wwPDB NMR Structure Validation Summary Report

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BMRB ID	:	6475
Title	:	Mannan Binding Module from Man5C
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Deposited on	:	2005-01-04

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

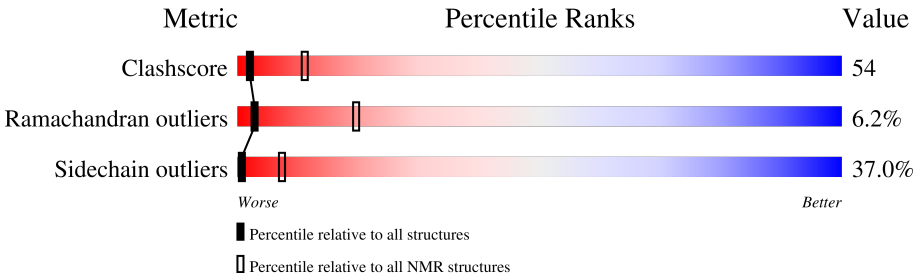
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 95%.

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	140	25% 40% 13% • • 17%

2 Ensemble composition and analysis

This entry contains 5 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:12-A:121 (110)	0.52	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, 3, 4
2	2, 5

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1709 atoms, of which 844 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ENDO-B1,4-MANNANASE 5C.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	116	1709	551	844	142	170	2	0

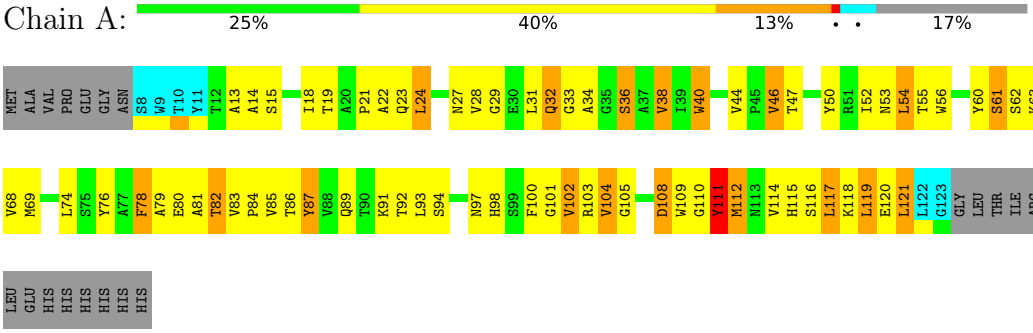
4 Residue-property plots

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: ENDO-B1,4-MANNANASE 5C

Chain A:

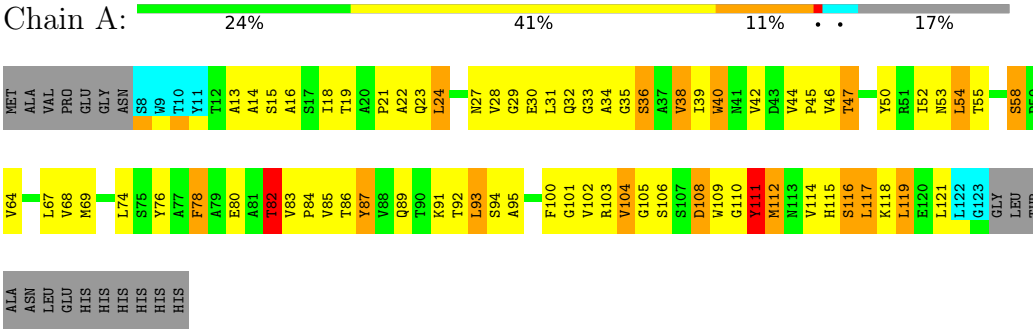


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

• Molecule 1: ENDO-B1,4-MANNANASE 5C

Chain A:



5 Refinement protocol and experimental data overview

Of the 80 calculated structures, 5 were deposited, based on the following criterion: *RANDOM 5 STRUCTURES FROM 20 LOWEST ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
Felix	structure solution	
CNS	structure solution	

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	1492
Number of shifts mapped to atoms	1395
Number of unparsed shifts	0
Number of shifts with mapping errors	97
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	95%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	814	799	797	86±9
All	All	4070	3995	3985	432

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 54.

5 of 220 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HD21	1:A:38:VAL:HG22	1.06	1.26	5	5
1:A:67:LEU:HD11	1:A:69:MET:CE	0.86	2.00	1	4
1:A:83:VAL:O	1:A:85:VAL:HG23	0.86	1.70	3	5
1:A:18:ILE:HD11	1:A:24:LEU:HD23	0.85	1.48	1	5
1:A:38:VAL:HG21	1:A:114:VAL:HG21	0.85	1.49	2	5

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	110/140 (79%)	86±2 (78±2%)	17±2 (15±2%)	7±1 (6±1%)	3	19
All	All	550/700 (79%)	431 (78%)	85 (15%)	34 (6%)	3	19

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	61	SER	5
1	A	84	PRO	5
1	A	111	TYR	5
1	A	78	PHE	3
1	A	33	GLY	3

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	88/113 (78%)	55±2 (63±3%)	33±2 (37±3%)	1	7
All	All	440/565 (78%)	277 (63%)	163 (37%)	1	7

5 of 54 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	24	LEU	5
1	A	36	SER	5
1	A	38	VAL	5
1	A	40	TRP	5
1	A	46	VAL	5

