wwPDB NMR Structure Validation Summary Report

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PDB ID	:	4AQZ
Title	:	B2 domain of Neisseria meningitidis Pilus assembly protein PilQ
Authors	:	Phelan, M.M.; Berry, J.L.; Derrick, J.P.; Lian, L.Y.
Deposited on	:	2012-04-20

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:

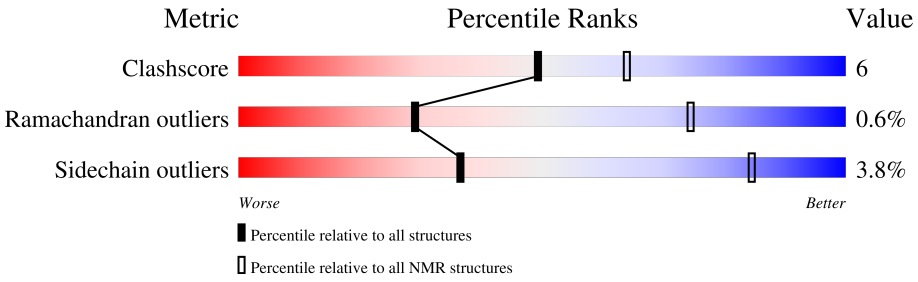
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 91%.

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	138	66% 9% 25%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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:225-A:327 (103)	0.45	15

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2073 atoms, of which 1005 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	138	2073	666	1005	202	196	4	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	MET	-	expression tag	UNP Q70M91
A	193	GLY	-	expression tag	UNP Q70M91
A	194	SER	-	expression tag	UNP Q70M91
A	195	SER	-	expression tag	UNP Q70M91
A	196	HIS	-	expression tag	UNP Q70M91
A	197	HIS	-	expression tag	UNP Q70M91
A	198	HIS	-	expression tag	UNP Q70M91
A	199	HIS	-	expression tag	UNP Q70M91
A	200	HIS	-	expression tag	UNP Q70M91
A	201	HIS	-	expression tag	UNP Q70M91
A	202	GLY	-	expression tag	UNP Q70M91
A	203	LEU	-	expression tag	UNP Q70M91
A	204	VAL	-	expression tag	UNP Q70M91
A	205	PRO	-	expression tag	UNP Q70M91
A	206	ARG	-	expression tag	UNP Q70M91
A	207	GLY	-	expression tag	UNP Q70M91
A	208	SER	-	expression tag	UNP Q70M91
A	209	HIS	-	expression tag	UNP Q70M91
A	210	MET	-	expression tag	UNP Q70M91
A	211	ALA	-	expression tag	UNP Q70M91
A	212	SER	-	expression tag	UNP Q70M91
A	213	MET	-	expression tag	UNP Q70M91
A	214	THR	-	expression tag	UNP Q70M91
A	215	GLY	-	expression tag	UNP Q70M91
A	216	GLY	-	expression tag	UNP Q70M91
A	217	GLN	-	expression tag	UNP Q70M91
A	218	GLN	-	expression tag	UNP Q70M91
A	219	MET	-	expression tag	UNP Q70M91
A	220	GLY	-	expression tag	UNP Q70M91
A	221	ARG	-	expression tag	UNP Q70M91

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Chain	Residue	Modelled	Actual	Comment	Reference
A	222	GLY	-	expression tag	UNP Q70M91
A	223	SER	-	expression tag	UNP Q70M91

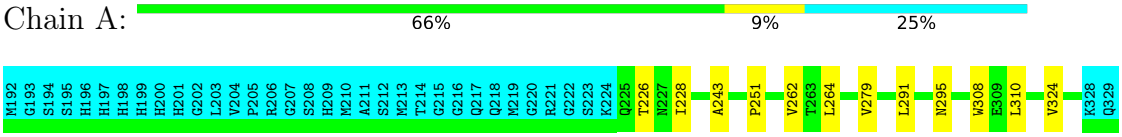
4 Residue-property plots (i)

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: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

Chain A:

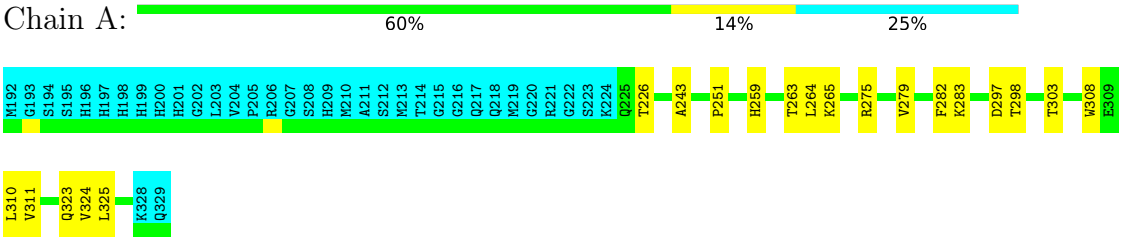


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 15. Colouring as in section 4.1 above.

• Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CYANA2.1 AND CNS1.2 WATER REFINEMENT*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
CYANA	refinement	
TopSpin	structure solution	
CcpNmr Analysis	structure solution	ANALYSIS
CYANA	structure solution	
CNS	structure solution	
TALOS+	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	1626
Number of shifts mapped to atoms	1556
Number of unparsed shifts	0
Number of shifts with mapping errors	70
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality

6.1 Standard geometry

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	0.89±0.03	0±0/822 (0.0± 0.0%)	0.71±0.03	0±0/1119 (0.0± 0.0%)
All	All	0.89	0/16440 (0.0%)	0.71	1/22380 (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	0.1±0.4
All	All	0	3

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	231	ARG	NE-CZ-NH2	-5.09	117.75	120.30	10	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	231	ARG	Sidechain	2
1	A	293	ARG	Sidechain	1

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	806	755	822	10±2
All	All	16120	15100	16440	197

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 6.

5 of 62 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:251:PRO:HB3	1:A:264:LEU:HD13	0.65	1.68	3	12
1:A:308:TRP:CZ3	1:A:310:LEU:HB2	0.64	2.28	15	11
1:A:279:VAL:HA	1:A:282:PHE:CD2	0.61	2.30	14	3
1:A:225:GLN:O	1:A:245:LEU:HD23	0.60	1.96	10	1
1:A:226:THR:HA	1:A:243:ALA:O	0.60	1.97	18	17

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	103/138 (75%)	99±2 (96±2%)	4±2 (4±2%)	1±1 (1±1%)	29	74
All	All	2060/2760 (75%)	1971 (96%)	77 (4%)	12 (1%)	29	74

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	295	ASN	6
1	A	279	VAL	5
1	A	225	GLN	1

6.3.2 Protein sidechains

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	89/116 (77%)	86±2 (96±2%)	3±2 (4±2%)	36 84
All	All	1780/2320 (77%)	1712 (96%)	68 (4%)	36 84

5 of 24 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	291	LEU	7
1	A	262	VAL	6
1	A	283	LYS	6
1	A	324	VAL	5
1	A	296	ASN	5

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

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 91% 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*

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	1626
Number of shifts mapped to atoms	1556
Number of unparsed shifts	0
Number of shifts with mapping errors	70
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 70) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	211	ALA	HB2	1.311	0.000	4
1	A	211	ALA	HB3	1.311	0.000	4
1	A	214	THR	HG22	1.112	0.001	4
1	A	214	THR	HG23	1.112	0.001	4
1	A	226	THR	HG22	1.071	0.000	4
1	A	226	THR	HG23	1.071	0.000	4
1	A	228	ILE	HD12	0.594	0.001	4
1	A	228	ILE	HD13	0.594	0.001	4
1	A	228	ILE	HG22	0.856	0.003	4
1	A	228	ILE	HG23	0.856	0.003	4
1	A	237	ALA	HB2	1.275	0.000	4
1	A	237	ALA	HB3	1.275	0.000	4
1	A	239	ILE	HD12	0.549	0.001	4
1	A	239	ILE	HD13	0.549	0.001	4

