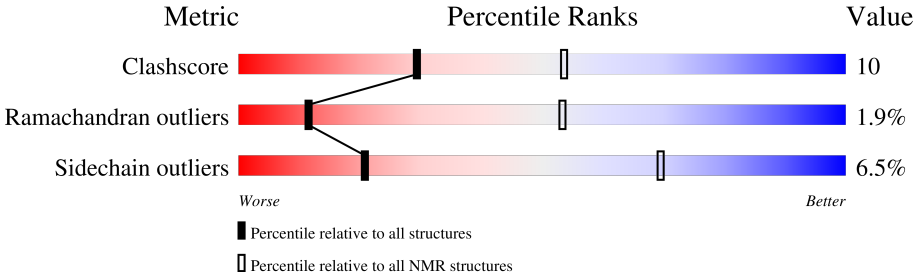
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 80%.

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	134	71% 20% • 7%

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 11 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:3-A:126 (124)	0.70	16

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 and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2141 atoms, of which 1074 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ABA-1A1 REPEAT UNIT.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	134	2141	672	1074	181	211	3	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q06811
A	-3	SER	-	expression tag	UNP Q06811
A	-2	PRO	-	expression tag	UNP Q06811
A	-1	GLU	-	expression tag	UNP Q06811
A	0	PHE	-	expression tag	UNP Q06811

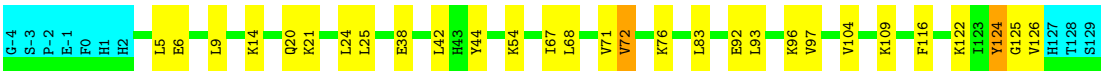
4 Residue-property plots (i)

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: ABA-1A1 REPEAT UNIT

Chain A: 71% 20% • 7%

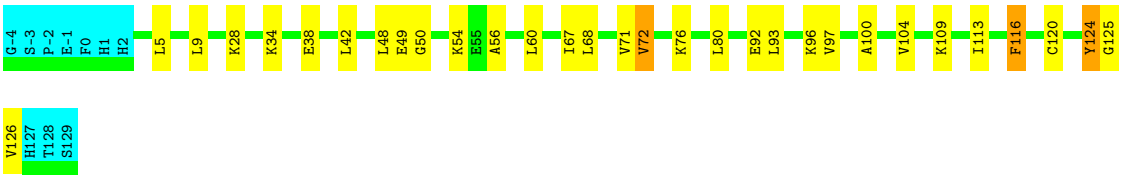


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

• Molecule 1: ABA-1A1 REPEAT UNIT

Chain A: 69% 21% • 7%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DEFAULT*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *EXPERIMENTALLY DERIVED RESTRAINT ENERGY*.

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

Software name	Classification	Version
ARIA2.3/CNS	refinement	
DANGLE	structure solution	1.1
CcpNmr Analysis	structure solution	2.1
CNS	structure solution	1.21
ARIA	structure solution	2.3
ANSIG	structure solution	
PALES	structure solution	1

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	1432
Number of shifts mapped to atoms	1432
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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	0.41±0.04	0±1/1000 (0.1± 0.1%)	0.49±0.01	0±0/1333 (0.0± 0.0%)
All	All	0.41	10/20000 (0.1%)	0.49	0/26660 (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	0.9±0.4
All	All	0	19

All 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	45	TYR	CE1-CZ	7.43	1.48	1.38	1	4
1	A	45	TYR	CE2-CZ	-6.98	1.29	1.38	1	4
1	A	44	TYR	CE2-CZ	6.45	1.47	1.38	8	1
1	A	44	TYR	CE1-CZ	-5.93	1.30	1.38	8	1

There are no bond-angle outliers.

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	124	TYR	Peptide	17
1	A	45	TYR	Sidechain	1
1	A	125	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	986	1007	1002	20±3
All	All	19720	20140	20040	404

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 10.

