wwPDB NMR Structure Validation Summary Report

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Title	:	Structure of the Self-Association Domain of Swallow
Authors	:	Loening, N.M.; Barbar, E.
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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:

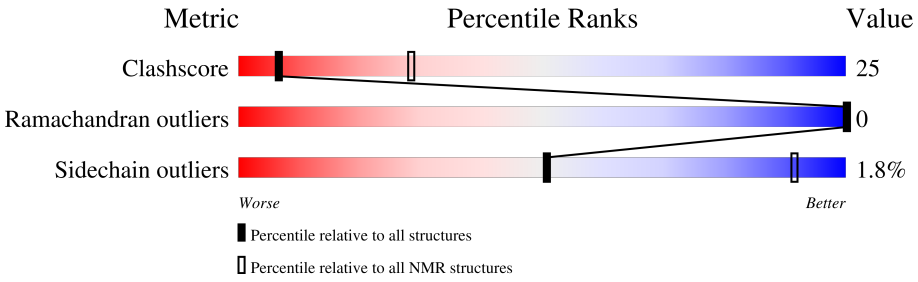
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 47%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	71	54% 24% 23%
1	B	71	54% 24% 23%

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:215-A:269, B:215-B:269 (110)	0.39	10

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 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2384 atoms, of which 1182 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein swallow.

Mol	Chain	Residues	Atoms						Trace
1	A	71	Total	C	H	N	O	S	0
			1192	367	591	110	123	1	
1	B	71	Total	C	H	N	O	S	0
			1192	367	591	110	123	1	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	GLU	ARG	engineered mutation	UNP P40688
A	244	ILE	LYS	engineered mutation	UNP P40688
A	253	ASP	CYS	engineered mutation	UNP P40688
A	265	ALA	CYS	engineered mutation	UNP P40688
B	224	GLU	ARG	engineered mutation	UNP P40688
B	244	ILE	LYS	engineered mutation	UNP P40688
B	253	ASP	CYS	engineered mutation	UNP P40688
B	265	ALA	CYS	engineered mutation	UNP P40688

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: Protein swallow

Chain A:

• Molecule 1: Protein swallow

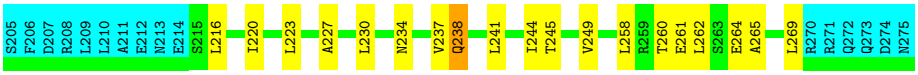
Chain B:

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

The representative model is number 10. Colouring as in section 4.1 above.

• Molecule 1: Protein swallow

Chain A:



• Molecule 1: Protein swallow

Chain B:

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	refinement	1.21
ARIA	structure calculation	2.3.2

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	969
Number of shifts mapped to atoms	969
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	47%

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	461	461	461	33±4
1	B	461	461	461	33±4
All	All	18440	18440	18440	917

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 25.

5 of 93 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:227:ALA:HB2	1:B:227:ALA:HB2	0.97	1.30	1	20
1:B:262:LEU:HA	1:B:265:ALA:HB3	0.70	1.64	11	20
1:A:262:LEU:HA	1:A:265:ALA:HB3	0.70	1.63	11	20
1:A:237:VAL:HG21	1:B:237:VAL:HG21	0.69	1.64	7	19
1:A:269:LEU:HD11	1:B:265:ALA:HB2	0.66	1.65	16	3

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	55/71 (77%)	52±1 (95±2%)	2±1 (5±2%)	0±0 (0±0%)	100	100
1	B	55/71 (77%)	53±1 (96±2%)	2±1 (4±2%)	0±0 (0±0%)	100	100
All	All	2200/2840 (77%)	2101 (96%)	99 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	52/67 (78%)	50±3 (97±6%)	1±1 (2±2%)	51	91
1	B	52/67 (78%)	51±1 (98±2%)	1±1 (2±2%)	51	91
All	All	2065/2680 (77%)	2027 (98%)	38 (2%)	51	91

5 of 20 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	264	GLU	3
1	B	264	GLU	3
1	A	217	GLN	3
1	B	217	GLN	3
1	A	267	GLN	2

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

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 47% for the well-defined parts and 47% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_ output*

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	969
Number of shifts mapped to atoms	969
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	71	-0.53 ± 0.14	Should be checked
$^{13}C_{\beta}$	70	0.24 ± 0.05	None needed (< 0.5 ppm)
$^{13}C'$	71	-0.64 ± 0.17	Should be applied
^{15}N	70	-0.72 ± 0.21	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 47%, i.e. 757 atoms were assigned a chemical shift out of a possible 1604. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	276/552 (50%)	111/222 (50%)	110/220 (50%)	55/110 (50%)
Sidechain	443/974 (45%)	291/618 (47%)	140/304 (46%)	12/52 (23%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	38/78 (49%)	19/38 (50%)	19/40 (48%)	0/0 (—%)
Overall	757/1604 (47%)	421/878 (48%)	269/564 (48%)	67/162 (41%)

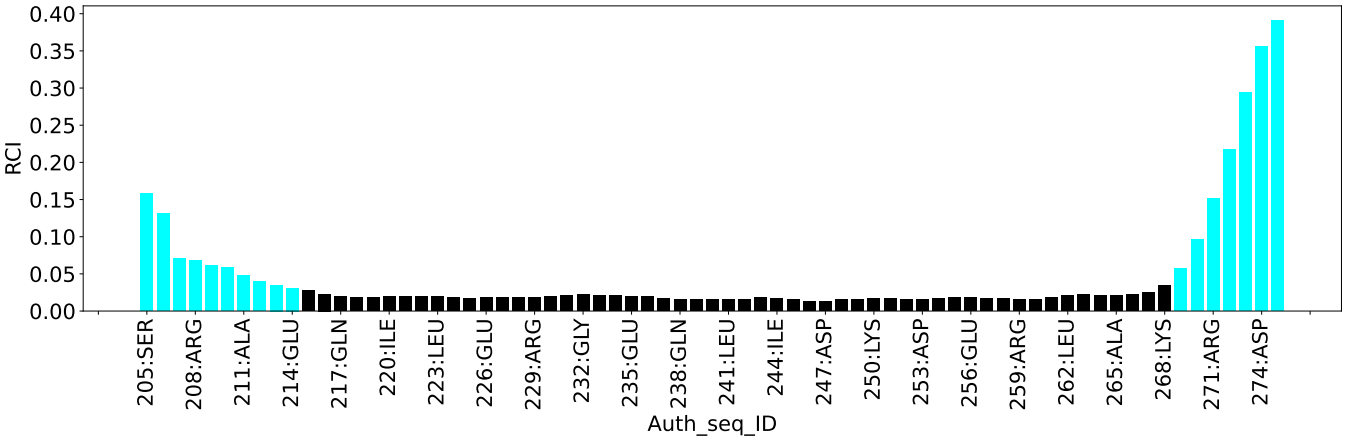
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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	5328
Intra-residue (|i-j|=0)	1738
Sequential (|i-j|=1)	1072
Medium range (|i-j|>1 and |i-j|<5)	1738
Long range (|i-j|≥5)	22
Inter-chain	758
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	256
Number of unmapped restraints	0
Number of restraints per residue	39.3
Number of long range restraints per residue[1]	0.2