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 95% for the well-defined parts and 95% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1492
Number of shifts mapped to atoms	1395
Number of unparsed shifts	0
Number of shifts with mapping errors	97
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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 97) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ALA	HA	4.038	0.02	1
1	A	2	ALA	HB1	1.396	0.02	1
1	A	2	ALA	HB2	1.396	0.02	1
1	A	2	ALA	HB3	1.396	0.02	1
1	A	2	ALA	C	173.63	0.1	1
1	A	2	ALA	CA	51.43	0.1	1
1	A	2	ALA	CB	19.17	0.1	1
1	A	3	VAL	H	8.4	0.02	1
1	A	3	VAL	HA	4.391	0.02	1
1	A	3	VAL	HB	2.01	0.02	1
1	A	3	VAL	HG11	0.889	0.02	1
1	A	3	VAL	HG12	0.889	0.02	1
1	A	3	VAL	HG13	0.889	0.02	1
1	A	3	VAL	HG21	0.828	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	VAL	HG22	0.828	0.02	1
1	A	3	VAL	HG23	0.828	0.02	1
1	A	3	VAL	C	174.31	0.1	1
1	A	3	VAL	CA	59.755	0.1	1
1	A	3	VAL	CB	32.147	0.1	1
1	A	3	VAL	CG1	20.817	0.1	1
1	A	3	VAL	CG2	19.887	0.1	1
1	A	3	VAL	N	120.35	0.1	1
1	A	4	PRO	HA	4.306	0.02	1
1	A	4	PRO	HB2	1.779	0.02	2
1	A	4	PRO	HB3	2.172	0.02	2
1	A	4	PRO	HG2	1.096	0.02	2
1	A	4	PRO	HG3	1.574	0.02	2
1	A	4	PRO	HD2	3.536	0.02	2
1	A	4	PRO	HD3	3.777	0.02	2
1	A	4	PRO	C	176.505	0.1	1
1	A	4	PRO	CA	63.023	0.1	1
1	A	4	PRO	CB	31.729	0.1	1
1	A	4	PRO	CG	27.163	0.1	1
1	A	4	PRO	CD	50.597	0.1	1
1	A	5	GLU	H	8.435	0.02	1
1	A	5	GLU	HA	4.144	0.02	1
1	A	5	GLU	HB2	1.847	0.02	2
1	A	5	GLU	HB3	1.914	0.02	2
1	A	5	GLU	HG2	2.194	0.02	1
1	A	5	GLU	HG3	2.194	0.02	1
1	A	5	GLU	C	176.856	0.1	1
1	A	5	GLU	CA	56.708	0.1	1
1	A	5	GLU	CB	30.066	0.1	1
1	A	5	GLU	CG	36.051	0.1	1
1	A	5	GLU	N	121.529	0.1	1
1	A	6	GLY	H	8.323	0.02	1
1	A	6	GLY	HA2	3.745	0.02	2
1	A	6	GLY	HA3	3.863	0.02	2
1	A	6	GLY	C	173.327	0.1	1
1	A	6	GLY	CA	44.981	0.1	1
1	A	6	GLY	N	109.932	0.1	1
1	A	7	ASN	H	8.027	0.02	1
1	A	7	ASN	HA	4.392	0.02	1
1	A	7	ASN	HB2	2.711	0.02	1
1	A	7	ASN	HB3	2.711	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	ASN	HD21	7.31	0.02	2
1	A	7	ASN	HD22	6.74	0.02	2
1	A	7	ASN	C	172.853	0.1	1
1	A	7	ASN	CA	52.597	0.1	1
1	A	7	ASN	CB	39.098	0.1	1
1	A	7	ASN	N	117.021	0.1	1
1	A	7	ASN	ND2	112.2	0.1	1
1	A	124	GLY	H	8.277	0.02	1
1	A	124	GLY	HA2	3.883	0.02	2
1	A	124	GLY	HA3	3.78	0.02	2
1	A	124	GLY	C	173.755	0.1	1
1	A	124	GLY	CA	44.976	0.1	1
1	A	124	GLY	N	108.728	0.1	1
1	A	125	LEU	H	7.931	0.02	1
1	A	125	LEU	HA	4.324	0.02	1
1	A	125	LEU	CA	55.29	0.1	1
1	A	125	LEU	N	108.16	0.1	1
1	A	126	THR	H	7.65	0.02	1
1	A	126	THR	HA	4.073	0.02	1
1	A	126	THR	HB	4.147	0.02	1
1	A	126	THR	HG21	1.048	0.02	1
1	A	126	THR	HG22	1.048	0.02	1
1	A	126	THR	HG23	1.048	0.02	1
1	A	126	THR	CA	62.721	0.1	1
1	A	126	THR	CB	70.54	0.1	1
1	A	126	THR	CG2	21.505	0.1	1
1	A	126	THR	N	119.17	0.1	1
1	A	127	ILE	HA	3.574	0.02	1
1	A	127	ILE	HB	1.877	0.02	1
1	A	127	ILE	HG12	1.365	0.02	2
1	A	127	ILE	HG13	1.164	0.02	2
1	A	127	ILE	HG21	0.901	0.02	1
1	A	127	ILE	HG22	0.901	0.02	1
1	A	127	ILE	HG23	0.901	0.02	1
1	A	127	ILE	HD11	0.834	0.02	1
1	A	127	ILE	HD12	0.834	0.02	1
1	A	127	ILE	HD13	0.834	0.02	1
1	A	127	ILE	CA	62.053	0.1	1
1	A	127	ILE	CB	38.203	0.1	1
1	A	127	ILE	CG1	26.891	0.1	1
1	A	127	ILE	CG2	17.192	0.1	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	ILE	CD1	13.562	0.1	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	126	-0.02 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	112	0.33 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	122	0.54 ± 0.14	Should be applied
^{15}N	119	-1.38 ± 0.47	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 95%, i.e. 1316 atoms were assigned a chemical shift out of a possible 1391. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	551/552 (100%)	226/226 (100%)	219/220 (100%)	106/106 (100%)
Sidechain	685/722 (95%)	470/480 (98%)	206/224 (92%)	9/18 (50%)
Aromatic	80/117 (68%)	39/56 (70%)	38/54 (70%)	3/7 (43%)
Overall	1316/1391 (95%)	735/762 (96%)	463/498 (93%)	118/131 (90%)

7.1.4 Statistically unusual chemical shifts

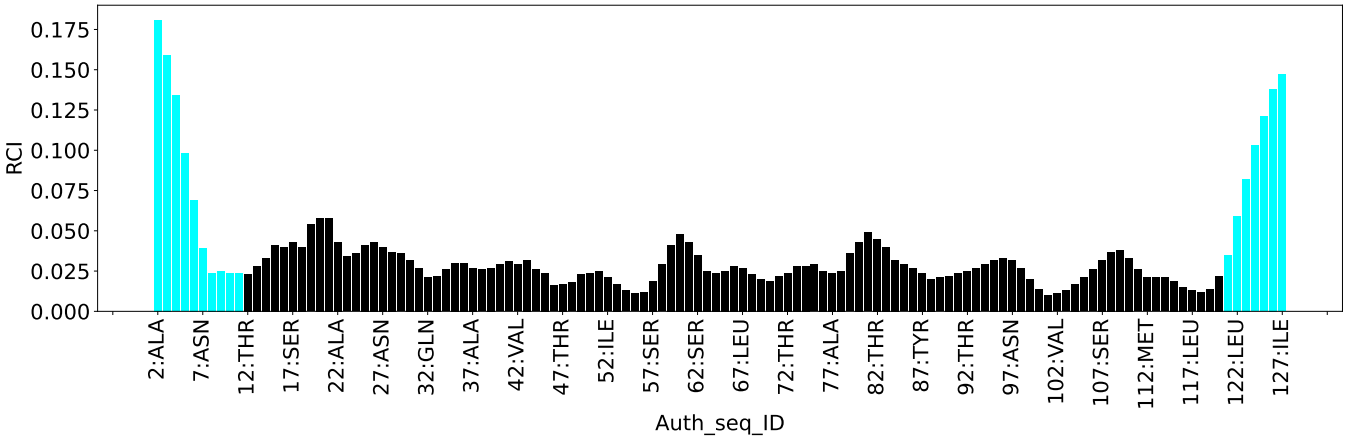
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	117	LEU	HB2	-0.58	-0.07 – 3.30	-6.5
1	A	16	ALA	HB1	-0.09	0.14 – 2.58	-5.9
1	A	16	ALA	HB2	-0.09	0.14 – 2.58	-5.9
1	A	16	ALA	HB3	-0.09	0.14 – 2.58	-5.9
1	A	76	TYR	HD1	5.29	5.49 – 8.39	-5.7
1	A	85	VAL	HB	0.32	0.43 – 3.54	-5.4