5 of 133 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:LEU:O	1:A:97:VAL:HB	0.78	1.79	8	7
1:A:122:LYS:HA	1:A:126:VAL:O	0.72	1.83	10	1
1:A:67:ILE:O	1:A:71:VAL:HB	0.70	1.87	5	4
1:A:96:LYS:O	1:A:99:GLU:HG3	0.70	1.87	6	1
1:A:92:GLU:O	1:A:96:LYS:HB2	0.67	1.90	20	14

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	124/134 (93%)	113±2 (91±2%)	9±2 (7±1%)	2±1 (2±1%)	11	53
All	All	2480/2680 (93%)	2259 (91%)	175 (7%)	46 (2%)	11	53

5 of 11 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	125	GLY	19
1	A	50	GLY	7
1	A	48	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	126	VAL	5
1	A	69	LYS	4

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	104/113 (92%)	97±3 (94±3%)	7±3 (6±3%)	21 69
All	All	2080/2260 (92%)	1945 (94%)	135 (6%)	21 69

5 of 37 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	116	PHE	14
1	A	72	VAL	13
1	A	54	LYS	12
1	A	83	LEU	9
1	A	97	VAL	8

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 80% for the well-defined parts and 79% 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	1432
Number of shifts mapped to atoms	1432
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	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
$^{13}C_{\alpha}$	134	-0.57 ± 0.06	Should be checked
$^{13}C_{\beta}$	125	0.16 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	124	-0.12 ± 0.23	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 80%, i.e. 1361 atoms were assigned a chemical shift out of a possible 1698. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	497/626 (79%)	252/255 (99%)	124/248 (50%)	121/123 (98%)
Sidechain	814/964 (84%)	540/618 (87%)	270/316 (85%)	4/30 (13%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	50/108 (46%)	25/52 (48%)	24/45 (53%)	1/11 (9%)
Overall	1361/1698 (80%)	817/925 (88%)	418/609 (69%)	126/164 (77%)

7.1.4 Statistically unusual chemical shifts (i)

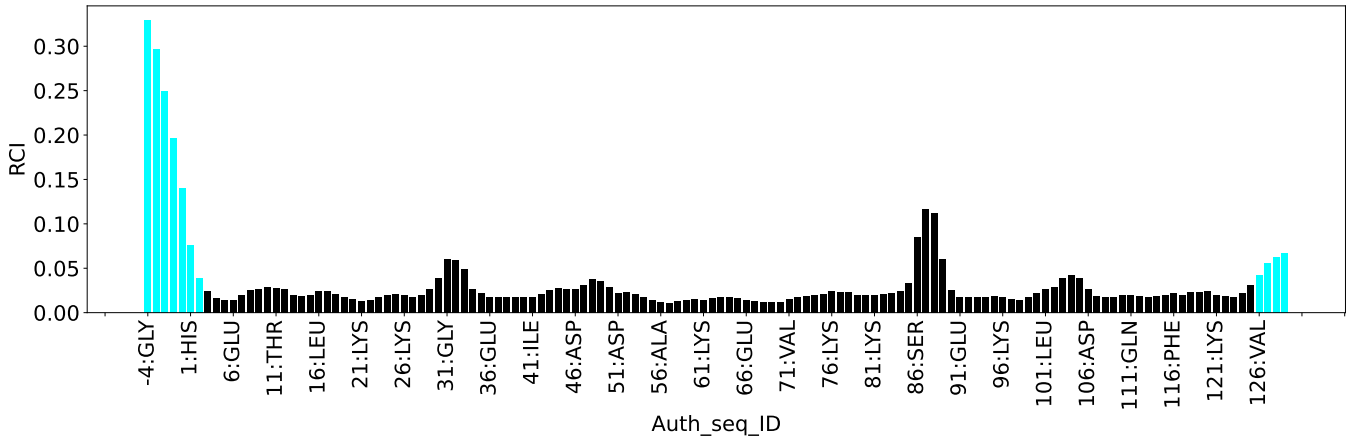
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	67	ILE	HG12	-0.86	-0.69 – 3.24	-5.4
1	A	61	LYS	HG2	0.13	0.13 – 2.61	-5.0

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	74404
Intra-residue (|i-j|=0)	4006
Sequential (|i-j|=1)	3682
Medium range (|i-j|>1 and |i-j|<5)	6486
Long range (|i-j|≥5)	60177
Inter-chain	0
Hydrogen bond restraints	52
Disulfide bond restraints	1
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	555.3
Number of long range restraints per residue[1]	449.1