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

8.2 Residual restraint violations

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)	84.0	0.2
0.2-0.5 (Medium)	189.3	0.5
>0.5 (Large)	192.8	2.61

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)	5.2	5.34
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

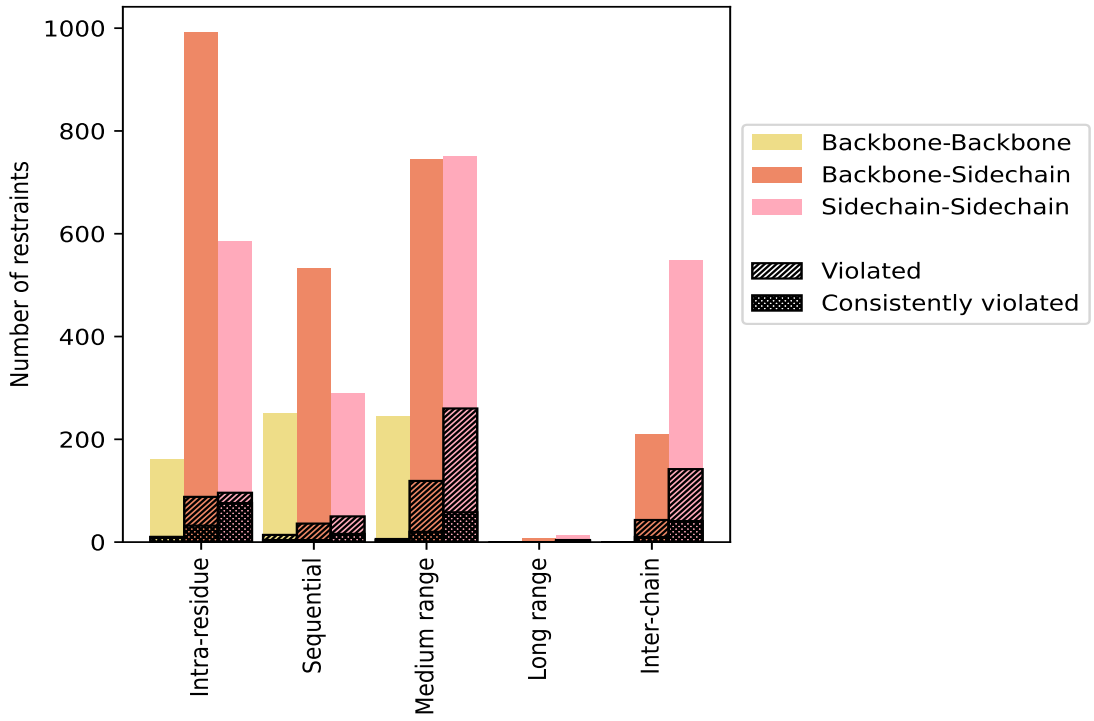
9.1 Summary of distance violations (i)

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)	1738	32.6	194	11.2	3.6	118	6.8	2.2
Backbone-Backbone	160	3.0	10	6.2	0.2	10	6.2	0.2
Backbone-Sidechain	992	18.6	88	8.9	1.7	32	3.2	0.6
Sidechain-Sidechain	586	11.0	96	16.4	1.8	76	13.0	1.4
Sequential (|i-j|=1)	1072	20.1	100	9.3	1.9	24	2.2	0.5
Backbone-Backbone	250	4.7	14	5.6	0.3	4	1.6	0.1
Backbone-Sidechain	532	10.0	36	6.8	0.7	4	0.8	0.1
Sidechain-Sidechain	290	5.4	50	17.2	0.9	16	5.5	0.3
Medium range (|i-j|>1 & |i-j|<5)	1738	32.6	385	22.2	7.2	82	4.7	1.5
Backbone-Backbone	244	4.6	6	2.5	0.1	4	1.6	0.1
Backbone-Sidechain	744	14.0	119	16.0	2.2	20	2.7	0.4
Sidechain-Sidechain	750	14.1	260	34.7	4.9	58	7.7	1.1
Long range (|i-j|≥5)	22	0.4	4	18.2	0.1	2	9.1	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	0.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	14	0.3	4	28.6	0.1	2	14.3	0.0
Inter-chain	758	14.2	185	24.4	3.5	51	6.7	1.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	210	3.9	43	20.5	0.8	10	4.8	0.2
Sidechain-Sidechain	548	10.3	142	25.9	2.7	41	7.5	0.8
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	5328	100.0	868	16.3	16.3	277	5.2	5.2
Backbone-Backbone	654	12.3	30	4.6	0.6	18	2.8	0.3
Backbone-Sidechain	2486	46.7	286	11.5	5.4	66	2.7	1.2
Sidechain-Sidechain	2188	41.1	552	25.2	10.4	193	8.8	3.6

[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	141	44	145	0	133	463	0.53	2.16	0.38	0.44
2	145	48	162	2	124	481	0.54	2.26	0.4	0.43
3	153	44	150	0	140	487	0.53	1.99	0.39	0.42
4	136	47	141	0	133	457	0.52	2.49	0.37	0.44
5	138	38	146	0	119	441	0.53	2.59	0.4	0.43
6	154	34	159	0	115	462	0.51	2.46	0.38	0.42
7	150	46	158	0	137	491	0.53	2.11	0.39	0.41
8	148	40	149	0	140	477	0.51	1.95	0.37	0.41
9	135	40	148	0	134	457	0.54	2.38	0.37	0.45
10	143	44	150	0	136	473	0.53	2.2	0.38	0.41