7.1.5 Random Coil Index (RCI) plots

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1830
Intra-residue (|i-j|=0)	697
Sequential (|i-j|=1)	324
Medium range (|i-j|>1 and |i-j|<5)	122
Long range (|i-j|≥5)	603
Inter-chain	0
Hydrogen bond restraints	84
Disulfide bond restraints	0
Total dihedral-angle restraints	158
Number of unmapped restraints	58
Number of restraints per residue	14.2
Number of long range restraints per residue[1]	4.9

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	15.2	0.2
0.2-0.5 (Medium)	2.8	0.4
>0.5 (Large)	0.2	0.52

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.8	2.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

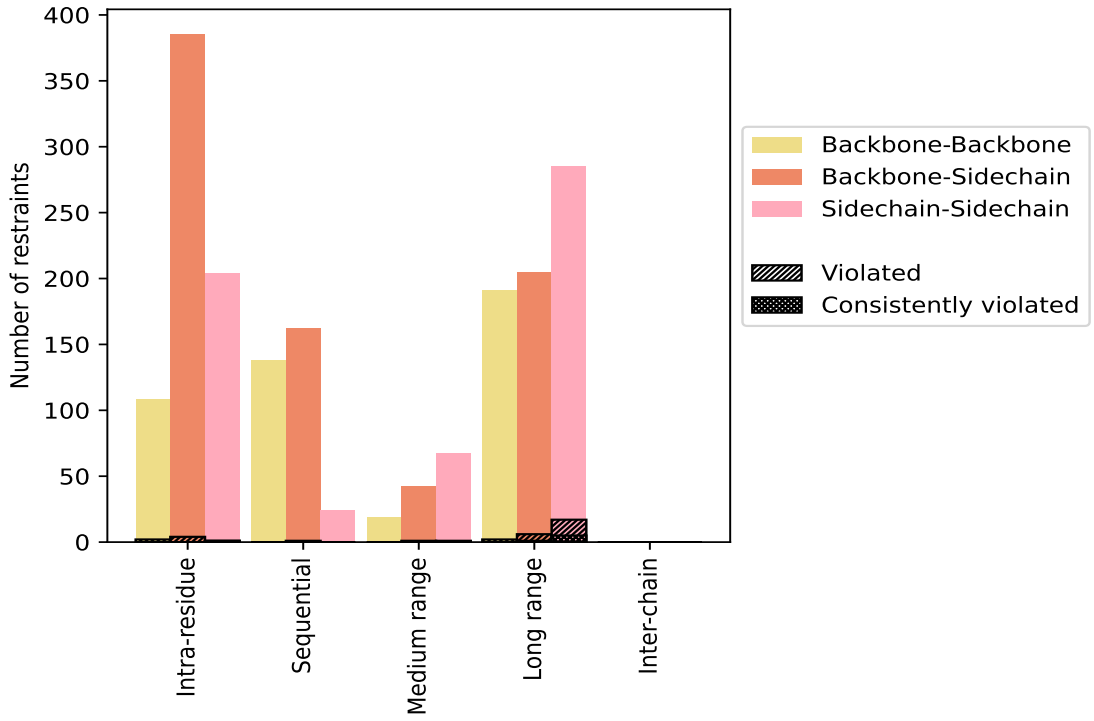
9.1 Summary of distance violations (i)

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)	697	38.1	7	1.0	0.4	1	0.1	0.1
Backbone-Backbone	108	5.9	2	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	385	21.0	4	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	204	11.1	1	0.5	0.1	1	0.5	0.1
Sequential (|i-j|=1)	324	17.7	1	0.3	0.1	0	0.0	0.0
Backbone-Backbone	138	7.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	162	8.9	1	0.6	0.1	0	0.0	0.0
Sidechain-Sidechain	24	1.3	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	122	6.7	2	1.6	0.1	0	0.0	0.0
Backbone-Backbone	13	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	42	2.3	1	2.4	0.1	0	0.0	0.0
Sidechain-Sidechain	67	3.7	1	1.5	0.1	0	0.0	0.0
Long range (|i-j|≥5)	603	33.0	24	4.0	1.3	6	1.0	0.3
Backbone-Backbone	113	6.2	1	0.9	0.1	0	0.0	0.0
Backbone-Sidechain	205	11.2	6	2.9	0.3	1	0.5	0.1
Sidechain-Sidechain	285	15.6	17	6.0	0.9	5	1.8	0.3
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	84	4.6	1	1.2	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1830	100.0	35	1.9	1.9	7	0.4	0.4
Backbone-Backbone	456	24.9	4	0.9	0.2	0	0.0	0.0
Backbone-Sidechain	794	43.4	12	1.5	0.7	1	0.1	0.1
Sidechain-Sidechain	580	31.7	19	3.3	1.0	6	1.0	0.3