[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)	553.6	0.2
0.2-0.5 (Medium)	1409.7	0.5
>0.5 (Large)	63704.2	46.58

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)

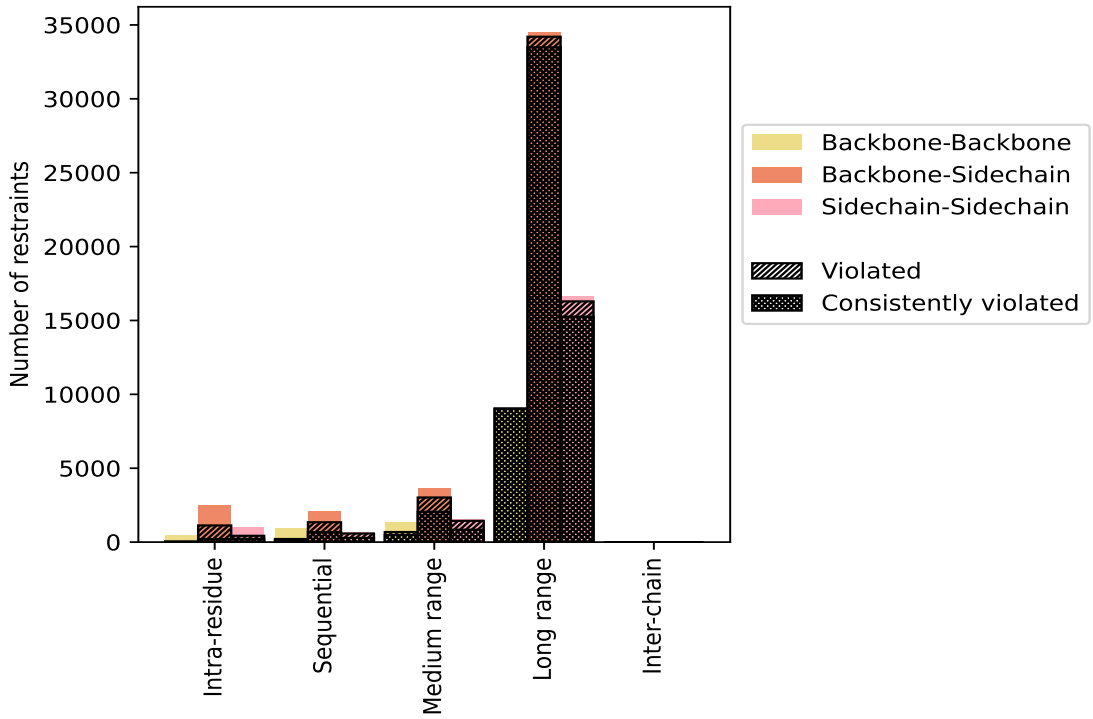
9.1 Summary of distance violations (i)

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)	4006	5.4	1591	39.7	2.1	453	11.3	0.6
Backbone-Backbone	477	0.6	37	7.8	0.0	27	5.7	0.0
Backbone-Sidechain	2508	3.4	1127	44.9	1.5	206	8.2	0.3
Sidechain-Sidechain	1021	1.4	427	41.8	0.6	220	21.5	0.3
Sequential (|i-j|=1)	3682	4.9	2134	58.0	2.9	1119	30.4	1.5
Backbone-Backbone	948	1.3	210	22.2	0.3	158	16.7	0.2
Backbone-Sidechain	2090	2.8	1343	64.3	1.8	678	32.4	0.9
Sidechain-Sidechain	644	0.9	581	90.2	0.8	283	43.9	0.4
Medium range (|i-j|>1 & |i-j|<5)	6486	8.7	5132	79.1	6.9	3371	52.0	4.5
Backbone-Backbone	1306	1.8	676	51.8	0.9	481	36.8	0.6
Backbone-Sidechain	3618	4.9	3019	83.4	4.1	2050	56.7	2.8
Sidechain-Sidechain	1562	2.1	1437	92.0	1.9	840	53.8	1.1
Long range (|i-j|≥5)	60177	80.9	59539	98.9	80.0	57768	96.0	77.6
Backbone-Backbone	9060	12.2	9046	99.8	12.2	9018	99.5	12.1
Backbone-Sidechain	34503	46.4	34203	99.1	46.0	33487	97.1	45.0
Sidechain-Sidechain	16614	22.3	16290	98.0	21.9	15263	91.9	20.5
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	52	0.1	7	13.5	0.0	0	0.0	0.0
Disulfide bond	1	0.0	1	100.0	0.0	0	0.0	0.0
Total	74404	100.0	68404	91.9	91.9	62711	84.3	84.3
Backbone-Backbone	11843	15.9	9976	84.2	13.4	9684	81.8	13.0
Backbone-Sidechain	42719	57.4	39692	92.9	53.3	36421	85.3	49.0
Sidechain-Sidechain	19842	26.7	18736	94.4	25.2	16606	83.7	22.3