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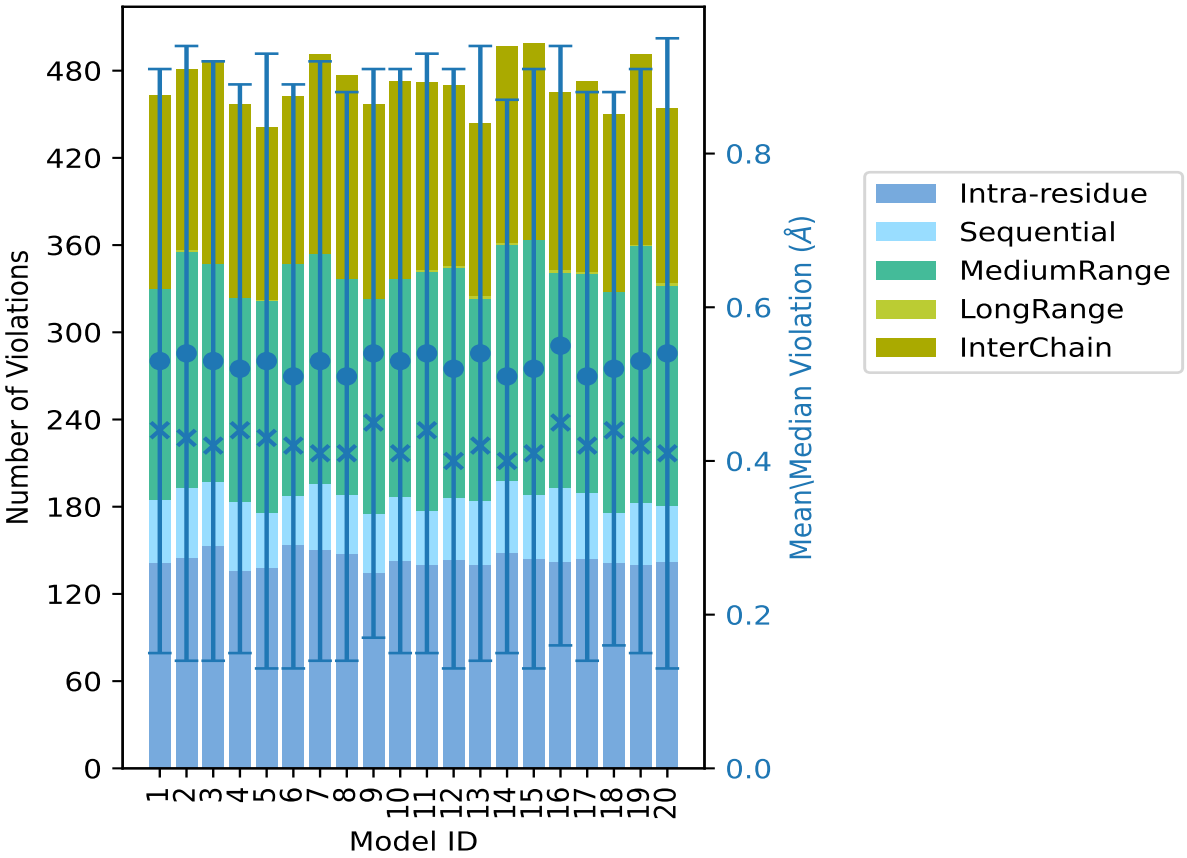
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	140	37	165	1	129	472	0.54	2.61	0.39	0.44
12	144	42	158	2	124	470	0.52	2.31	0.39	0.4
13	140	44	139	2	119	444	0.54	2.12	0.4	0.42
14	148	50	162	2	135	497	0.51	2.27	0.36	0.4
15	144	44	176	0	135	499	0.52	2.06	0.39	0.41
16	142	51	148	2	122	465	0.55	2.22	0.39	0.45
17	144	46	150	2	131	473	0.51	2.28	0.37	0.42
18	141	35	152	0	122	450	0.52	2.26	0.36	0.44
19	140	43	177	0	131	491	0.53	2.17	0.38	0.42
20	142	39	151	2	120	454	0.54	2.27	0.41	0.41

[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

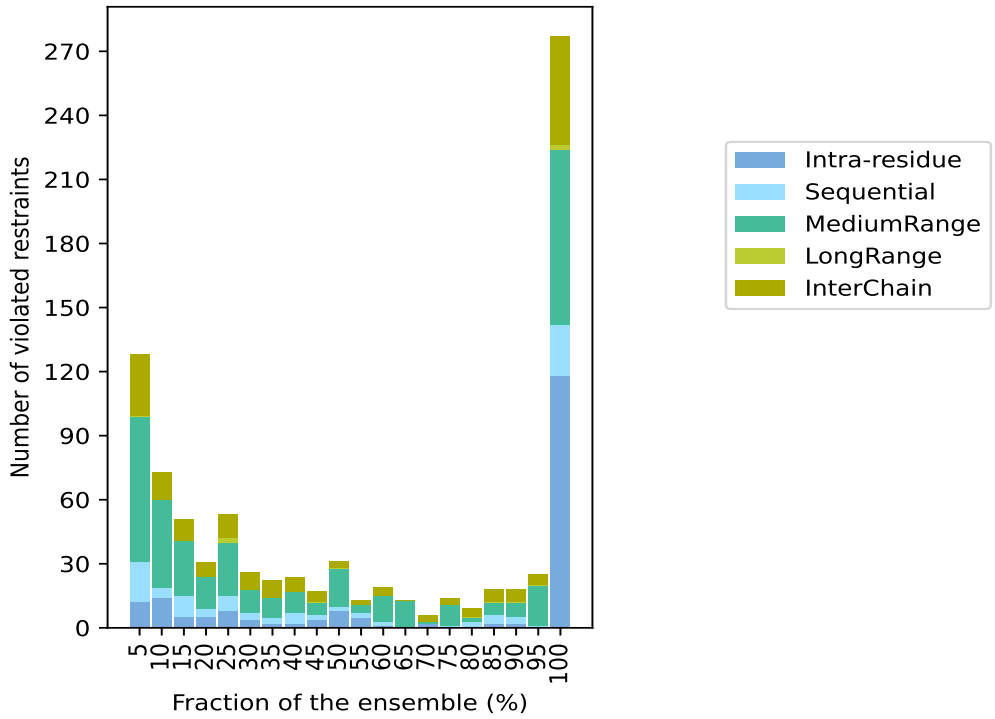
9.3 Distance violation statistics for the ensemble (i)