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	239	ILE	HG22	0.468	0.002	4
1	A	239	ILE	HG23	0.468	0.002	4
1	A	240	ILE	HD12	1.017	0.001	4
1	A	240	ILE	HD13	1.017	0.001	4
1	A	240	ILE	HG22	0.923	0.003	4
1	A	240	ILE	HG23	0.923	0.003	4
1	A	242	LEU	HD12	0.722	0.005	2
1	A	242	LEU	HD13	0.722	0.005	2
1	A	242	LEU	HD22	0.733	0.000	2
1	A	242	LEU	HD23	0.733	0.000	2
1	A	243	ALA	HB2	1.106	0.000	4
1	A	243	ALA	HB3	1.106	0.000	4
1	A	244	ALA	HB2	0.598	0.000	4
1	A	244	ALA	HB3	0.598	0.000	4
1	A	245	LEU	HD12	0.687	0.007	2
1	A	245	LEU	HD13	0.687	0.007	2
1	A	245	LEU	HD22	0.806	0.002	2
1	A	245	LEU	HD23	0.806	0.002	2
1	A	248	ALA	HB2	1.179	0.000	4
1	A	248	ALA	HB3	1.179	0.000	4
1	A	253	ILE	HD12	0.845	0.002	4
1	A	253	ILE	HD13	0.845	0.002	4
1	A	253	ILE	HG22	0.601	0.004	4
1	A	253	ILE	HG23	0.601	0.004	4
1	A	260	ILE	HD12	-0.011	0.001	4
1	A	260	ILE	HD13	-0.011	0.001	4
1	A	260	ILE	HG22	0.502	0.001	4
1	A	260	ILE	HG23	0.502	0.001	4
1	A	261	ILE	HD12	0.725	0.001	4
1	A	261	ILE	HD13	0.725	0.001	4
1	A	261	ILE	HG22	0.610	0.007	4
1	A	261	ILE	HG23	0.610	0.007	4
1	A	262	VAL	HG12	0.048	0.001	2
1	A	262	VAL	HG13	0.048	0.001	2
1	A	262	VAL	HG22	0.375	0.001	2
1	A	262	VAL	HG23	0.375	0.001	2
1	A	263	THR	HG22	0.969	0.000	4
1	A	263	THR	HG23	0.969	0.000	4
1	A	264	LEU	HD12	-0.345	0.001	2
1	A	264	LEU	HD13	-0.345	0.001	2
1	A	264	LEU	HD22	0.061	0.001	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	264	LEU	HD23	0.061	0.001	2
1	A	268	THR	HG22	0.938	0.001	4
1	A	268	THR	HG23	0.938	0.001	4
1	A	269	LEU	HD12	0.527	0.001	2
1	A	269	LEU	HD13	0.527	0.001	2
1	A	269	LEU	HD22	0.825	0.002	2
1	A	269	LEU	HD23	0.825	0.002	2
1	A	271	THR	HG22	1.233	0.002	4
1	A	271	THR	HG23	1.233	0.002	4
1	A	272	THR	HG22	1.225	0.000	4
1	A	272	THR	HG23	1.225	0.000	4
1	A	273	LEU	HD12	0.883	0.003	2
1	A	273	LEU	HD13	0.883	0.003	2
1	A	273	LEU	HD22	0.991	0.001	2
1	A	273	LEU	HD23	0.991	0.001	2
1	A	277	LEU	HD12	0.755	0.002	2
1	A	277	LEU	HD13	0.755	0.002	2
1	A	277	LEU	HD22	0.690	0.001	2
1	A	277	LEU	HD23	0.690	0.001	2
1	A	279	VAL	HG12	-0.580	0.000	2
1	A	279	VAL	HG13	-0.580	0.000	2
1	A	279	VAL	HG22	0.070	0.001	2
1	A	279	VAL	HG23	0.070	0.001	2
1	A	280	ALA	HB2	1.446	0.000	4
1	A	280	ALA	HB3	1.446	0.000	4
1	A	284	THR	HG22	1.001	0.002	4
1	A	284	THR	HG23	1.001	0.002	4
1	A	286	VAL	HG12	0.415	0.001	2
1	A	286	VAL	HG13	0.415	0.001	2
1	A	286	VAL	HG22	0.703	0.001	2
1	A	286	VAL	HG23	0.703	0.001	2
1	A	289	VAL	HG12	0.617	0.001	2
1	A	289	VAL	HG13	0.617	0.001	2
1	A	289	VAL	HG22	0.718	0.001	2
1	A	289	VAL	HG23	0.718	0.001	2
1	A	290	THR	HG22	1.061	0.001	4
1	A	290	THR	HG23	1.061	0.001	4
1	A	291	LEU	HD12	0.638	0.003	2
1	A	291	LEU	HD13	0.638	0.003	2
1	A	291	LEU	HD22	0.739	0.001	2
1	A	291	LEU	HD23	0.739	0.001	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	294	LEU	HD12	0.728	0.005	2
1	A	294	LEU	HD13	0.728	0.005	2
1	A	294	LEU	HD22	0.730	0.000	2
1	A	294	LEU	HD23	0.730	0.000	2
1	A	298	THR	HG22	0.917	0.011	4
1	A	298	THR	HG23	0.917	0.011	4
1	A	300	LEU	HD12	0.483	0.004	2
1	A	300	LEU	HD13	0.483	0.004	2
1	A	300	LEU	HD22	0.663	0.001	2
1	A	300	LEU	HD23	0.663	0.001	2
1	A	301	ILE	HD12	0.660	0.002	4
1	A	301	ILE	HD13	0.660	0.002	4
1	A	301	ILE	HG22	0.658	0.002	4
1	A	301	ILE	HG23	0.658	0.002	4
1	A	302	ILE	HD12	0.343	0.001	4
1	A	302	ILE	HD13	0.343	0.001	4
1	A	302	ILE	HG22	0.540	0.001	4
1	A	302	ILE	HG23	0.540	0.001	4
1	A	303	THR	HG22	1.047	0.001	4
1	A	303	THR	HG23	1.047	0.001	4
1	A	304	THR	HG22	-0.216	0.001	4
1	A	304	THR	HG23	-0.216	0.001	4
1	A	305	ALA	HB2	1.218	0.000	4
1	A	305	ALA	HB3	1.218	0.000	4
1	A	310	LEU	HD12	0.901	0.001	2
1	A	310	LEU	HD13	0.901	0.001	2
1	A	310	LEU	HD22	0.901	0.001	2
1	A	310	LEU	HD23	0.901	0.001	2
1	A	311	VAL	HG12	0.840	0.005	2
1	A	311	VAL	HG13	0.840	0.005	2
1	A	311	VAL	HG22	0.871	0.000	2
1	A	311	VAL	HG23	0.871	0.000	2
1	A	315	ALA	HB2	1.152	0.000	4
1	A	315	ALA	HB3	1.152	0.000	4
1	A	316	ALA	HB2	1.167	0.000	4
1	A	316	ALA	HB3	1.167	0.000	4
1	A	321	THR	HG22	0.912	0.002	4
1	A	321	THR	HG23	0.912	0.002	4
1	A	324	VAL	HG12	0.431	0.004	2
1	A	324	VAL	HG13	0.431	0.004	2
1	A	324	VAL	HG22	0.460	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	324	VAL	HG23	0.460	0.000	2
1	A	325	LEU	HD12	0.822	0.001	2
1	A	325	LEU	HD13	0.822	0.001	2
1	A	325	LEU	HD22	0.822	0.000	2
1	A	325	LEU	HD23	0.822	0.000	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 70) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	228	ILE	HG12	1.465	0.001	2
1	A	228	ILE	HG13	0.905	0.000	2
1	A	228	ILE	HG21	0.856	0.003	4
1	A	228	ILE	HG22	0.856	0.003	4
1	A	228	ILE	HG23	0.856	0.003	4
1	A	239	ILE	HG12	1.079	0.001	2
1	A	239	ILE	HG13	0.688	0.002	2
1	A	239	ILE	HG21	0.468	0.002	4
1	A	239	ILE	HG22	0.468	0.002	4
1	A	239	ILE	HG23	0.468	0.002	4
1	A	240	ILE	HG12	1.641	0.001	2
1	A	240	ILE	HG13	1.364	0.001	2
1	A	240	ILE	HG21	0.923	0.003	4
1	A	240	ILE	HG22	0.923	0.003	4
1	A	240	ILE	HG23	0.923	0.003	4
1	A	253	ILE	HG12	0.734	0.007	2
1	A	253	ILE	HG13	1.446	0.009	2
1	A	253	ILE	HG21	0.601	0.004	4
1	A	253	ILE	HG22	0.601	0.004	4
1	A	253	ILE	HG23	0.601	0.004	4
1	A	260	ILE	HG12	0.655	0.000	2
1	A	260	ILE	HG13	1.129	0.001	2
1	A	260	ILE	HG21	0.502	0.001	4
1	A	260	ILE	HG22	0.502	0.001	4
1	A	260	ILE	HG23	0.502	0.001	4
1	A	261	ILE	HG12	0.911	0.002	2
1	A	261	ILE	HG13	1.424	0.003	2
1	A	261	ILE	HG21	0.61	0.007	4
1	A	261	ILE	HG22	0.61	0.007	4