[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 (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	958	1640	4323	58742	0	65663	13.61	42.79	8.75	12.94
2	960	1658	4317	58732	0	65667	13.84	46.58	8.88	13.19
3	942	1673	4309	58716	0	65640	13.72	42.71	8.8	13.09
4	935	1661	4339	58772	0	65707	14.02	43.3	9.04	13.32
5	935	1654	4348	58761	0	65698	13.83	44.2	8.98	13.06
6	982	1673	4300	58723	0	65678	13.49	43.16	8.65	12.87
7	973	1652	4356	58711	0	65692	13.89	44.1	8.95	13.21
8	956	1615	4297	58744	0	65612	13.79	43.86	8.84	13.16
9	955	1646	4331	58746	0	65678	13.63	41.91	8.72	13.02
10	940	1672	4326	58715	0	65653	13.63	42.56	8.7	13.02
11	962	1669	4338	58755	0	65724	13.82	44.12	8.83	13.2

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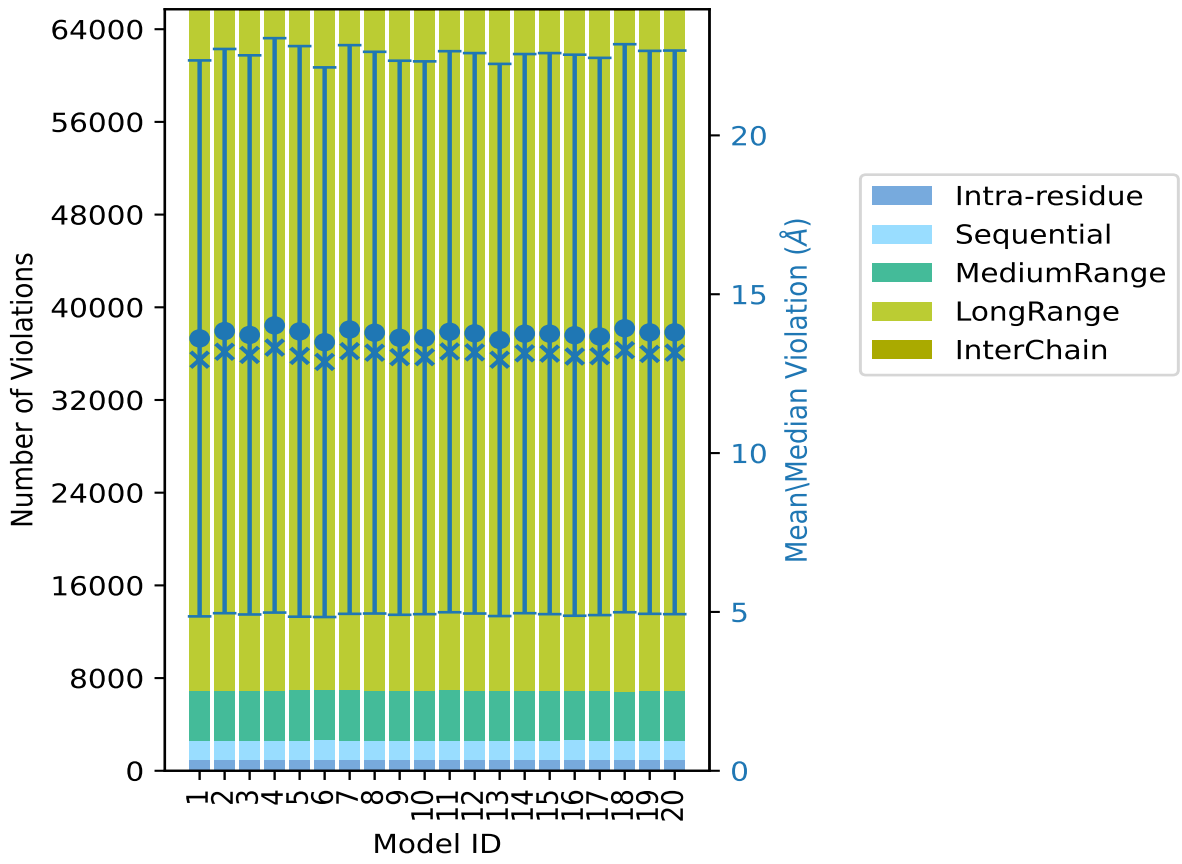
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	958	1651	4313	58757	0	65679	13.77	41.67	8.82	13.17
13	935	1677	4317	58721	0	65650	13.56	41.45	8.69	12.94
14	942	1650	4324	58789	0	65705	13.76	42.85	8.8	13.14
15	948	1626	4306	58710	0	65590	13.76	44.12	8.83	13.13
16	981	1644	4312	58744	0	65681	13.71	43.66	8.83	13.04
17	956	1668	4321	58727	0	65672	13.67	43.38	8.77	13.05
18	953	1612	4250	58776	0	65591	13.93	42.45	8.94	13.24
19	946	1635	4323	58756	0	65660	13.8	43.29	8.86	13.12
20	936	1677	4309	58789	0	65711	13.8	43.27	8.87	13.16