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

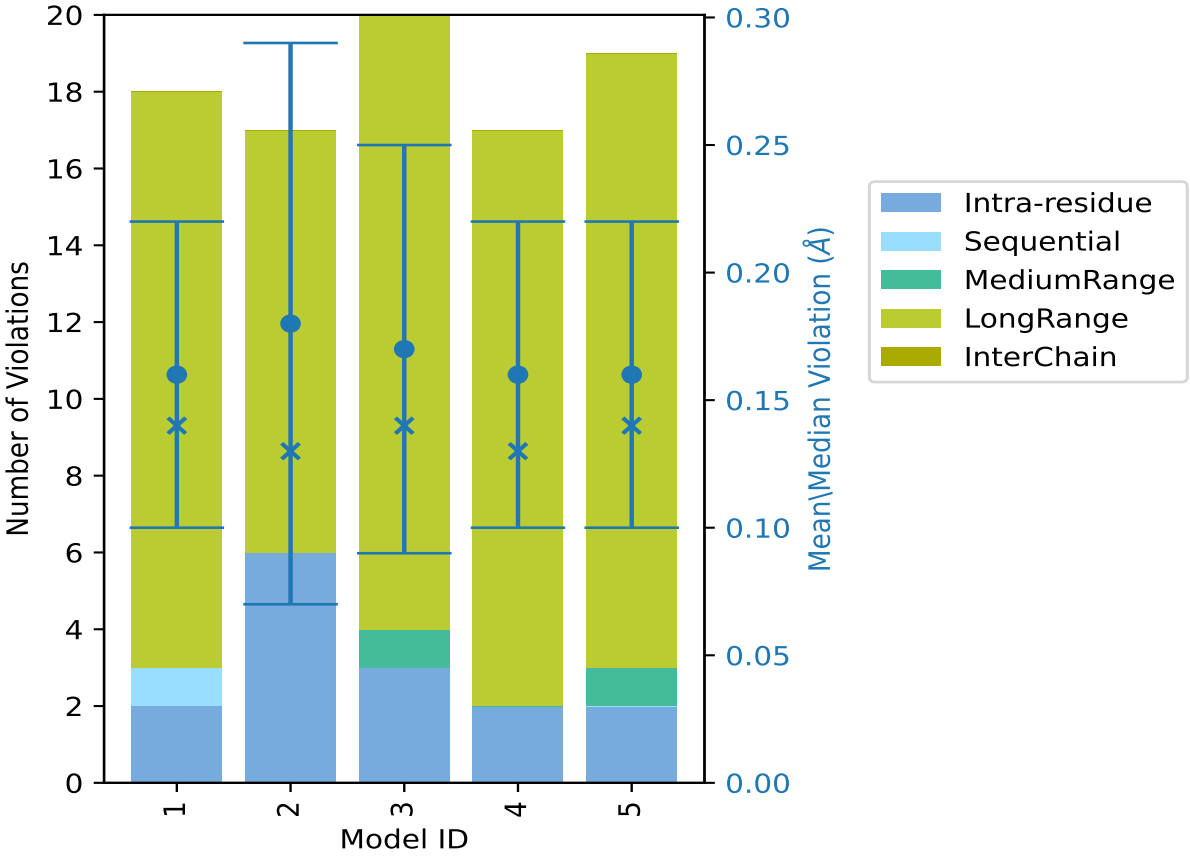
9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	2	1	0	15	0	18	0.16	0.37	0.06	0.14
2	6	0	0	11	0	17	0.18	0.52	0.11	0.13
3	3	0	1	16	0	20	0.17	0.4	0.08	0.14
4	2	0	0	15	0	17	0.16	0.38	0.06	0.13
5	2	0	1	16	0	19	0.16	0.34	0.06	0.14

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

9.3 Distance violation statistics for the ensemble

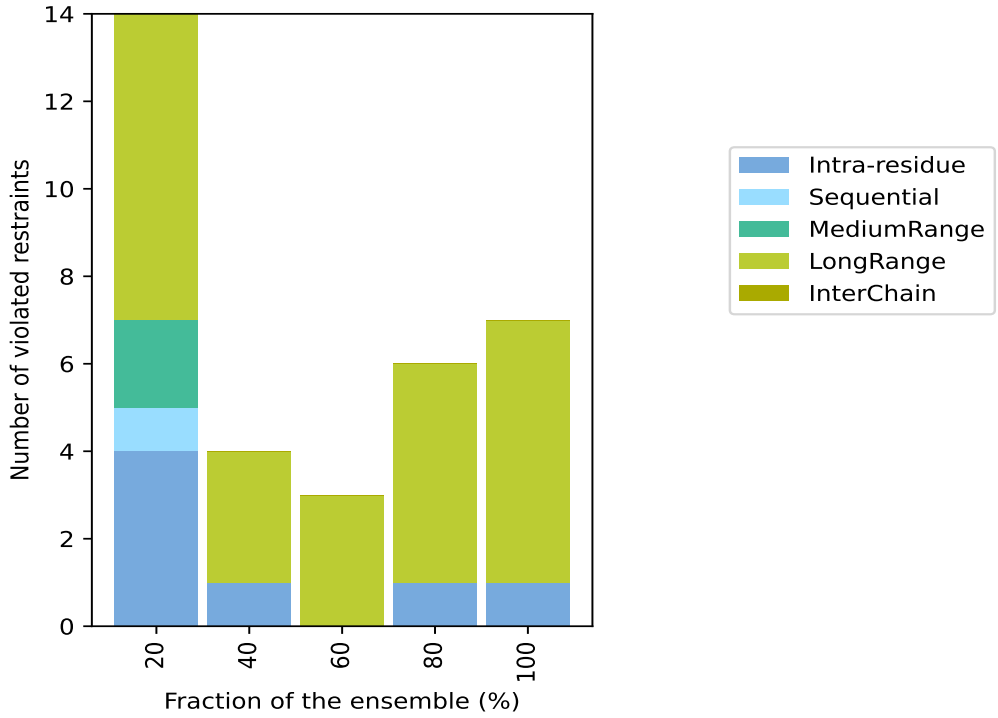
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1712(IR:690, SQ:323, MR:120, LR:579, IC:0) restraints are 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]	%
4	1	2	7	0	14	1	20.0
1	0	0	3	0	4	2	40.0
0	0	0	3	0	3	3	60.0
1	0	0	5	0	6	4	80.0
1	0	0	6	0	7	5	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints,

