



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 10:39 AM UTC

PDB ID : 5A4G / pdb_00005a4g
BMRB ID : 25658
Title : NMR structure of a 180 residue construct encompassing the N-terminal metal-binding site and the membrane proximal domain of SilB from Cupriavidus metallidurans CH34
Authors : Bersch, B.; Urbina Fernandez, P.; Vandenbussche, G.
Deposited on : 2015-06-09

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 ⓘ 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 ⓘ](#)) 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

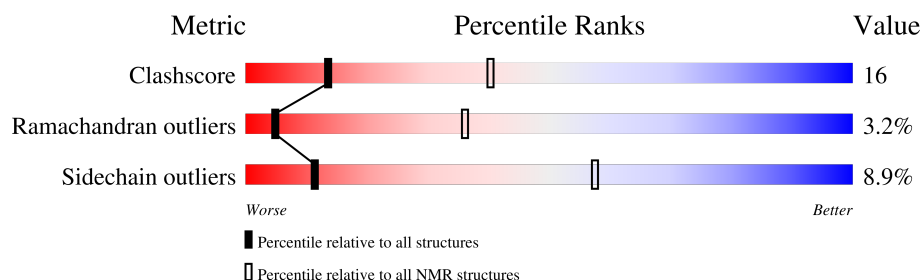
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	180	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:25-A:59 (35)	0.44	14
2	A:80-A:87, A:93-A:149 (65)	0.63	2
3	A:152-A:166 (15)	2.64	3

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. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2684 atoms, of which 1347 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SILB, SILVER EFFLUX PROTEIN, MFP COMPONENT OF THE THREE COMPONENTS PROTON ANTIPTORER METAL EFFLUX SYSTEM.

Mol	Chain	Residues	Atoms						Trace
1	A	180	Total	C	H	N	O	S	0
			2683	829	1347	240	261	6	

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q58AF3
A	175	LEU	-	expression tag	UNP Q58AF3
A	176	GLU	-	expression tag	UNP Q58AF3
A	177	VAL	-	expression tag	UNP Q58AF3
A	178	LEU	-	expression tag	UNP Q58AF3
A	179	PHE	-	expression tag	UNP Q58AF3
A	180	GLN	-	expression tag	UNP Q58AF3
A	90	GLY	-	linker	UNP Q58AF3
A	91	SER	-	linker	UNP Q58AF3

- Molecule 2 is SILVER ION (CCD ID: AG) (formula: Ag).

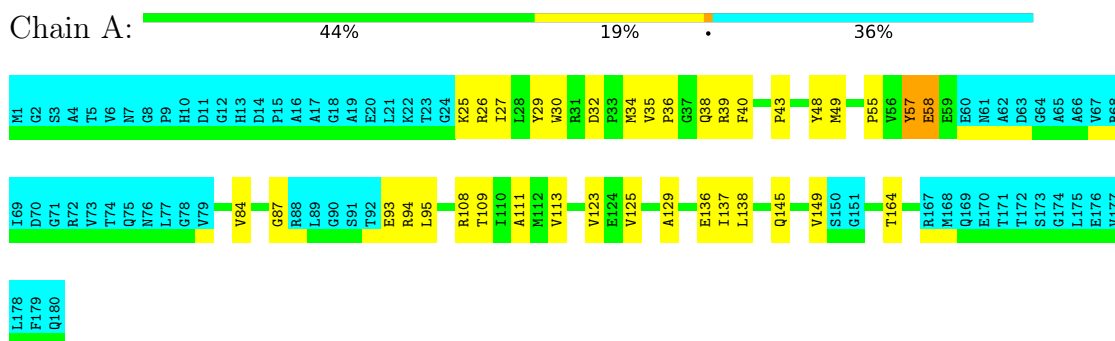
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ag
			1	1

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.