[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

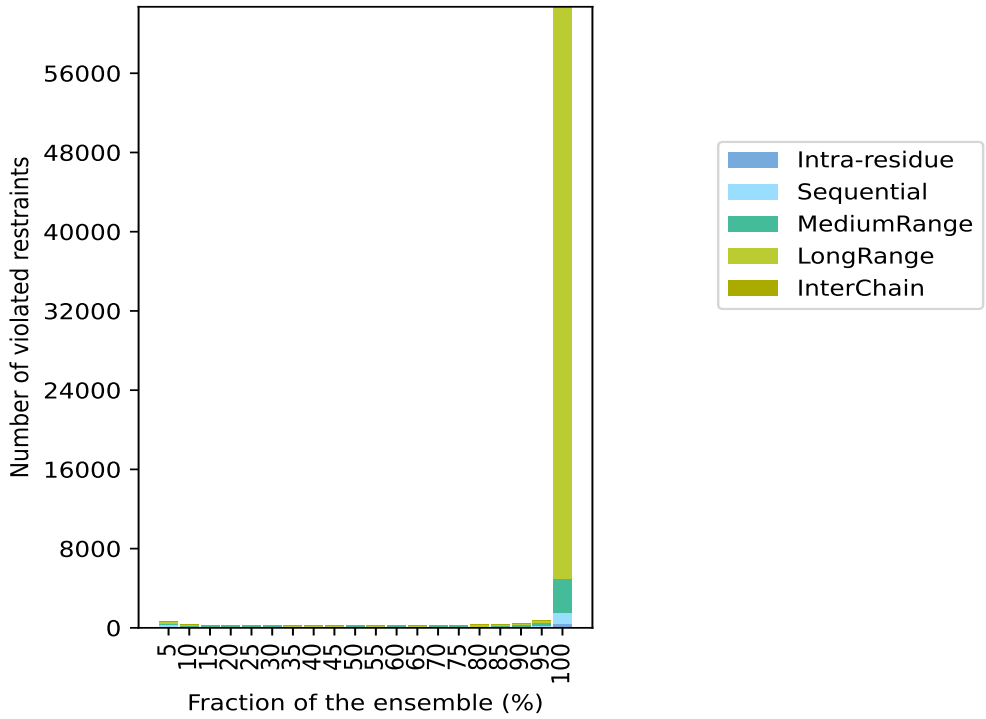
9.3 Distance violation statistics for the ensemble (i)