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	261	ILE	HG23	0.61	0.007	4
1	A	262	VAL	HG11	0.048	0.001	2
1	A	262	VAL	HG12	0.048	0.001	2
1	A	262	VAL	HG21	0.375	0.001	2
1	A	262	VAL	HG22	0.375	0.001	2
1	A	262	VAL	HG23	0.375	0.001	2
1	A	279	VAL	HG11	-0.58	0.000	2
1	A	279	VAL	HG12	-0.58	0.000	2
1	A	279	VAL	HG21	0.07	0.001	2
1	A	279	VAL	HG22	0.07	0.001	2
1	A	279	VAL	HG23	0.07	0.001	2
1	A	286	VAL	HG11	0.415	0.001	2
1	A	286	VAL	HG12	0.415	0.001	2
1	A	286	VAL	HG21	0.703	0.001	2
1	A	286	VAL	HG22	0.703	0.001	2
1	A	286	VAL	HG23	0.703	0.001	2
1	A	289	VAL	HG11	0.617	0.001	2
1	A	289	VAL	HG12	0.617	0.001	2
1	A	289	VAL	HG21	0.718	0.001	2
1	A	289	VAL	HG22	0.718	0.001	2
1	A	289	VAL	HG23	0.718	0.001	2
1	A	301	ILE	HG12	1.29	0.000	2
1	A	301	ILE	HG13	0.865	0.002	2
1	A	301	ILE	HG21	0.658	0.002	4
1	A	301	ILE	HG22	0.658	0.002	4
1	A	301	ILE	HG23	0.658	0.002	4
1	A	302	ILE	HG12	0.611	0.002	2
1	A	302	ILE	HG13	1.333	0.000	2
1	A	302	ILE	HG21	0.54	0.001	4
1	A	302	ILE	HG22	0.54	0.001	4
1	A	302	ILE	HG23	0.54	0.001	4
1	A	311	VAL	HG11	0.84	0.005	2
1	A	311	VAL	HG12	0.84	0.005	2
1	A	311	VAL	HG21	0.871	0.000	2
1	A	311	VAL	HG22	0.871	0.000	2
1	A	311	VAL	HG23	0.871	0.000	2
1	A	324	VAL	HG11	0.431	0.004	2
1	A	324	VAL	HG12	0.431	0.004	2
1	A	324	VAL	HG21	0.46	0.000	2
1	A	324	VAL	HG22	0.46	0.000	2
1	A	324	VAL	HG23	0.46	0.000	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
$^{13}C_{\alpha}$	123	-0.07 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	113	0.08 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	123	-1.80 ± 0.27	Should be applied
^{15}N	116	-0.83 ± 0.45	None needed (imprecise)

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 91%, i.e. 1297 atoms were assigned a chemical shift out of a possible 1424. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	511/511 (100%)	207/207 (100%)	206/206 (100%)	98/98 (100%)
Sidechain	722/818 (88%)	492/532 (92%)	225/254 (89%)	5/32 (16%)
Aromatic	64/95 (67%)	32/47 (68%)	31/41 (76%)	1/7 (14%)
Overall	1297/1424 (91%)	731/786 (93%)	462/501 (92%)	104/137 (76%)

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.

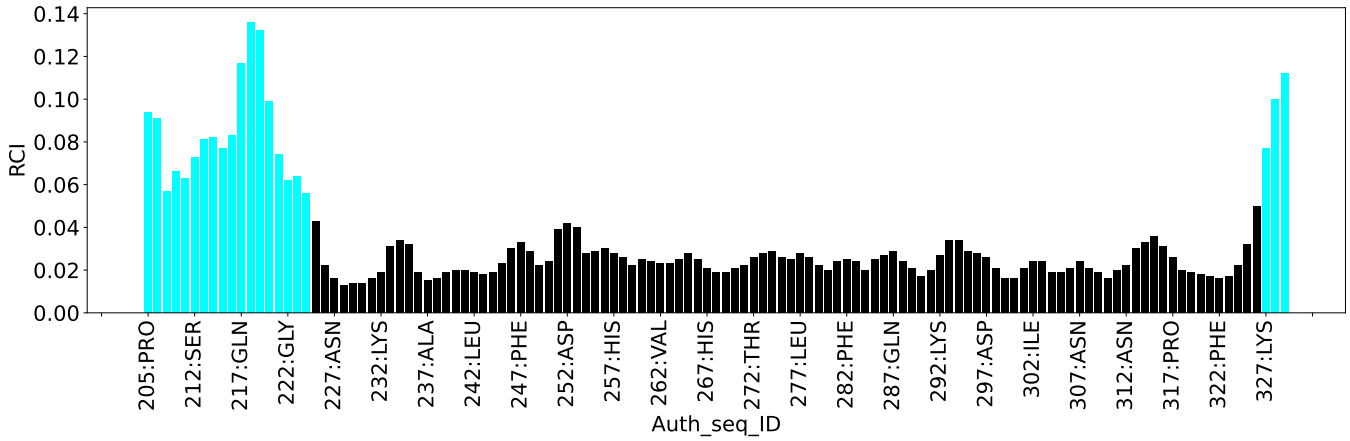
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	304	THR	HG21	-0.22	0.08 – 2.19	-6.4
1	A	304	THR	HG22	-0.22	0.08 – 2.19	-6.4
1	A	304	THR	HG23	-0.22	0.08 – 2.19	-6.4
1	A	279	VAL	HG11	-0.58	-0.48 – 2.12	-5.4
1	A	279	VAL	HG12	-0.58	-0.48 – 2.12	-5.4
1	A	279	VAL	HG13	-0.58	-0.48 – 2.12	-5.4