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, 4460(IR:1544, SQ:972, MR:1353, LR:18, IC:573) 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]	%
12	19	68	0	29	128	1	5.0
14	5	41	0	13	73	2	10.0
5	10	26	0	10	51	3	15.0
5	4	15	0	7	31	4	20.0
8	7	25	2	11	53	5	25.0
4	3	11	0	8	26	6	30.0
2	3	9	0	8	22	7	35.0
2	5	10	0	7	24	8	40.0
4	2	6	0	5	17	9	45.0
8	2	18	0	3	31	10	50.0
5	2	4	0	2	13	11	55.0
1	2	12	0	4	19	12	60.0
0	0	13	0	0	13	13	65.0
2	0	1	0	3	6	14	70.0
0	1	10	0	3	14	15	75.0
0	3	2	0	4	9	16	80.0
2	4	6	0	6	18	17	85.0
2	3	7	0	6	18	18	90.0
0	1	19	0	5	25	19	95.0
118	24	82	2	51	277	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

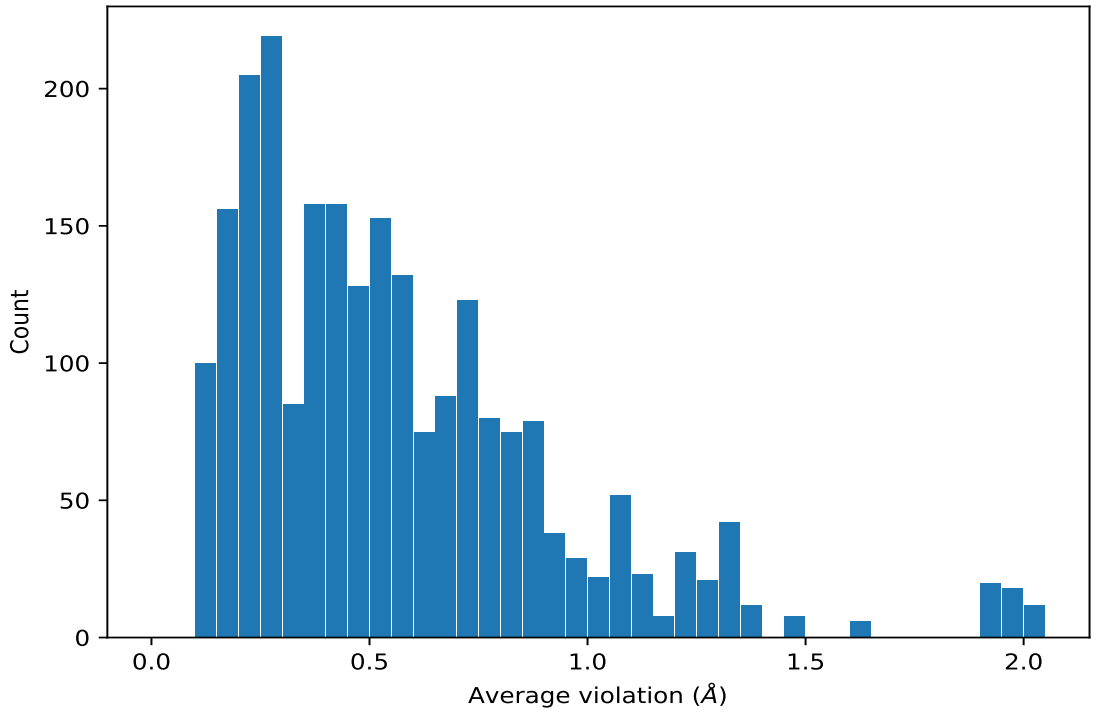
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(1,2162)	1:251:B:MET:HE3	1:254:A:ASN:HB2	20	2.0	0.22	2.01
(1,2162)	1:251:B:MET:HE3	1:254:B:ASN:HB2	20	2.0	0.22	2.01
(1,2162)	1:251:B:MET:HE1	1:254:A:ASN:HB2	20	2.0	0.22	2.01
(1,2162)	1:251:B:MET:HE2	1:254:B:ASN:HB2	20	2.0	0.22	2.01
(1,2162)	1:251:B:MET:HE1	1:254:B:ASN:HB2	20	2.0	0.22	2.01
(1,2162)	1:251:B:MET:HE2	1:254:A:ASN:HB2	20	2.0	0.22	2.01
(1,2161)	1:251:A:MET:HE3	1:254:B:ASN:HB2	20	2.0	0.22	2.0
(1,2161)	1:251:A:MET:HE3	1:254:A:ASN:HB2	20	2.0	0.22	2.0
(1,2161)	1:251:A:MET:HE1	1:254:B:ASN:HB2	20	2.0	0.22	2.0
(1,2161)	1:251:A:MET:HE2	1:254:A:ASN:HB2	20	2.0	0.22	2.0
(1,2161)	1:251:A:MET:HE1	1:254:A:ASN:HB2	20	2.0	0.22	2.0
(1,2161)	1:251:A:MET:HE2	1:254:B:ASN:HB2	20	2.0	0.22	2.0
(3,238)	1:244:B:ILE:HG23	1:241:A:LEU:HD12	20	1.98	0.17	1.96
(3,238)	1:244:B:ILE:HG23	1:241:A:LEU:HD13	20	1.98	0.17	1.96
(3,238)	1:244:B:ILE:HG21	1:241:A:LEU:HD12	20	1.98	0.17	1.96
(3,238)	1:244:B:ILE:HG22	1:241:A:LEU:HD13	20	1.98	0.17	1.96