[5]Inter-chain restraints, [6] Number of models with violations

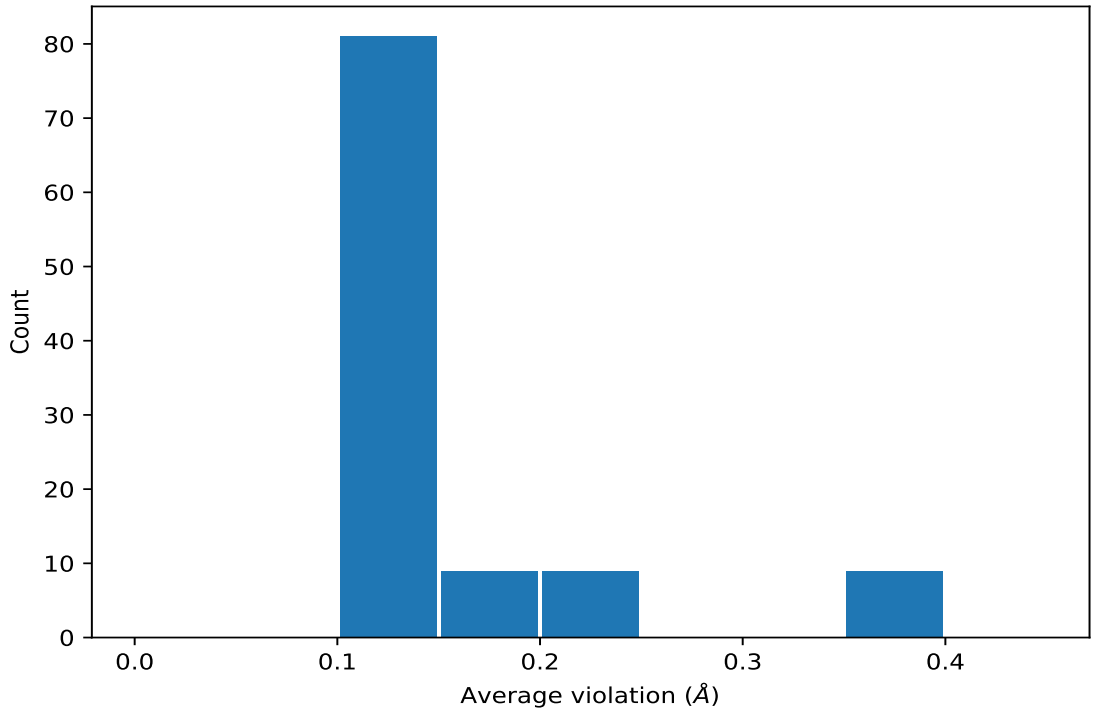
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG21	5	0.37	0.02	0.37
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG22	5	0.37	0.02	0.37
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG23	5	0.37	0.02	0.37
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG21	5	0.37	0.02	0.37
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG22	5	0.37	0.02	0.37
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG23	5	0.37	0.02	0.37
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG21	5	0.37	0.02	0.37
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG22	5	0.37	0.02	0.37
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG23	5	0.37	0.02	0.37
(1,221)	1:A:18:ILE:HG12	1:A:24:LEU:HG	5	0.19	0.02	0.19
(1,221)	1:A:18:ILE:HG13	1:A:24:LEU:HG	5	0.19	0.02	0.19
(1,1565)	1:A:104:VAL:HB	1:A:109:TRP:HE3	5	0.18	0.01	0.18
(1,478)	1:A:34:ALA:HA	1:A:104:VAL:HG11	5	0.17	0.05	0.18
(1,478)	1:A:34:ALA:HA	1:A:104:VAL:HG12	5	0.17	0.05	0.18
(1,478)	1:A:34:ALA:HA	1:A:104:VAL:HG13	5	0.17	0.05	0.18
(1,1540)	1:A:102:VAL:HG11	1:A:117:LEU:HG	5	0.16	0.02	0.15

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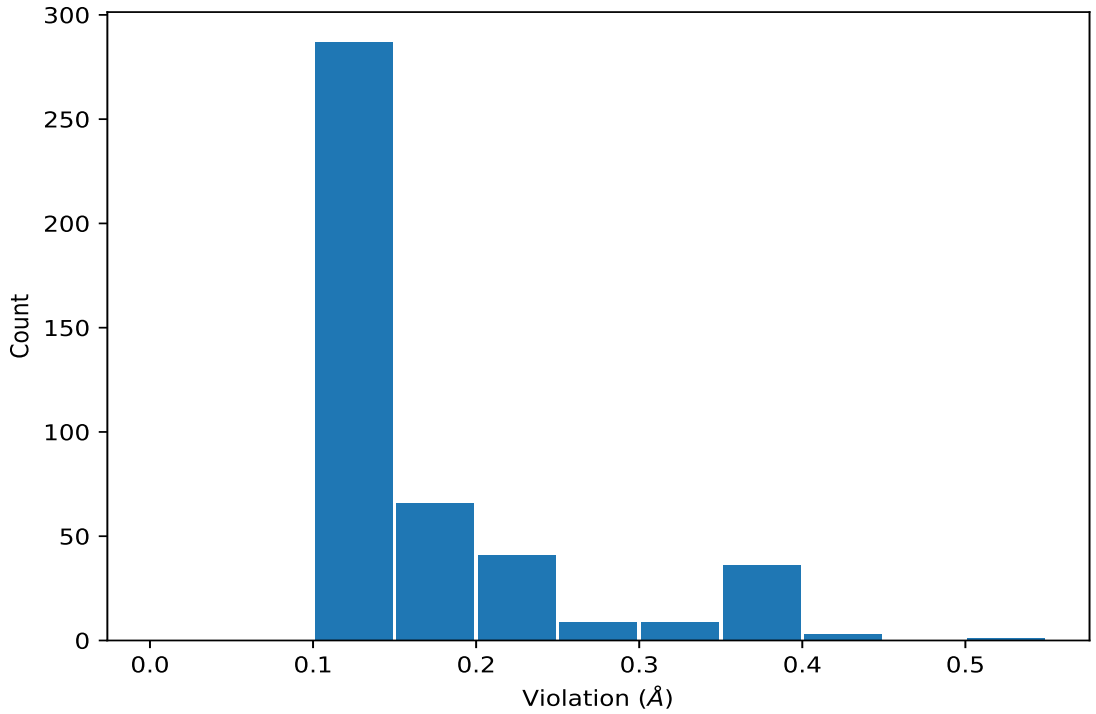
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1540)	1:A:102:VAL:HG12	1:A:117:LEU:HG	5	0.16	0.02	0.15
(1,1540)	1:A:102:VAL:HG13	1:A:117:LEU:HG	5	0.16	0.02	0.15
(1,288)	1:A:22:ALA:HB1	1:A:31:LEU:HD21	5	0.13	0.01	0.13
(1,288)	1:A:22:ALA:HB1	1:A:31:LEU:HD22	5	0.13	0.01	0.13
(1,288)	1:A:22:ALA:HB1	1:A:31:LEU:HD23	5	0.13	0.01	0.13
(1,288)	1:A:22:ALA:HB2	1:A:31:LEU:HD21	5	0.13	0.01	0.13
(1,288)	1:A:22:ALA:HB2	1:A:31:LEU:HD22	5	0.13	0.01	0.13
(1,288)	1:A:22:ALA:HB2	1:A:31:LEU:HD23	5	0.13	0.01	0.13
(1,288)	1:A:22:ALA:HB3	1:A:31:LEU:HD21	5	0.13	0.01	0.13
(1,288)	1:A:22:ALA:HB3	1:A:31:LEU:HD22	5	0.13	0.01	0.13
(1,288)	1:A:22:ALA:HB3	1:A:31:LEU:HD23	5	0.13	0.01	0.13
(1,1537)	1:A:102:VAL:HG21	1:A:112:MET:HE1	5	0.12	0.01	0.12
(1,1537)	1:A:102:VAL:HG21	1:A:112:MET:HE2	5	0.12	0.01	0.12
(1,1537)	1:A:102:VAL:HG21	1:A:112:MET:HE3	5	0.12	0.01	0.12
(1,1537)	1:A:102:VAL:HG22	1:A:112:MET:HE1	5	0.12	0.01	0.12
(1,1537)	1:A:102:VAL:HG22	1:A:112:MET:HE2	5	0.12	0.01	0.12
(1,1537)	1:A:102:VAL:HG22	1:A:112:MET:HE3	5	0.12	0.01	0.12
(1,1537)	1:A:102:VAL:HG23	1:A:112:MET:HE1	5	0.12	0.01	0.12
(1,1537)	1:A:102:VAL:HG23	1:A:112:MET:HE2	5	0.12	0.01	0.12
(1,1537)	1:A:102:VAL:HG23	1:A:112:MET:HE3	5	0.12	0.01	0.12
(1,828)	1:A:52:ILE:HG21	1:A:67:LEU:HD11	4	0.24	0.02	0.24
(1,828)	1:A:52:ILE:HG21	1:A:67:LEU:HD12	4	0.24	0.02	0.24
(1,828)	1:A:52:ILE:HG21	1:A:67:LEU:HD13	4	0.24	0.02	0.24
(1,828)	1:A:52:ILE:HG22	1:A:67:LEU:HD11	4	0.24	0.02	0.24
(1,828)	1:A:52:ILE:HG22	1:A:67:LEU:HD12	4	0.24	0.02	0.24
(1,828)	1:A:52:ILE:HG22	1:A:67:LEU:HD13	4	0.24	0.02	0.24
(1,828)	1:A:52:ILE:HG23	1:A:67:LEU:HD11	4	0.24	0.02	0.24
(1,828)	1:A:52:ILE:HG23	1:A:67:LEU:HD12	4	0.24	0.02	0.24
(1,828)	1:A:52:ILE:HG23	1:A:67:LEU:HD13	4	0.24	0.02	0.24
(1,271)	1:A:21:PRO:HG2	1:A:31:LEU:HB2	4	0.14	0.03	0.14
(1,271)	1:A:21:PRO:HG2	1:A:31:LEU:HB3	4	0.14	0.03	0.14
(1,271)	1:A:21:PRO:HG3	1:A:31:LEU:HB2	4	0.14	0.03	0.14
(1,271)	1:A:21:PRO:HG3	1:A:31:LEU:HB3	4	0.14	0.03	0.14
(1,229)	1:A:18:ILE:HG12	1:A:31:LEU:HD21	4	0.12	0.01	0.12