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

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	2607
Intra-residue (|i-j|=0)	523
Sequential (|i-j|=1)	667
Medium range (|i-j|>1 and |i-j|<5)	274
Long range (|i-j|≥5)	1143
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	154
Number of unmapped restraints	331
Number of restraints per residue	20.0
Number of long range restraints per residue[1]	8.3

[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)	17.4	0.2
0.2-0.5 (Medium)	21.4	0.5
>0.5 (Large)	110.0	6.47

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)	5.5	3.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

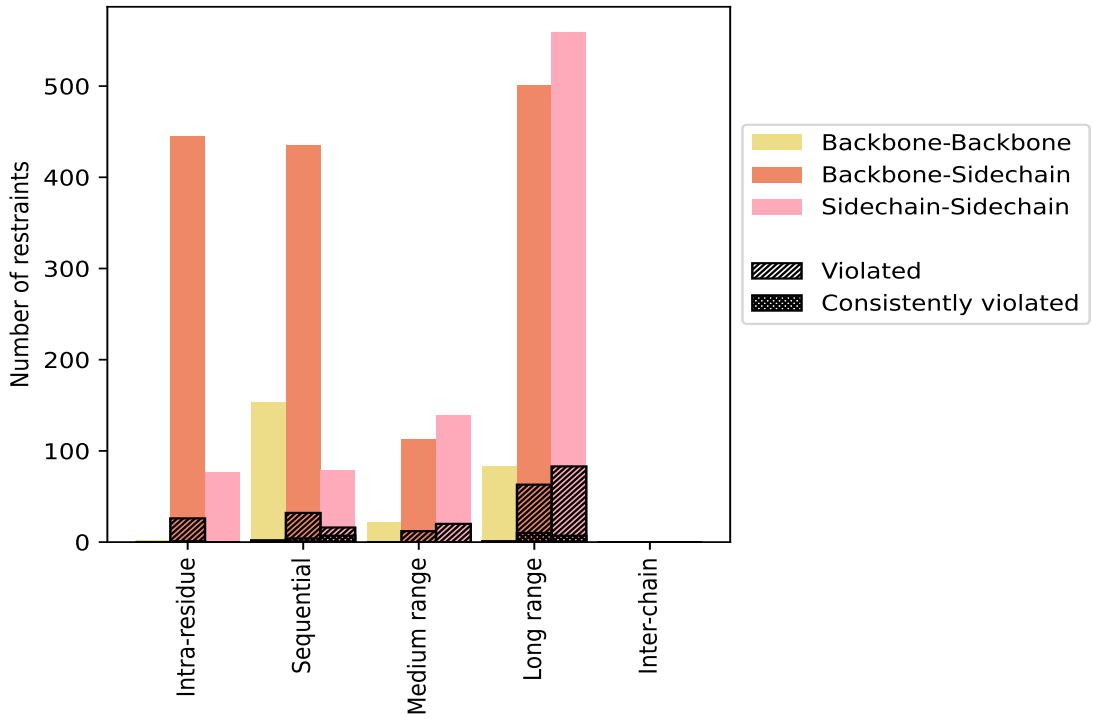
9.1 Summary of distance violations (i)

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)	523	20.1	26	5.0	1.0	1	0.2	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	445	17.1	26	5.8	1.0	1	0.2	0.0
Sidechain-Sidechain	76	2.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	667	25.6	50	7.5	1.9	11	1.6	0.4
Backbone-Backbone	153	5.9	2	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	435	16.7	32	7.4	1.2	4	0.9	0.2
Sidechain-Sidechain	79	3.0	16	20.3	0.6	7	8.9	0.3
Medium range (|i-j|>1 & |i-j|<5)	274	10.5	32	11.7	1.2	0	0.0	0.0
Backbone-Backbone	22	0.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	113	4.3	12	10.6	0.5	0	0.0	0.0
Sidechain-Sidechain	139	5.3	20	14.4	0.8	0	0.0	0.0
Long range (|i-j|≥5)	1143	43.8	147	12.9	5.6	17	1.5	0.7
Backbone-Backbone	83	3.2	1	1.2	0.0	0	0.0	0.0
Backbone-Sidechain	501	19.2	63	12.6	2.4	10	2.0	0.4
Sidechain-Sidechain	559	21.4	83	14.8	3.2	7	1.3	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	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	2607	100.0	255	9.8	9.8	29	1.1	1.1
Backbone-Backbone	260	10.0	3	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	1494	57.3	133	8.9	5.1	15	1.0	0.6
Sidechain-Sidechain	853	32.7	119	14.0	4.6	14	1.6	0.5

[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	14	31	16	79	0	140	1.35	3.91	0.99	1.02
2	12	35	23	92	0	162	1.35	4.23	1.06	1.09
3	10	32	23	77	0	142	1.2	4.15	0.95	0.94
4	17	33	21	75	0	146	1.31	3.44	0.9	1.1
5	14	34	20	81	0	149	1.36	4.95	0.98	1.19
6	15	26	22	82	0	145	1.12	3.85	0.88	1.02
7	9	30	18	82	0	139	1.32	6.23	1.14	1.0
8	14	30	23	85	0	152	1.4	4.02	0.98	1.27
9	6	34	19	88	0	147	1.48	6.47	1.23	1.21
10	14	36	19	90	0	159	1.37	4.0	1.05	1.21
11	15	31	20	82	0	148	1.31	4.12	0.94	1.07

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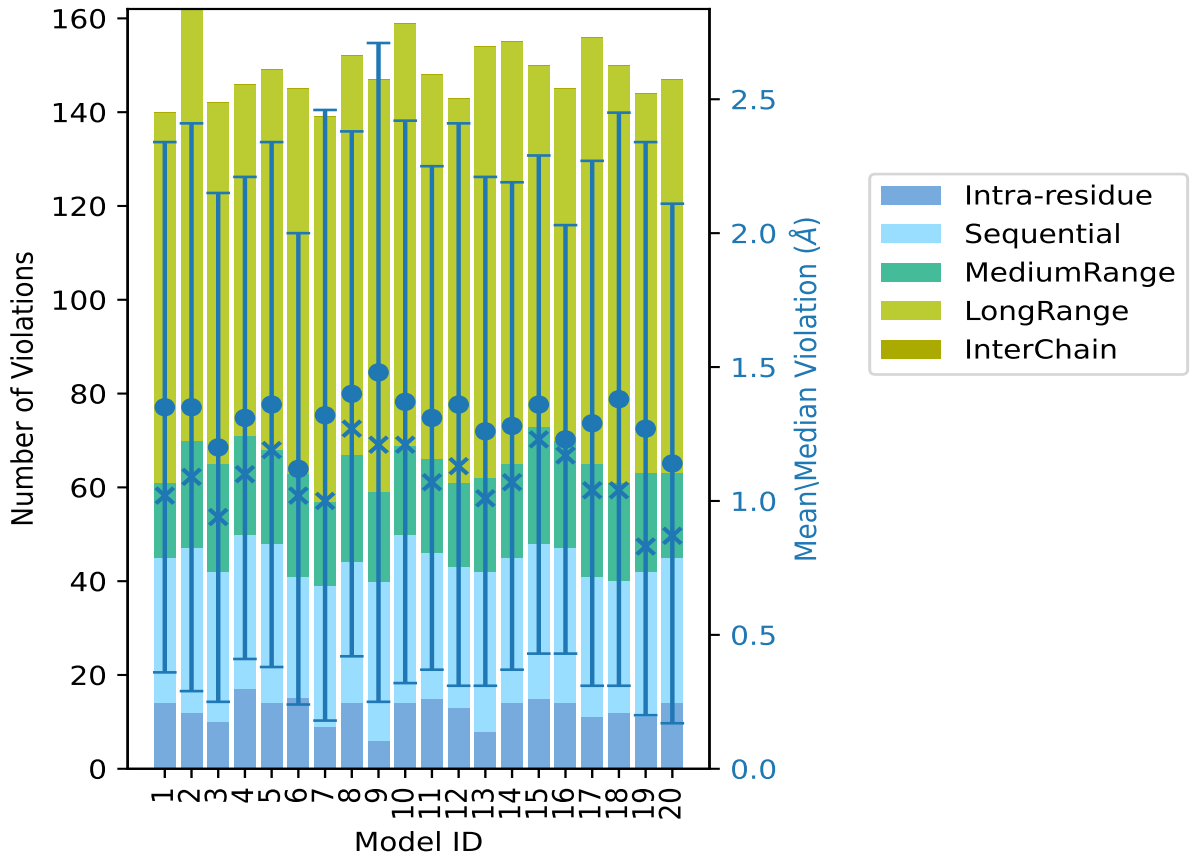
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	13	30	18	82	0	143	1.36	4.57	1.05	1.13
13	8	34	20	92	0	154	1.26	3.85	0.95	1.01
14	14	31	20	90	0	155	1.28	3.56	0.91	1.07
15	15	33	25	77	0	150	1.36	3.69	0.93	1.23
16	14	33	23	75	0	145	1.23	3.32	0.8	1.17
17	11	30	24	91	0	156	1.29	3.87	0.98	1.04
18	12	28	21	89	0	150	1.38	4.81	1.07	1.04
19	11	31	21	81	0	144	1.27	4.19	1.07	0.83
20	14	31	18	84	0	147	1.14	4.25	0.97	0.87