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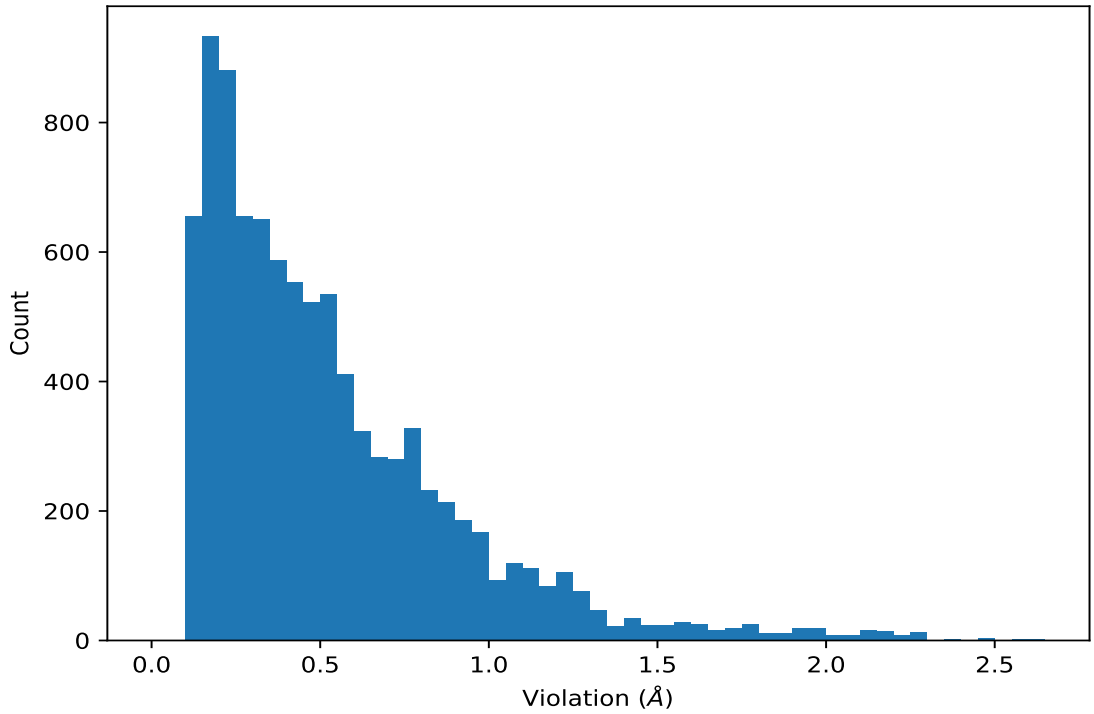
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,238)	1:244:B:ILE:HG21	1:241:A:LEU:HD11	20	1.98	0.17	1.96
(3,238)	1:244:B:ILE:HG23	1:241:A:LEU:HD11	20	1.98	0.17	1.96
(3,238)	1:244:B:ILE:HG22	1:241:A:LEU:HD12	20	1.98	0.17	1.96
(3,237)	1:244:A:ILE:HG23	1:241:B:LEU:HD12	20	1.97	0.17	1.96
(3,237)	1:244:A:ILE:HG23	1:241:B:LEU:HD13	20	1.97	0.17	1.96
(3,237)	1:244:A:ILE:HG21	1:241:B:LEU:HD12	20	1.97	0.17	1.96
(3,237)	1:244:A:ILE:HG22	1:241:B:LEU:HD13	20	1.97	0.17	1.96
(3,237)	1:244:A:ILE:HG21	1:241:B:LEU:HD11	20	1.97	0.17	1.96
(3,237)	1:244:A:ILE:HG23	1:241:B:LEU:HD11	20	1.97	0.17	1.96
(3,237)	1:244:A:ILE:HG22	1:241:B:LEU:HD12	20	1.97	0.17	1.96
(1,75)	1:255:A:PHE:HD2	1:257:A:THR:HG21	20	1.91	0.36	2.0
(1,75)	1:255:A:PHE:HD1	1:257:A:THR:HG23	20	1.91	0.36	2.0
(1,75)	1:255:A:PHE:HD2	1:257:B:THR:HG21	20	1.91	0.36	2.0
(1,75)	1:255:A:PHE:HD2	1:257:A:THR:HG22	20	1.91	0.36	2.0
(1,75)	1:255:A:PHE:HD2	1:257:A:THR:HG23	20	1.91	0.36	2.0
(1,75)	1:255:A:PHE:HD1	1:257:B:THR:HG21	20	1.91	0.36	2.0
(1,75)	1:255:A:PHE:HD2	1:257:B:THR:HG22	20	1.91	0.36	2.0
(1,75)	1:255:A:PHE:HD1	1:257:B:THR:HG22	20	1.91	0.36	2.0
(1,75)	1:255:A:PHE:HD1	1:257:A:THR:HG21	20	1.91	0.36	2.0
(1,75)	1:255:A:PHE:HD1	1:257:B:THR:HG23	20	1.91	0.36	2.0
(1,76)	1:255:B:PHE:HD2	1:257:B:THR:HG21	20	1.91	0.36	2.0
(1,76)	1:255:B:PHE:HD1	1:257:B:THR:HG23	20	1.91	0.36	2.0
(1,76)	1:255:B:PHE:HD2	1:257:A:THR:HG21	20	1.91	0.36	2.0
(1,76)	1:255:B:PHE:HD2	1:257:B:THR:HG22	20	1.91	0.36	2.0
(1,76)	1:255:B:PHE:HD2	1:257:B:THR:HG23	20	1.91	0.36	2.0
(1,76)	1:255:B:PHE:HD1	1:257:A:THR:HG21	20	1.91	0.36	2.0
(1,76)	1:255:B:PHE:HD2	1:257:A:THR:HG22	20	1.91	0.36	2.0
(1,76)	1:255:B:PHE:HD1	1:257:A:THR:HG22	20	1.91	0.36	2.0
(1,76)	1:255:B:PHE:HD1	1:257:B:THR:HG21	20	1.91	0.36	2.0
(1,76)	1:255:B:PHE:HD1	1:257:A:THR:HG23	20	1.91	0.36	2.0
(3,1201)	1:244:A:ILE:HD13	1:240:A:ARG:HG2	20	1.62	0.17	1.66
(3,1201)	1:244:A:ILE:HD12	1:240:A:ARG:HG2	20	1.62	0.17	1.66
(3,1201)	1:244:A:ILE:HD11	1:240:A:ARG:HG2	20	1.62	0.17	1.66
(3,1202)	1:244:B:ILE:HD13	1:240:B:ARG:HG2	20	1.62	0.17	1.66
(3,1202)	1:244:B:ILE:HD12	1:240:B:ARG:HG2	20	1.62	0.17	1.66
(3,1202)	1:244:B:ILE:HD11	1:240:B:ARG:HG2	20	1.62	0.17	1.66
(1,2239)	1:244:A:ILE:HG21	1:251:B:MET:HB2	20	1.46	0.7	1.08
(1,2239)	1:244:A:ILE:HG22	1:251:B:MET:HB2	20	1.46	0.7	1.08
(1,2239)	1:244:A:ILE:HG23	1:251:B:MET:HB2	20	1.46	0.7	1.08
(1,2239)	1:244:A:ILE:HG22	1:251:B:MET:HG3	20	1.46	0.7	1.08
(1,2240)	1:244:B:ILE:HG21	1:251:A:MET:HB2	20	1.45	0.69	1.08