[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)
(1,1338)	1:A:83:VAL:HB	1:A:83:VAL:H	2	0.52
(1,1446)	1:A:93:LEU:HA	1:A:93:LEU:HD21	3	0.4
(1,1446)	1:A:93:LEU:HA	1:A:93:LEU:HD22	3	0.4
(1,1446)	1:A:93:LEU:HA	1:A:93:LEU:HD23	3	0.4
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG21	3	0.39
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG22	3	0.39
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG23	3	0.39
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG21	3	0.39
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG22	3	0.39
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG23	3	0.39
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG21	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG22	3	0.39
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG23	3	0.39
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG21	4	0.38
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG22	4	0.38
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG23	4	0.38
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG21	4	0.38
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG22	4	0.38
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG23	4	0.38
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG21	4	0.38
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG22	4	0.38
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG23	4	0.38
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG21	1	0.37
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG22	1	0.37
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG23	1	0.37
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG21	1	0.37
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG22	1	0.37
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG23	1	0.37
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG21	1	0.37
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG22	1	0.37
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG23	1	0.37
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG21	2	0.36
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG22	2	0.36
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG23	2	0.36
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG21	2	0.36
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG22	2	0.36
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG23	2	0.36
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG21	2	0.36
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG22	2	0.36
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG23	2	0.36
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG21	5	0.34
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG22	5	0.34
(1,207)	1:A:18:ILE:HD11	1:A:18:ILE:HG23	5	0.34
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG21	5	0.34
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG22	5	0.34
(1,207)	1:A:18:ILE:HD12	1:A:18:ILE:HG23	5	0.34
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG21	5	0.34
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG22	5	0.34
(1,207)	1:A:18:ILE:HD13	1:A:18:ILE:HG23	5	0.34
(1,828)	1:A:52:ILE:HG21	1:A:67:LEU:HD11	3	0.26
(1,828)	1:A:52:ILE:HG21	1:A:67:LEU:HD12	3	0.26
(1,828)	1:A:52:ILE:HG21	1:A:67:LEU:HD13	3	0.26
(1,828)	1:A:52:ILE:HG22	1:A:67:LEU:HD11	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:A:52:ILE:HG22	1:A:67:LEU:HD12	3	0.26
(1,828)	1:A:52:ILE:HG22	1:A:67:LEU:HD13	3	0.26
(1,828)	1:A:52:ILE:HG23	1:A:67:LEU:HD11	3	0.26
(1,828)	1:A:52:ILE:HG23	1:A:67:LEU:HD12	3	0.26
(1,828)	1:A:52:ILE:HG23	1:A:67:LEU:HD13	3	0.26
(1,828)	1:A:52:ILE:HG21	1:A:67:LEU:HD11	1	0.24
(1,828)	1:A:52:ILE:HG21	1:A:67:LEU:HD12	1	0.24
(1,828)	1:A:52:ILE:HG21	1:A:67:LEU:HD13	1	0.24
(1,828)	1:A:52:ILE:HG22	1:A:67:LEU:HD11	1	0.24
(1,828)	1:A:52:ILE:HG22	1:A:67:LEU:HD12	1	0.24
(1,828)	1:A:52:ILE:HG22	1:A:67:LEU:HD13	1	0.24
(1,828)	1:A:52:ILE:HG23	1:A:67:LEU:HD11	1	0.24
(1,828)	1:A:52:ILE:HG23	1:A:67:LEU:HD12	1	0.24
(1,828)	1:A:52:ILE:HG23	1:A:67:LEU:HD13	1	0.24
(1,828)	1:A:52:ILE:HG21	1:A:67:LEU:HD11	5	0.23