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, 5955(IR:2415, SQ:1548, MR:1354, LR:638, 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]	%
154	116	183	151	0	604	1	5.0
105	65	101	114	0	385	2	10.0
49	40	85	77	0	251	3	15.0
51	46	71	77	0	245	4	20.0
61	32	63	75	0	231	5	25.0
83	44	77	63	0	267	6	30.0
52	27	67	66	0	212	7	35.0
60	39	49	56	0	204	8	40.0
39	34	50	68	0	191	9	45.0
47	50	69	62	0	228	10	50.0
45	32	53	63	0	193	11	55.0
44	45	74	48	0	211	12	60.0
45	41	69	62	0	217	13	65.0
39	43	90	67	0	239	14	70.0
34	41	78	82	0	235	15	75.0
28	45	111	105	0	289	16	80.0
43	61	88	109	0	301	17	85.0
54	73	135	170	0	432	18	90.0
105	141	248	256	0	750	19	95.0
453	1119	3371	57768	0	62711	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

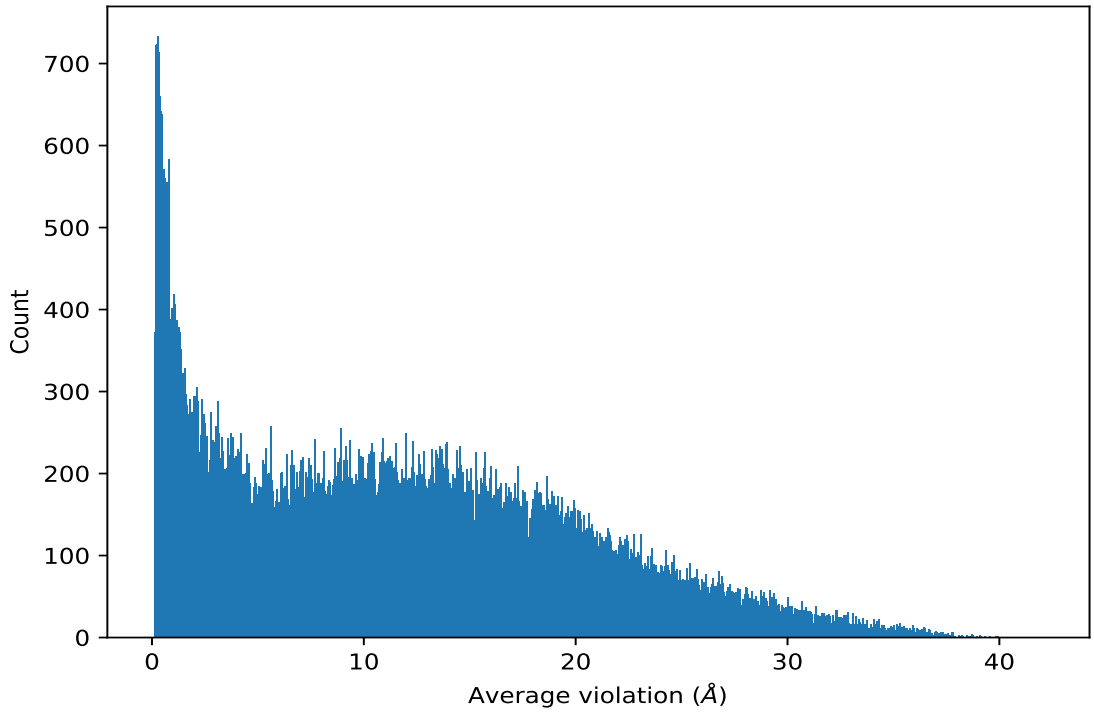
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