[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)
(3,1972)	1:225:B:VAL:HG21	1:229:B:ARG:HG3	11	2.61
(3,1971)	1:225:A:VAL:HG21	1:229:A:ARG:HG3	11	2.6
(3,1971)	1:225:A:VAL:HG23	1:229:A:ARG:HG3	5	2.59
(3,1972)	1:225:B:VAL:HG23	1:229:B:ARG:HG3	5	2.58
(1,2239)	1:244:A:ILE:HG21	1:251:B:MET:HB2	4	2.49
(1,2240)	1:244:B:ILE:HG21	1:251:A:MET:HB2	4	2.47
(1,76)	1:255:B:PHE:HD2	1:257:B:THR:HG23	6	2.46
(1,75)	1:255:A:PHE:HD2	1:257:A:THR:HG23	6	2.46
(1,2162)	1:251:B:MET:HE1	1:254:B:ASN:HB2	9	2.38
(1,2161)	1:251:A:MET:HE1	1:254:A:ASN:HB2	9	2.38

10 Dihedral-angle violation analysis

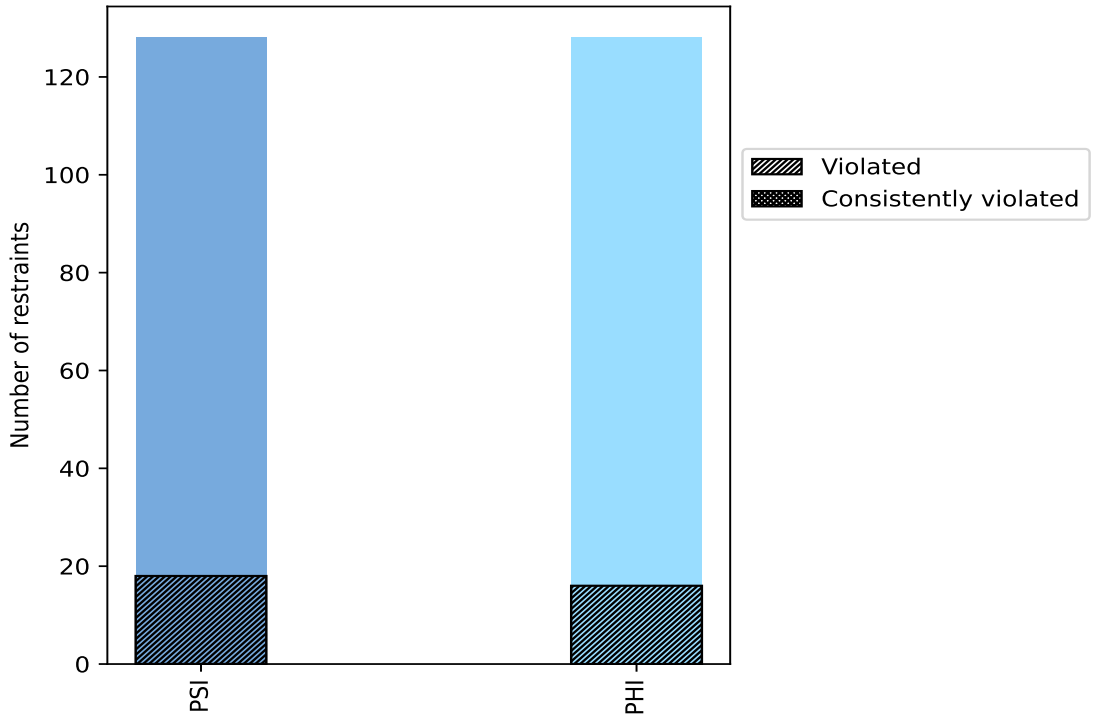
10.1 Summary of dihedral-angle violations

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]
PSI	128	50.0	18	14.1	7.0	0	0.0	0.0
PHI	128	50.0	16	12.5	6.2	0	0.0	0.0
Total	256	100.0	34	13.3	13.3	0	0.0	0.0