10 Dihedral-angle violation analysis

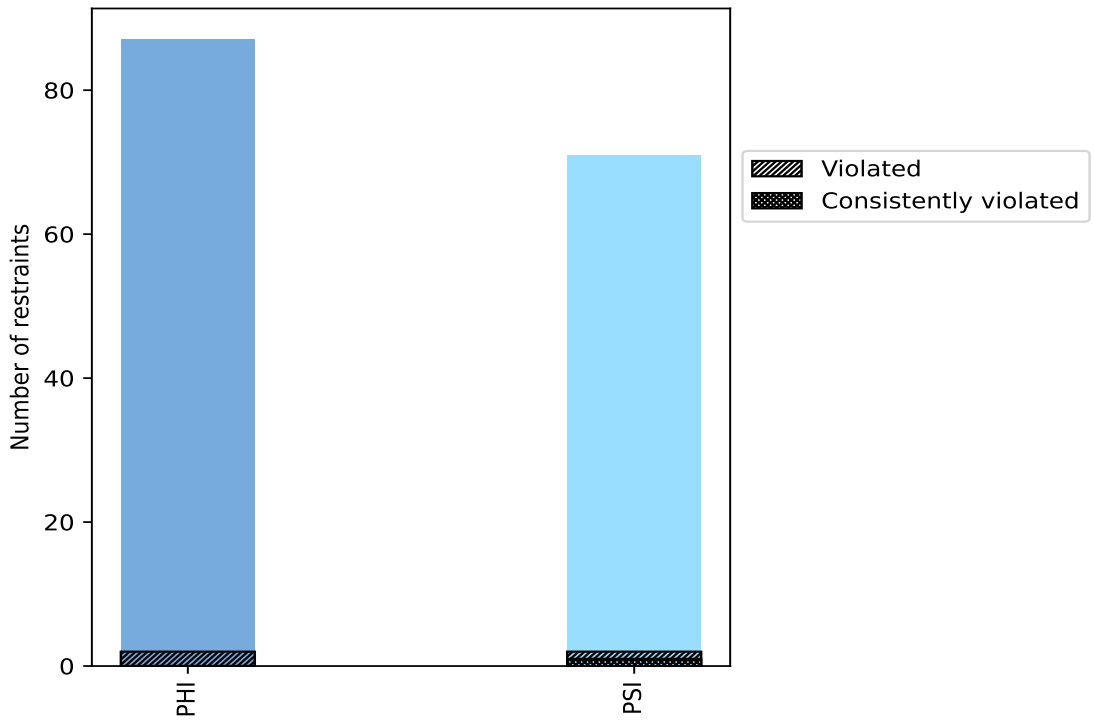
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	87	55.1	2	2.3	1.3	0	0.0	0.0
PSI	71	44.9	2	2.8	1.3	1	1.4	0.6
Total	158	100.0	4	2.5	2.5	1	0.6	0.6

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



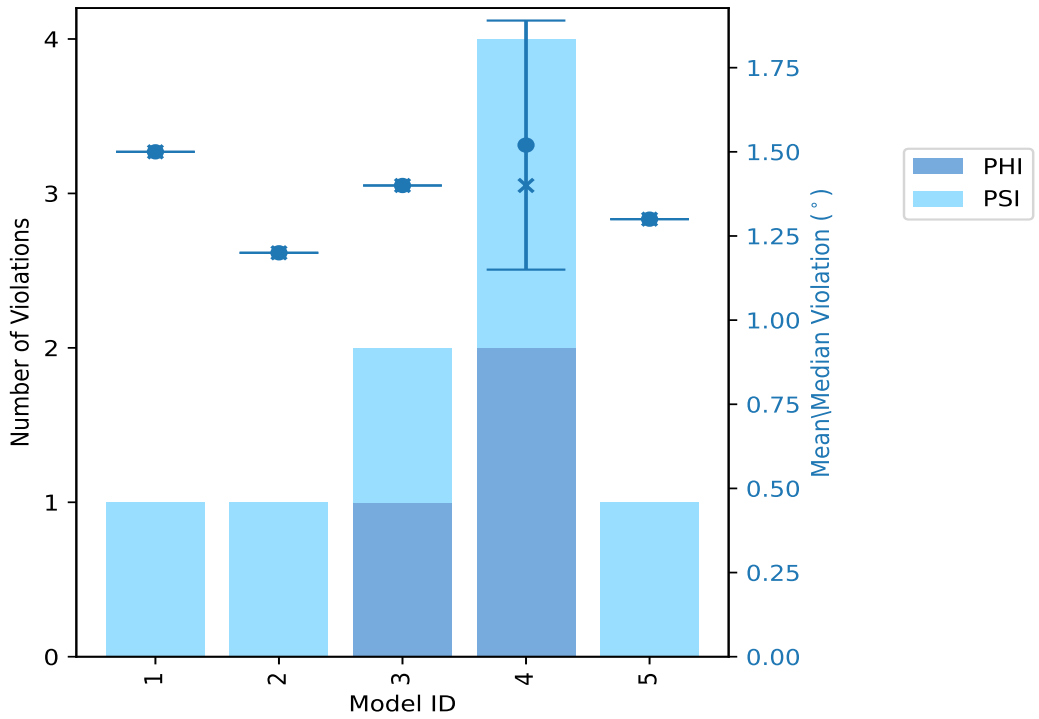
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	1	1	1.5	1.5	0.0	1.5
2	0	1	1	1.2	1.2	0.0	1.2
3	1	1	2	1.4	1.4	0.0	1.4
4	2	2	4	1.52	2.1	0.37	1.4
5	0	1	1	1.3	1.3	0.0	1.3

10.2.1 Bar graph : Dihedral violation statistics for each model



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

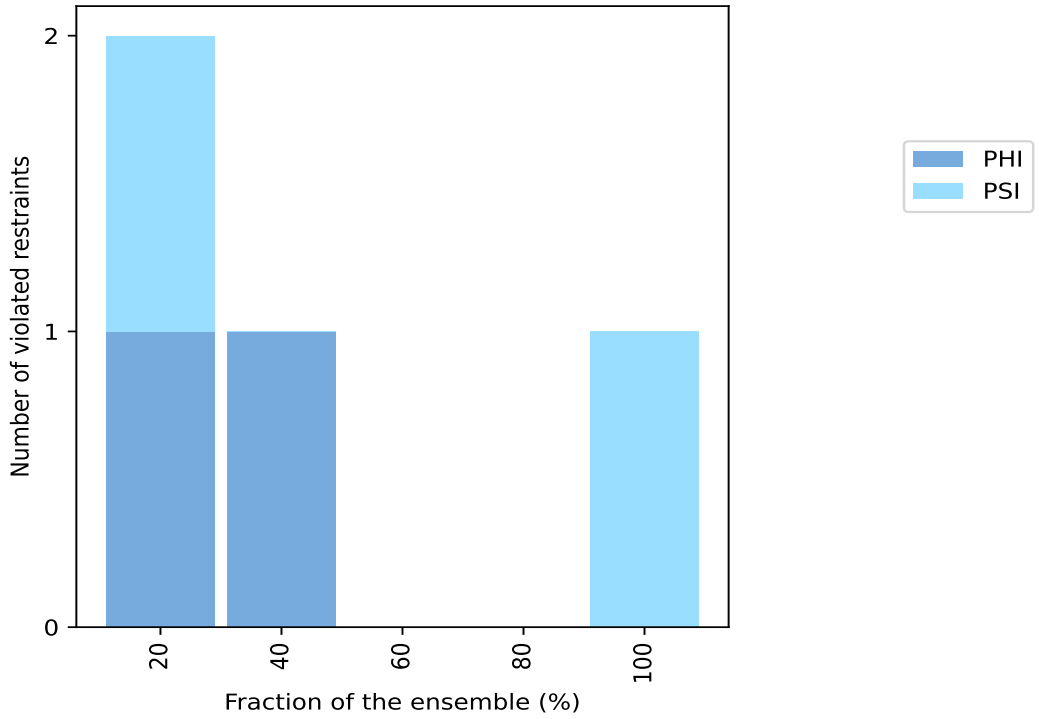
10.3 Dihedral-angle violation statistics for the ensemble