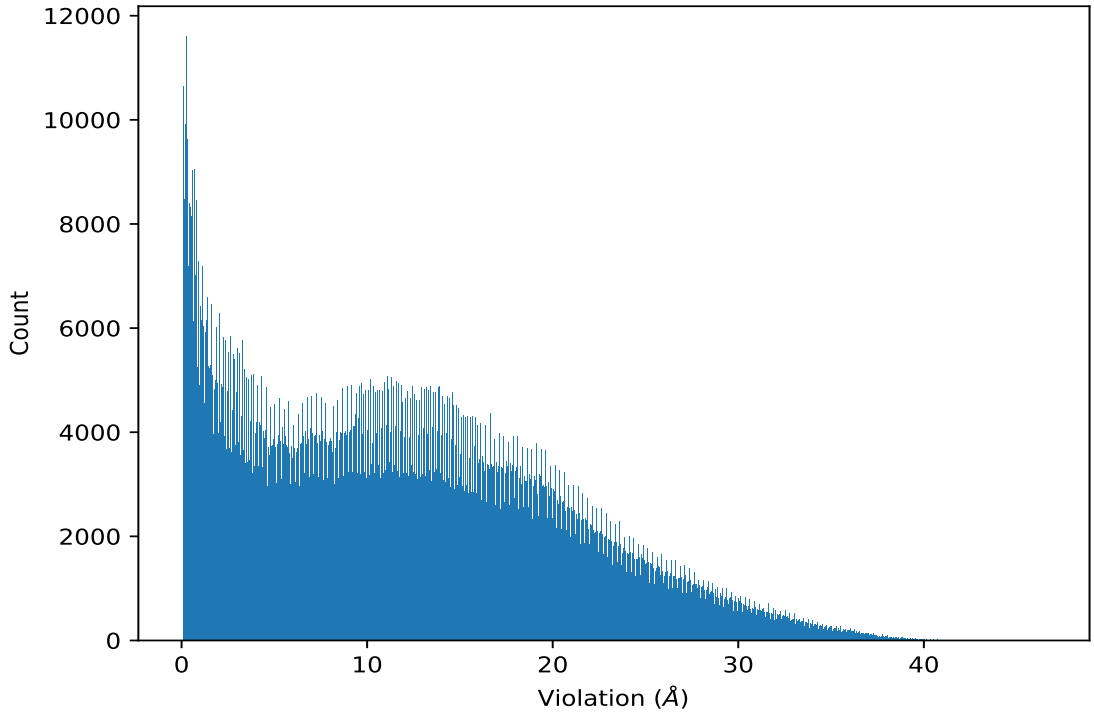
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(9,27685)	1:A:86:SER:HB3	1:A:30:ASP:HB2	20	42.1	0.77	42.38
(9,27691)	1:A:86:SER:HB2	1:A:30:ASP:HB2	20	41.9	1.11	41.78
(9,27715)	1:A:86:SER:HB3	1:A:30:ASP:HB3	20	41.86	1.22	41.9
(9,27688)	1:A:86:SER:HB2	1:A:30:ASP:HB3	20	41.67	1.12	41.74
(9,18615)	1:A:30:ASP:HB2	1:A:86:SER:HA	20	41.64	0.79	41.67
(9,18613)	1:A:30:ASP:HB3	1:A:86:SER:HA	20	41.46	0.95	41.16
(9,36420)	1:A:31:GLY:H	1:A:86:SER:HA	20	40.33	0.62	40.11
(7,12347)	1:A:31:GLY:H	1:A:86:SER:HB3	20	40.22	0.78	40.08
(7,5471)	1:A:30:ASP:H	1:A:86:SER:HB3	20	40.12	0.78	40.02
(7,12359)	1:A:31:GLY:H	1:A:86:SER:HB2	20	40.01	0.99	39.83

[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)
(7,17274)	1:A:87:GLY:H	1:A:-4:GLY:HA3	2	46.58
(7,17287)	1:A:87:GLY:H	1:A:-4:GLY:HA2	2	46.54
(7,15703)	1:A:88:ALA:H	1:A:-4:GLY:HA3	2	45.66
(7,15717)	1:A:88:ALA:H	1:A:-4:GLY:HA2	2	45.55
(9,27691)	1:A:86:SER:HB2	1:A:30:ASP:HB2	5	44.2
(9,27715)	1:A:86:SER:HB3	1:A:30:ASP:HB3	11	44.12
(9,27715)	1:A:86:SER:HB3	1:A:30:ASP:HB3	15	44.12
(7,15811)	1:A:-4:GLY:HA3	1:A:129:SER:H	7	44.1
(7,22029)	1:A:86:SER:H	1:A:-4:GLY:HA2	2	44.05
(7,22040)	1:A:86:SER:H	1:A:-4:GLY:HA3	2	44.04

10 Dihedral-angle violation analysis (i)

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