[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

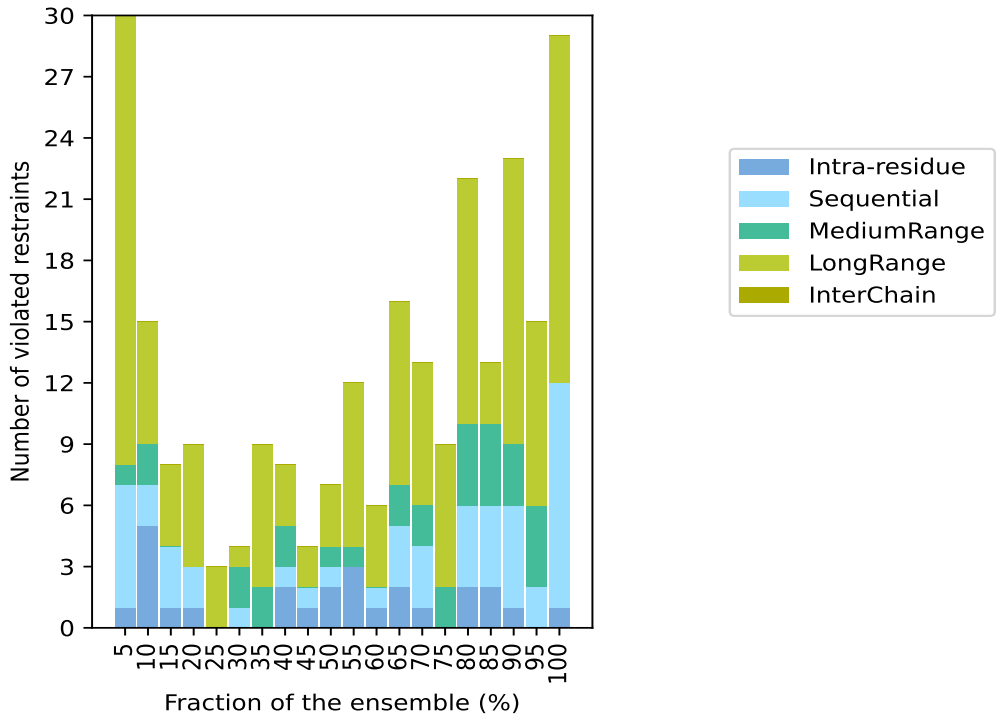
9.3 Distance violation statistics for the ensemble (i)

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, 2352(IR:497, SQ:617, MR:242, LR:996, 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	6	1	22	0	30	1	5.0
5	2	2	6	0	15	2	10.0
1	3	0	4	0	8	3	15.0
1	2	0	6	0	9	4	20.0
0	0	0	3	0	3	5	25.0
0	1	2	1	0	4	6	30.0
0	0	2	7	0	9	7	35.0
2	1	2	3	0	8	8	40.0
1	1	0	2	0	4	9	45.0
2	1	1	3	0	7	10	50.0
3	0	1	8	0	12	11	55.0
1	1	0	4	0	6	12	60.0
2	3	2	9	0	16	13	65.0
1	3	2	7	0	13	14	70.0
0	0	2	7	0	9	15	75.0
2	4	4	12	0	22	16	80.0
2	4	4	3	0	13	17	85.0
1	5	3	14	0	23	18	90.0
0	2	4	9	0	15	19	95.0
1	11	0	17	0	29	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

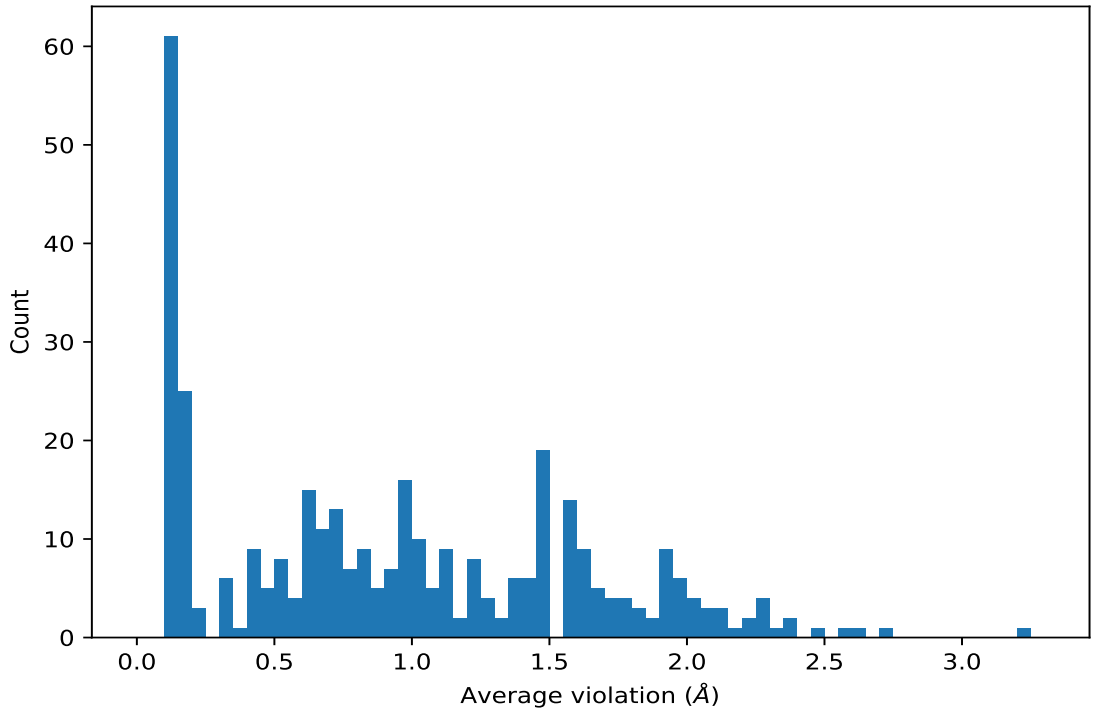
9.3.1 Bar graph : Distance violation statistics for the ensemble



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.