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
1	1	2	1	20.0
1	0	1	2	40.0
0	0	0	3	60.0
0	0	0	4	80.0
0	1	1	5	100.0

[1] Number of models with violations

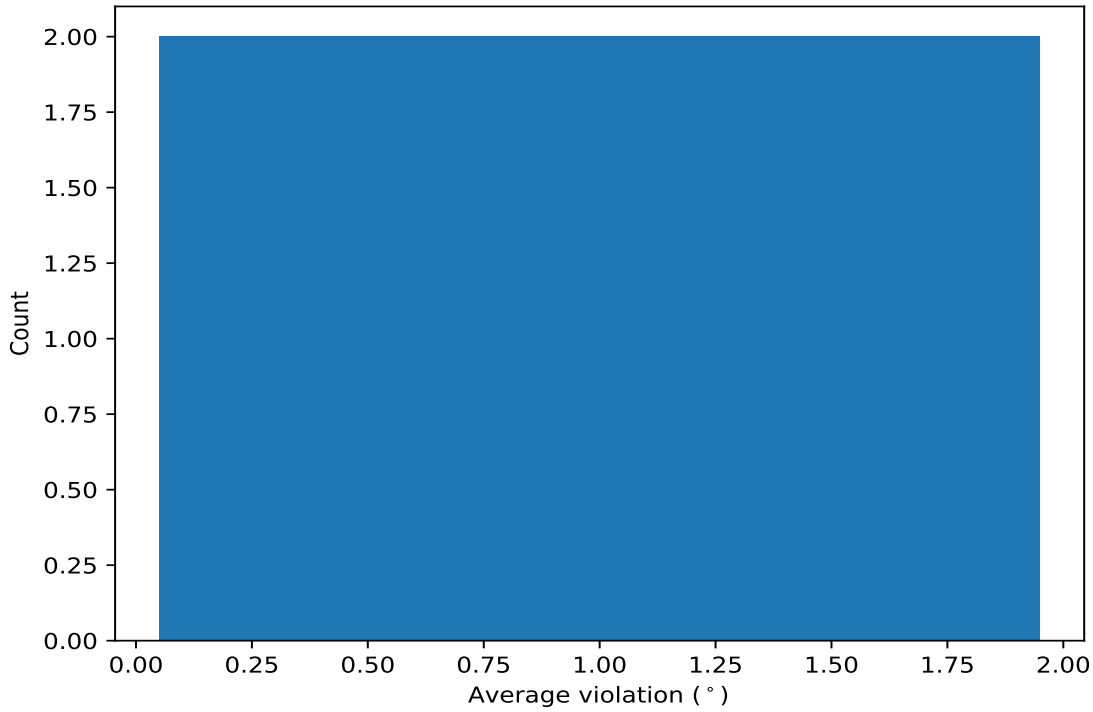
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

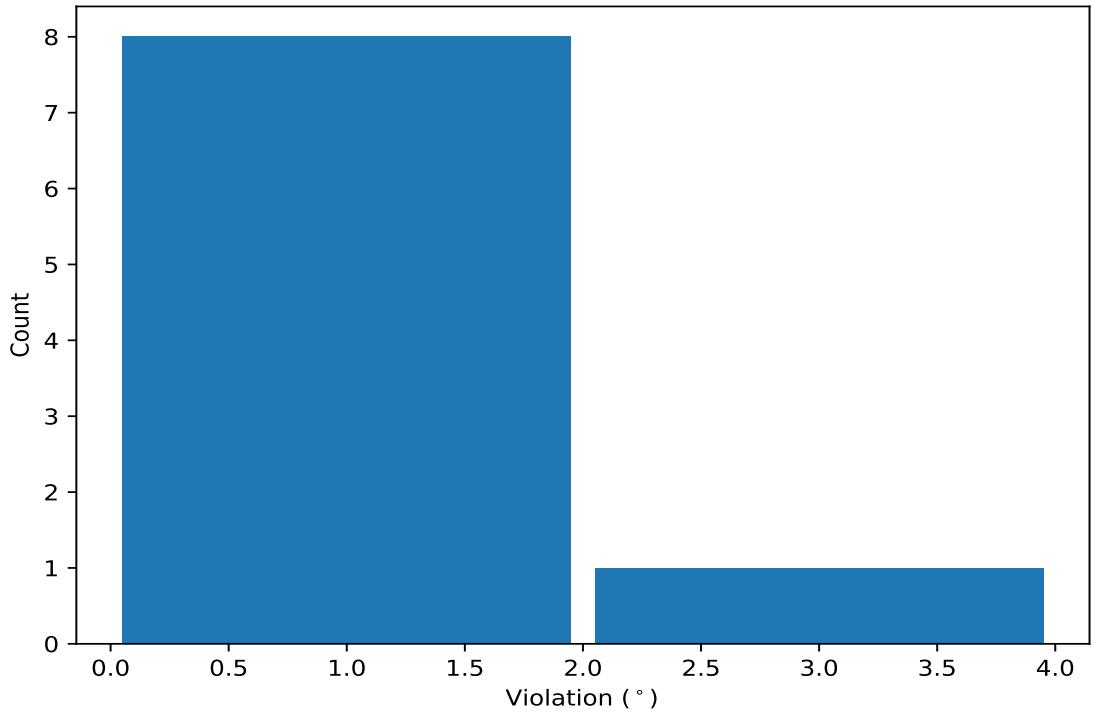
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,86)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ILE:N	5	1.5	0.32	1.4
(1,46)	1:A:89:GLN:C	1:A:90:THR:N	1:A:90:THR:CA	1:A:90:THR:C	2	1.5	0.1	1.5

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ILE:N	4	2.1
(1,46)	1:A:89:GLN:C	1:A:90:THR:N	1:A:90:THR:CA	1:A:90:THR:C	4	1.6
(1,86)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ILE:N	1	1.5
(1,86)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ILE:N	3	1.4
(1,46)	1:A:89:GLN:C	1:A:90:THR:N	1:A:90:THR:CA	1:A:90:THR:C	3	1.4
(1,86)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ILE:N	5	1.3
(1,86)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ILE:N	2	1.2
(1,66)	1:A:9:TRP:N	1:A:9:TRP:CA	1:A:9:TRP:C	1:A:10:THR:N	4	1.2
(1,59)	1:A:117:LEU:C	1:A:118:LYS:N	1:A:118:LYS:CA	1:A:118:LYS:C	4	1.2