[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



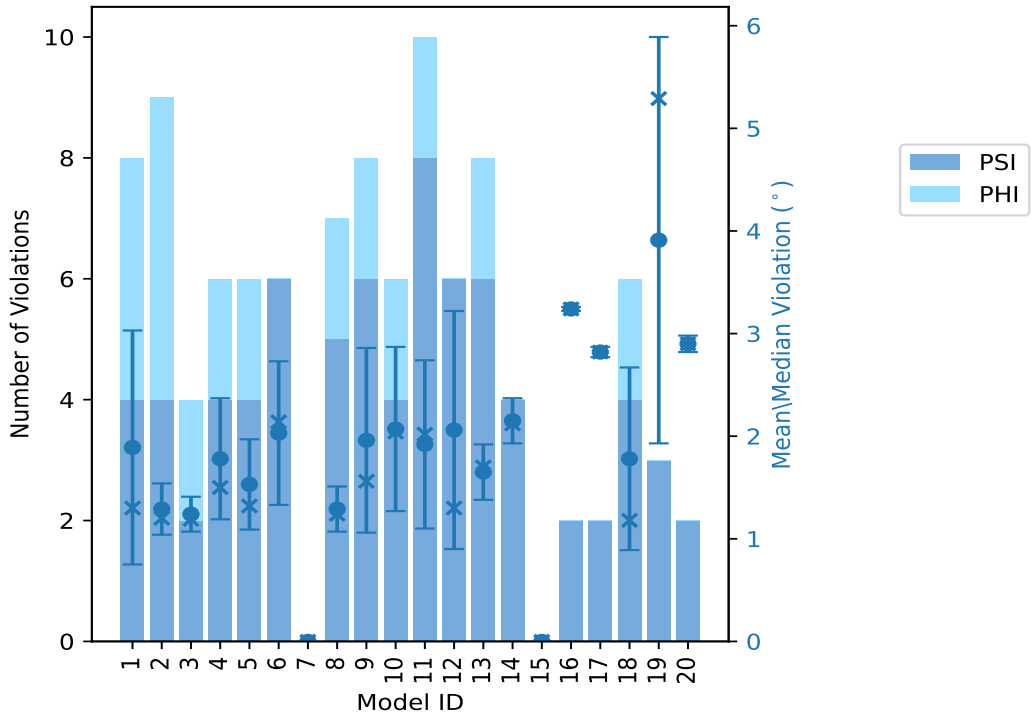
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	4	4	8	1.89	3.95	1.14	1.3
2	4	5	9	1.29	1.77	0.25	1.2
3	2	2	4	1.24	1.49	0.17	1.19
4	4	2	6	1.78	2.64	0.59	1.5
5	4	2	6	1.53	2.14	0.44	1.32
6	6	0	6	2.03	2.91	0.7	2.14
7	0	0	0	0.0	0.0	0.0	0.0
8	5	2	7	1.29	1.64	0.22	1.24
9	6	2	8	1.96	3.52	0.9	1.56
10	4	2	6	2.07	3.07	0.8	2.04
11	8	2	10	1.92	3.28	0.82	2.02
12	6	0	6	2.06	3.76	1.16	1.3
13	6	2	8	1.65	1.97	0.27	1.7
14	4	0	4	2.15	2.44	0.22	2.12
15	0	0	0	0.0	0.0	0.0	0.0
16	2	0	2	3.24	3.26	0.02	3.24
17	2	0	2	2.82	2.87	0.05	2.82
18	4	2	6	1.78	3.05	0.89	1.18
19	3	0	3	3.91	5.34	1.98	5.29
20	2	0	2	2.9	2.97	0.08	2.9

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	
PSI	PHI	Total	Count[1]	%
7	9	16	1	5.0
3	3	6	2	10.0
2	4	6	3	15.0
2	0	2	4	20.0
0	0	0	5	25.0
1	0	1	6	30.0
1	0	1	7	35.0
0	0	0	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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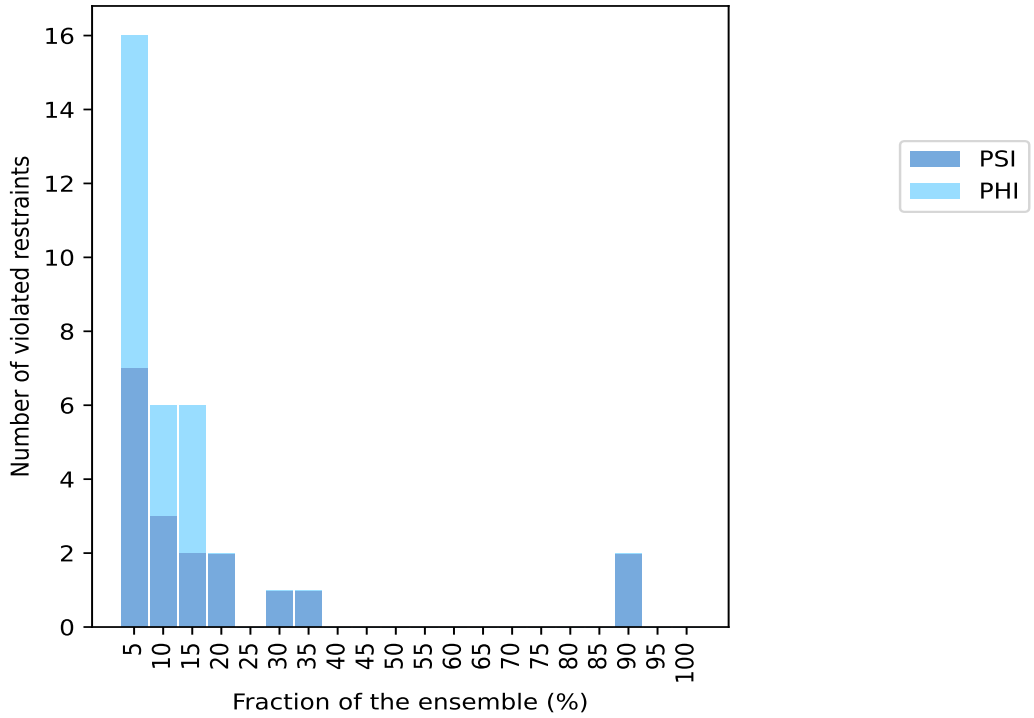
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
2	0	2	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