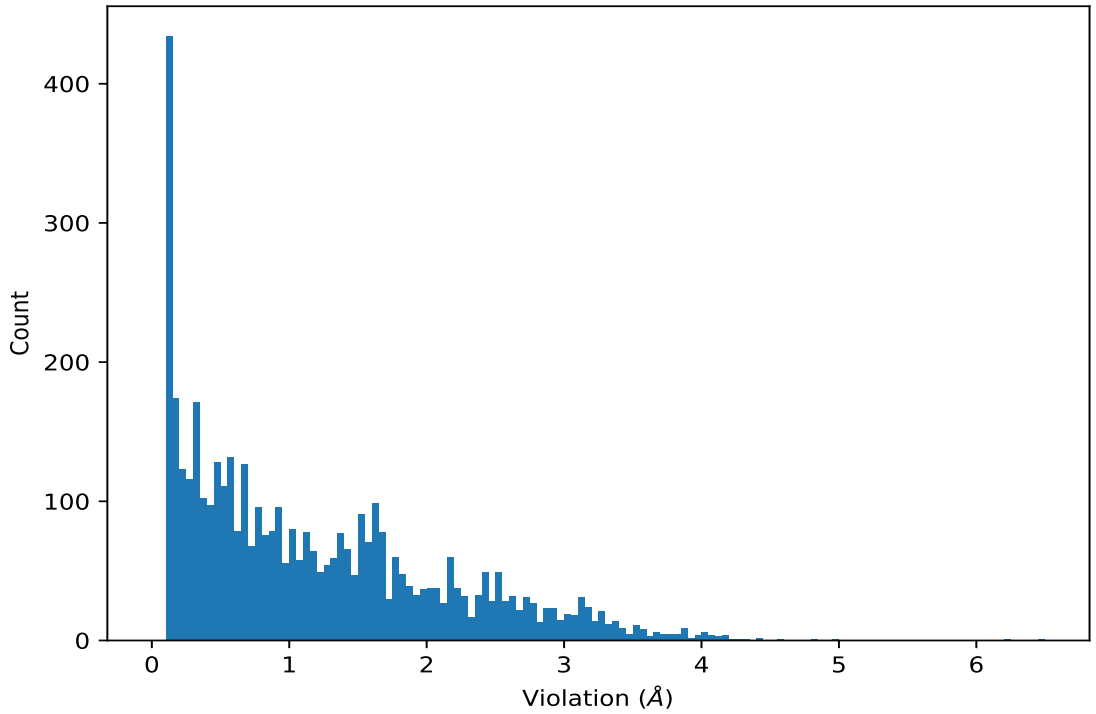
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2047)	1:A:240:ILE:HB	1:A:324:VAL:HG13	20	2.64	1.31	3.28
(1,2133)	1:A:252:ASP:HB2	1:A:262:VAL:HG13	20	2.56	0.89	2.66
(1,2119)	1:A:251:PRO:HA	1:A:262:VAL:HG13	20	2.27	1.3	3.13
(1,2417)	1:A:286:VAL:HG13	1:A:322:PHE:HB2	20	2.2	0.73	2.15
(1,2362)	1:A:279:VAL:HG13	1:A:286:VAL:HA	20	2.17	1.28	1.82
(1,2186)	1:A:262:VAL:HG13	1:A:263:THR:HB	20	2.12	0.82	2.46
(1,2356)	1:A:279:VAL:HG13	1:A:280:ALA:HA	20	2.11	0.64	2.23
(1,2366)	1:A:279:VAL:HG13	1:A:287:GLN:HB2	20	1.97	1.05	2.08
(1,2366)	1:A:279:VAL:HG13	1:A:287:GLN:HB3	20	1.97	1.05	2.08
(1,2408)	1:A:286:VAL:HG13	1:A:287:GLN:HB2	20	1.95	0.83	1.9
(1,2408)	1:A:286:VAL:HG13	1:A:287:GLN:HB3	20	1.95	0.83	1.9
(1,2518)	1:A:309:GLU:H	1:A:324:VAL:HG13	20	1.87	1.15	1.7

[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)
(1,2363)	1:A:279:VAL:HG13	1:A:286:VAL:HG13	9	6.47
(1,2363)	1:A:279:VAL:HG13	1:A:286:VAL:HG13	7	6.23
(1,2363)	1:A:279:VAL:HG13	1:A:286:VAL:HG13	5	4.95
(1,2363)	1:A:279:VAL:HG13	1:A:286:VAL:HG13	18	4.81
(1,2420)	1:A:286:VAL:HG13	1:A:324:VAL:HG13	12	4.57
(1,2412)	1:A:286:VAL:HG13	1:A:289:VAL:H	7	4.4
(1,2362)	1:A:279:VAL:HG13	1:A:286:VAL:HA	5	4.4
(1,2412)	1:A:286:VAL:HG13	1:A:289:VAL:H	9	4.34
(1,2363)	1:A:279:VAL:HG13	1:A:286:VAL:HG13	20	4.25
(1,2420)	1:A:286:VAL:HG13	1:A:324:VAL:HG13	2	4.23

10 Dihedral-angle violation analysis

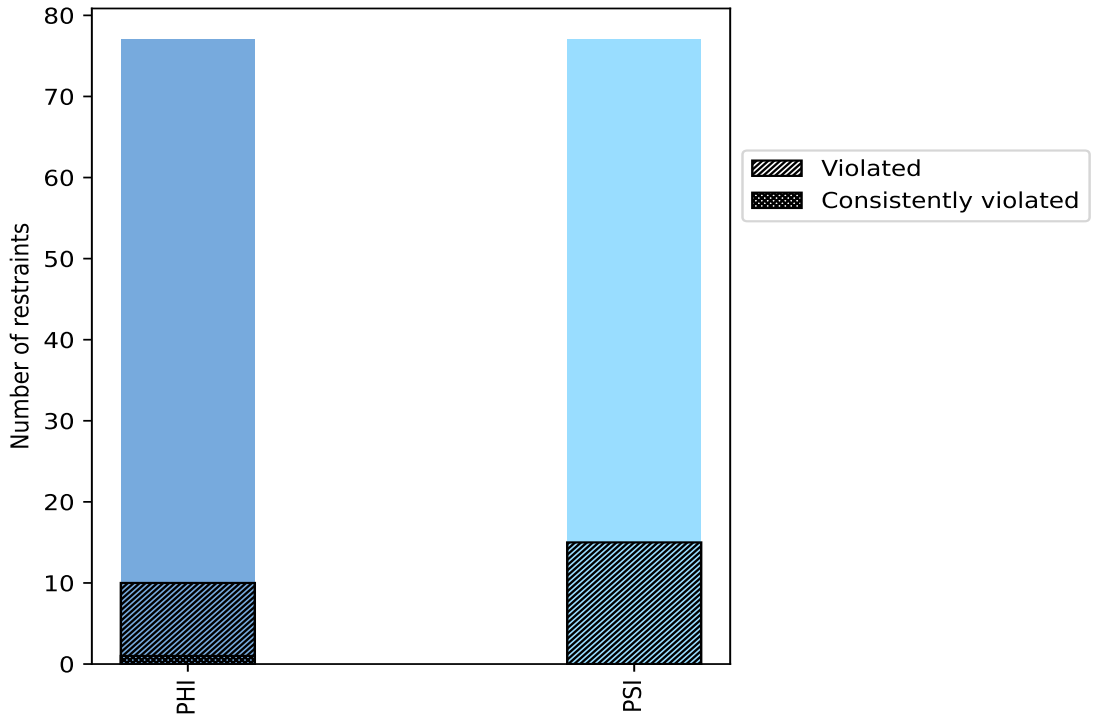
10.1 Summary of dihedral-angle violations