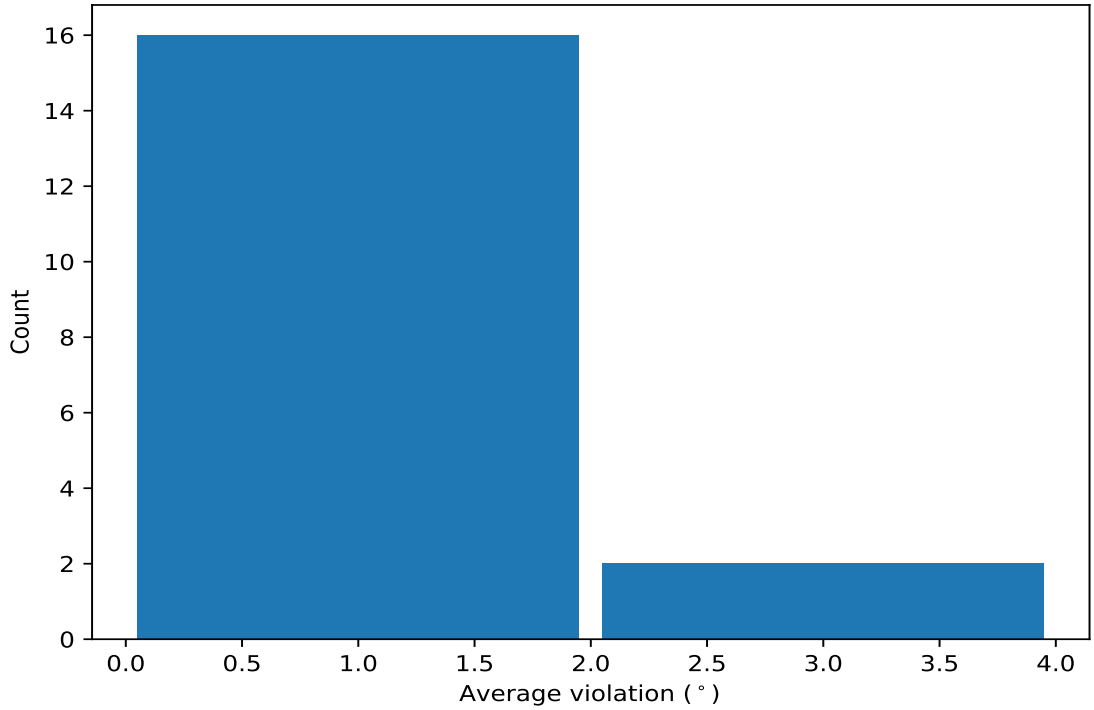


10.4 Most violated dihedral-angle restraints in the ensemble

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

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.

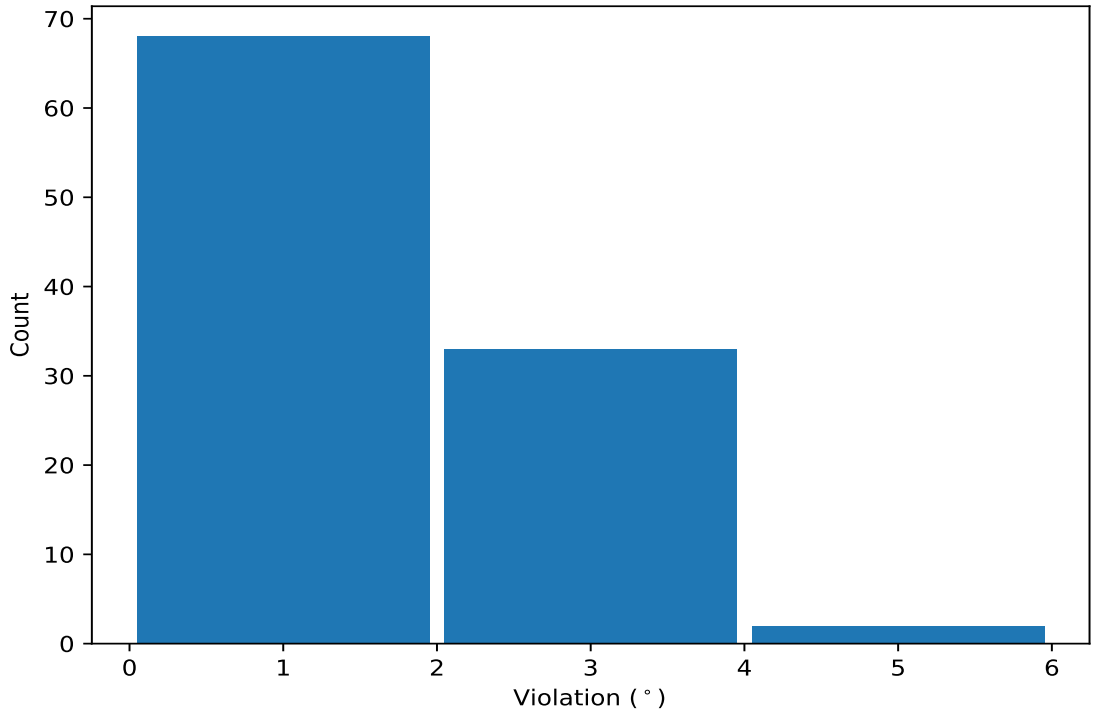
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(2,40)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:ALA:N	18	2.79	1.0	2.92
(1,40)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:ALA:N	18	2.79	1.0	2.86
(2,68)	1:240:B:ARG:N	1:240:B:ARG:CA	1:240:B:ARG:C	1:241:B:LEU:N	7	1.27	0.21	1.13
(1,68)	1:240:A:ARG:N	1:240:A:ARG:CA	1:240:A:ARG:C	1:241:A:LEU:N	6	1.25	0.15	1.17
(2,46)	1:229:B:ARG:N	1:229:B:ARG:CA	1:229:B:ARG:C	1:230:B:LEU:N	4	1.82	0.13	1.84
(1,46)	1:229:A:ARG:N	1:229:A:ARG:CA	1:229:A:ARG:C	1:230:A:LEU:N	4	1.79	0.16	1.81
(1,96)	1:254:A:ASN:N	1:254:A:ASN:CA	1:254:A:ASN:C	1:255:A:PHE:N	3	1.89	0.47	2.18
(2,96)	1:254:B:ASN:N	1:254:B:ASN:CA	1:254:B:ASN:C	1:255:B:PHE:N	3	1.75	0.5	2.11
(2,123)	1:267:B:GLN:C	1:268:B:LYS:N	1:268:B:LYS:CA	1:268:B:LYS:C	3	1.28	0.11	1.31
(1,123)	1:267:A:GLN:C	1:268:A:LYS:N	1:268:A:LYS:CA	1:268:A:LYS:C	3	1.22	0.02	1.22

[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 violations for 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 (°)
(1,40)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:ALA:N	19	5.34
(2,40)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:ALA:N	19	5.29
(2,40)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:ALA:N	1	3.95
(1,40)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:ALA:N	1	3.78
(1,40)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:ALA:N	12	3.76
(2,40)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:ALA:N	12	3.62
(2,40)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:ALA:N	9	3.52
(1,40)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:ALA:N	9	3.42
(1,40)	1:226:A:GLU:N	1:226:A:GLU:CA	1:226:A:GLU:C	1:227:A:ALA:N	11	3.28
(2,40)	1:226:B:GLU:N	1:226:B:GLU:CA	1:226:B:GLU:C	1:227:B:ALA:N	11	3.26