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	77	50.0	10	13.0	6.5	1	1.3	0.6
PSI	77	50.0	15	19.5	9.7	0	0.0	0.0
Total	154	100.0	25	16.2	16.2	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



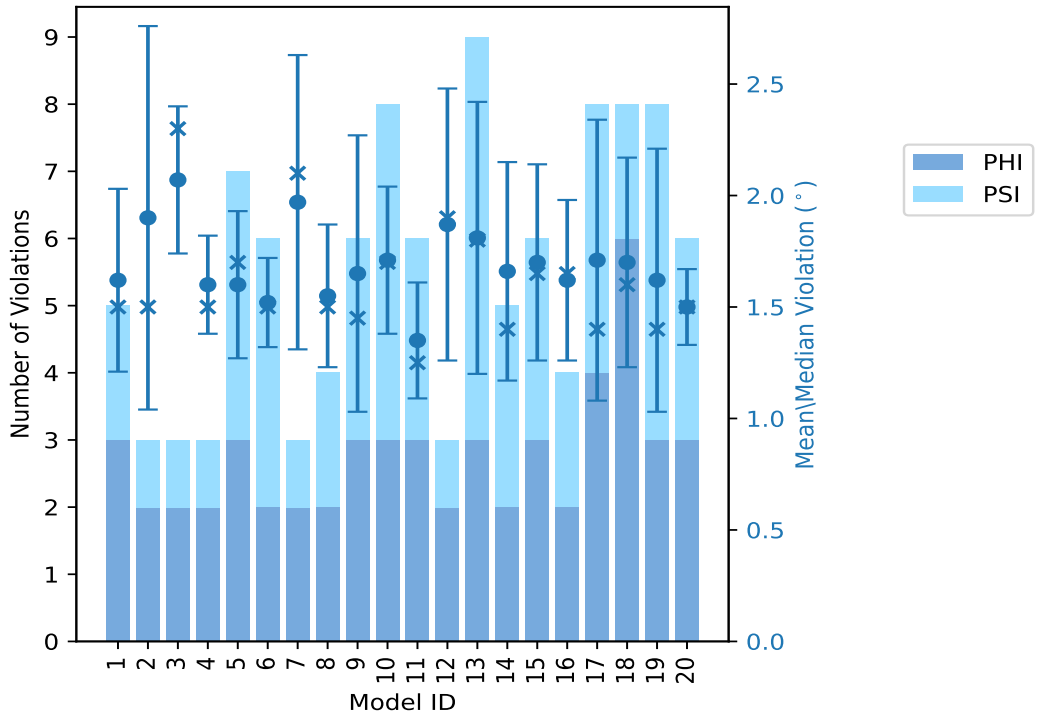
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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	3	2	5	1.62	2.4	0.41	1.5
2	2	1	3	1.9	3.1	0.86	1.5
3	2	1	3	2.07	2.3	0.33	2.3
4	2	1	3	1.6	1.9	0.22	1.5
5	3	4	7	1.6	2.0	0.33	1.7
6	2	4	6	1.52	1.8	0.2	1.5
7	2	1	3	1.97	2.7	0.66	2.1
8	2	2	4	1.55	2.0	0.32	1.5
9	3	3	6	1.65	3.0	0.62	1.45
10	3	5	8	1.71	2.1	0.33	1.7
11	3	3	6	1.35	1.8	0.26	1.25
12	2	1	3	1.87	2.6	0.61	1.9
13	3	6	9	1.81	2.7	0.61	1.8
14	2	3	5	1.66	2.3	0.49	1.4
15	3	3	6	1.7	2.4	0.44	1.65
16	2	2	4	1.62	2.1	0.36	1.65
17	4	4	8	1.71	2.9	0.63	1.4
18	6	2	8	1.7	2.6	0.47	1.6
19	3	5	8	1.62	2.8	0.59	1.4
20	3	3	6	1.5	1.7	0.17	1.5

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]	%
2	6	8	1	5.0
2	2	4	2	10.0
4	1	5	3	15.0
0	2	2	4	20.0
0	0	0	5	25.0
0	2	2	6	30.0
0	0	0	7	35.0
0	1	1	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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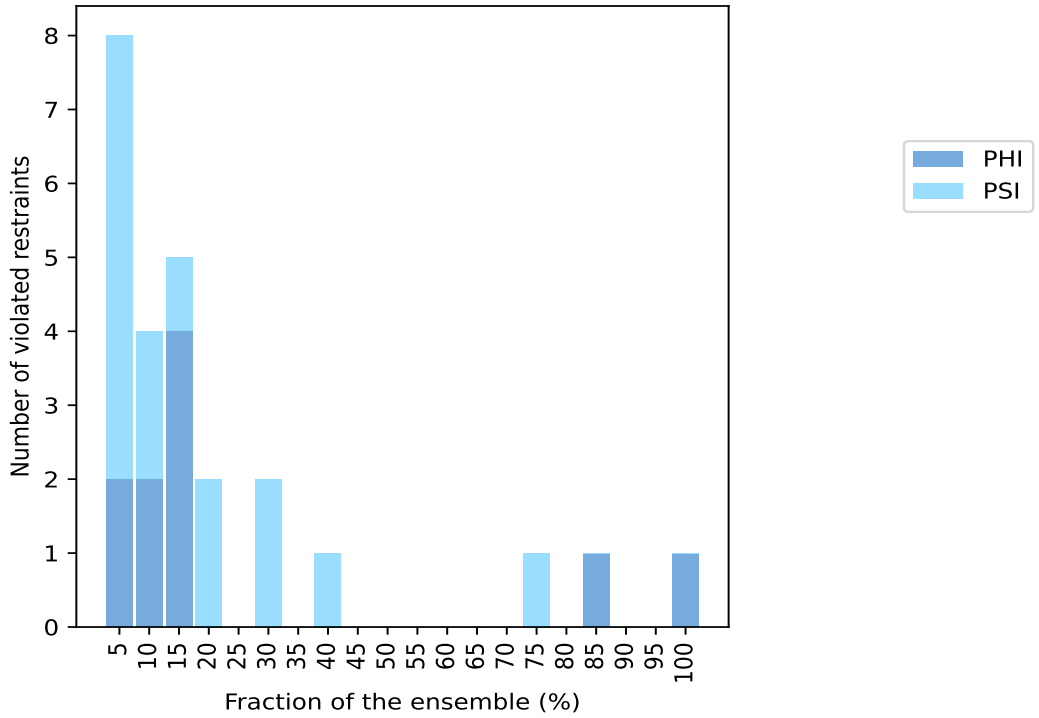
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	1	1	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
1	0	1	20	100.0

[1] Number of models with violations

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

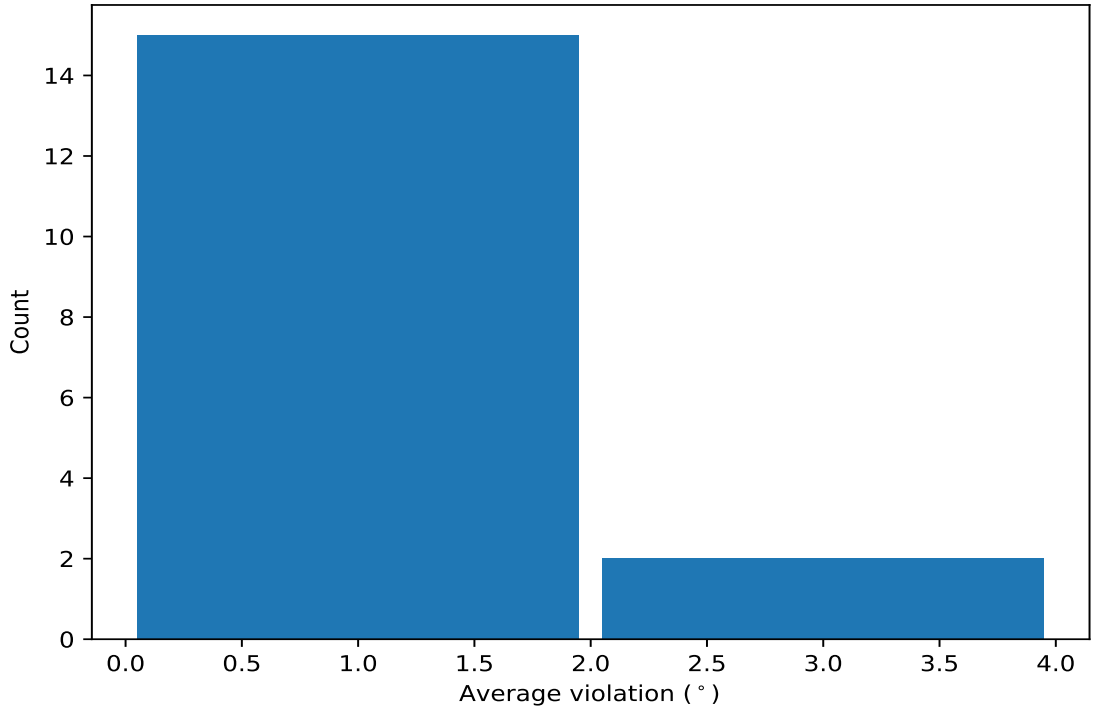


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

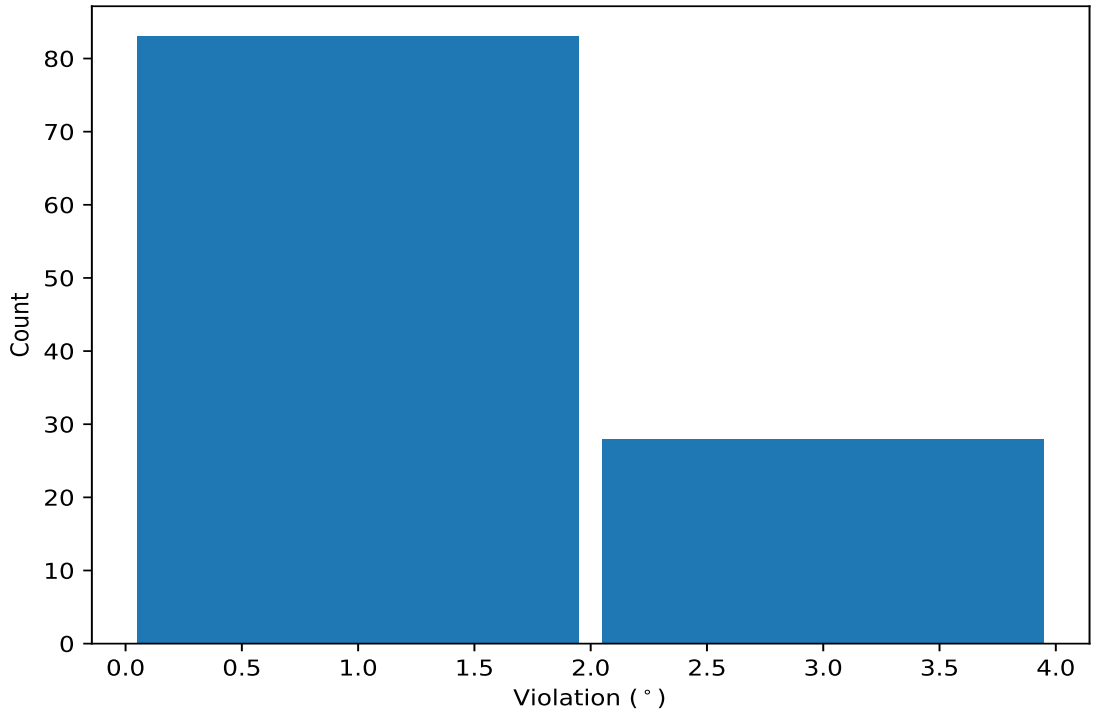
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,51)	1:A:259:HIS:C	1:A:260:ILE:N	1:A:260:ILE:CA	1:A:260:ILE:C	20	2.16	0.52	2.2
(1,142)	1:A:320:PHE:C	1:A:321:THR:N	1:A:321:THR:CA	1:A:321:THR:C	17	1.62	0.41	1.5
(1,27)	1:A:244:ALA:N	1:A:244:ALA:CA	1:A:244:ALA:C	1:A:245:LEU:N	15	1.62	0.33	1.6
(1,105)	1:A:296:ASN:N	1:A:296:ASN:CA	1:A:296:ASN:C	1:A:297:ASP:N	8	2.11	0.45	2.05
(1,83)	1:A:283:LYS:N	1:A:283:LYS:CA	1:A:283:LYS:C	1:A:284:THR:N	6	1.47	0.31	1.3
(1,5)	1:A:229:ASP:N	1:A:229:ASP:CA	1:A:229:ASP:C	1:A:230:PHE:N	6	1.37	0.2	1.35
(1,113)	1:A:301:ILE:N	1:A:301:ILE:CA	1:A:301:ILE:C	1:A:302:ILE:N	4	1.78	0.23	1.8
(1,91)	1:A:288:LYS:N	1:A:288:LYS:CA	1:A:288:LYS:C	1:A:289:VAL:N	4	1.68	0.68	1.4
(1,129)	1:A:311:VAL:N	1:A:311:VAL:CA	1:A:311:VAL:C	1:A:312:ASN:N	3	1.8	0.59	1.6
(1,6)	1:A:228:ILE:C	1:A:229:ASP:N	1:A:229:ASP:CA	1:A:229:ASP:C	3	1.5	0.22	1.6

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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

The following table provides the list of violationsfor 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,51)	1:A:259:HIS:C	1:A:260:ILE:N	1:A:260:ILE:CA	1:A:260:ILE:C	2	3.1
(1,51)	1:A:259:HIS:C	1:A:260:ILE:N	1:A:260:ILE:CA	1:A:260:ILE:C	9	3.0
(1,105)	1:A:296:ASN:N	1:A:296:ASN:CA	1:A:296:ASN:C	1:A:297:ASP:N	17	2.9
(1,91)	1:A:288:LYS:N	1:A:288:LYS:CA	1:A:288:LYS:C	1:A:289:VAL:N	19	2.8
(1,51)	1:A:259:HIS:C	1:A:260:ILE:N	1:A:260:ILE:CA	1:A:260:ILE:C	7	2.7
(1,51)	1:A:259:HIS:C	1:A:260:ILE:N	1:A:260:ILE:CA	1:A:260:ILE:C	13	2.7
(1,51)	1:A:259:HIS:C	1:A:260:ILE:N	1:A:260:ILE:CA	1:A:260:ILE:C	12	2.6
(1,129)	1:A:311:VAL:N	1:A:311:VAL:CA	1:A:311:VAL:C	1:A:312:ASN:N	13	2.6
(1,105)	1:A:296:ASN:N	1:A:296:ASN:CA	1:A:296:ASN:C	1:A:297:ASP:N	18	2.6
(1,51)	1:A:259:HIS:C	1:A:260:ILE:N	1:A:260:ILE:CA	1:A:260:ILE:C	17	2.5