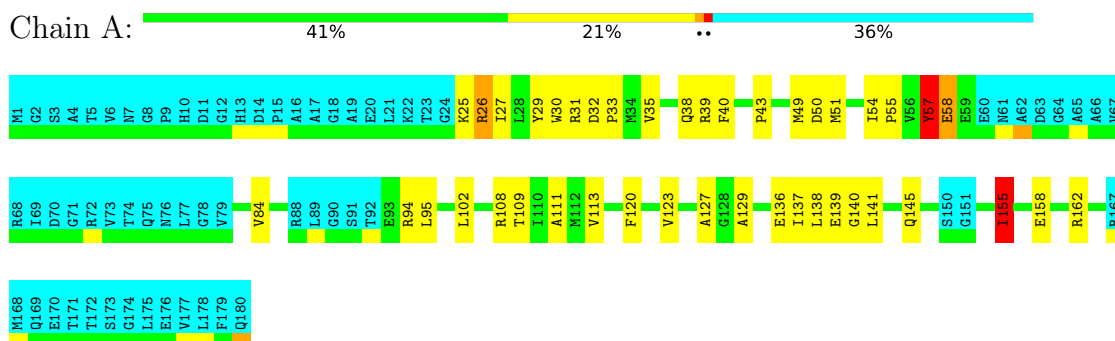
- Molecule 1: SILB, SILVER EFFLUX PROTEIN, MFP COMPONENT OF THE THREE COMPONENTS PROTON ANTIPOINTER METAL EFFLUX SYSTEM



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

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: SILB, SILVER EFFLUX PROTEIN, MFP COMPONENT OF THE THREE COMPONENTS PROTON ANTIPOINTER METAL EFFLUX SYSTEM



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *TOTAL ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	1.1
NMRDraw	structure solution	ANY
NMRPipe	structure solution	ANY
CcpNmr Analysis	structure solution	2.3
CcpNmr Analysis	structure solution	2.4
NMRView	structure solution	ANY
CYANA	structure solution	ANY

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	1807
Number of shifts mapped to atoms	1807
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AG

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	0.53±0.02	0±0/890 (0.0± 0.0%)	0.81±0.03	0±1/1203 (0.0± 0.1%)
All	All	0.53	0/17800 (0.0%)	0.81	5/24060 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	155	ILE	N-CA-C	-5.47	107.40	112.43	8	1
1	A	42	LYS	CA-C-N	5.39	125.40	119.90	12	2
1	A	42	LYS	C-N-CA	5.39	125.40	119.90	12	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	874	900	900	28±4
All	All	17500	18000	18000	569

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 16.

5 of 196 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ASP:HB3	1:A:34:MET:SD	0.91	2.06	19	1
1:A:129:ALA:HB3	1:A:136:GLU:HB2	0.91	1.42	13	18
1:A:84:VAL:HG23	1:A:143:ALA:HA	0.88	1.42	18	1
1:A:48:TYR:HB2	1:A:49:MET:HE2	0.81	1.50	8	5
1:A:32:ASP:HB3	1:A:35:VAL:HG22	0.80	1.53	10	16

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	115/180 (64%)	99±3 (86±2%)	13±3 (11±2%)	4±1 (3±1%)	5	36
All	All	2300/3600 (64%)	1976 (86%)	251 (11%)	73 (3%)	5	36

5 of 15 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	57	TYR	20
1	A	87	GLY	11
1	A	164	THR	9
1	A	155	ILE	6
1	A	43	PRO	5

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	91/138 (66%)	83±2 (91±2%)	8±2 (9±2%)	11	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1820/2760 (66%)	1658 (91%)	162 (9%)	11 57

5 of 33 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	57	TYR	19
1	A	34	MET	16
1	A	125	VAL	12
1	A	58	GLU	11
1	A	108	ARG	11

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 82% for the well-defined parts and 77% 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	1807
Number of shifts mapped to atoms	1807
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	167	-0.04 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	145	-0.02 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	151	-0.10 ± 0.06	None needed (< 0.5 ppm)
^{15}N	157	-0.21 ± 0.42	None needed (< 0.5 ppm)

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 82%, i.e. 1283 atoms were assigned a chemical shift out of a possible 1556. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	534/572 (93%)	223/235 (95%)	210/230 (91%)	101/107 (94%)
Sidechain	701/915 (77%)	469/598 (78%)	231/281 (82%)	1/36 (3%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	48/69 (70%)	24/33 (73%)	23/35 (66%)	1/1 (100%)
Overall	1283/1556 (82%)	716/866 (83%)	464/546 (85%)	103/144 (72%)

7.1.4 Statistically unusual chemical shifts [i](#)

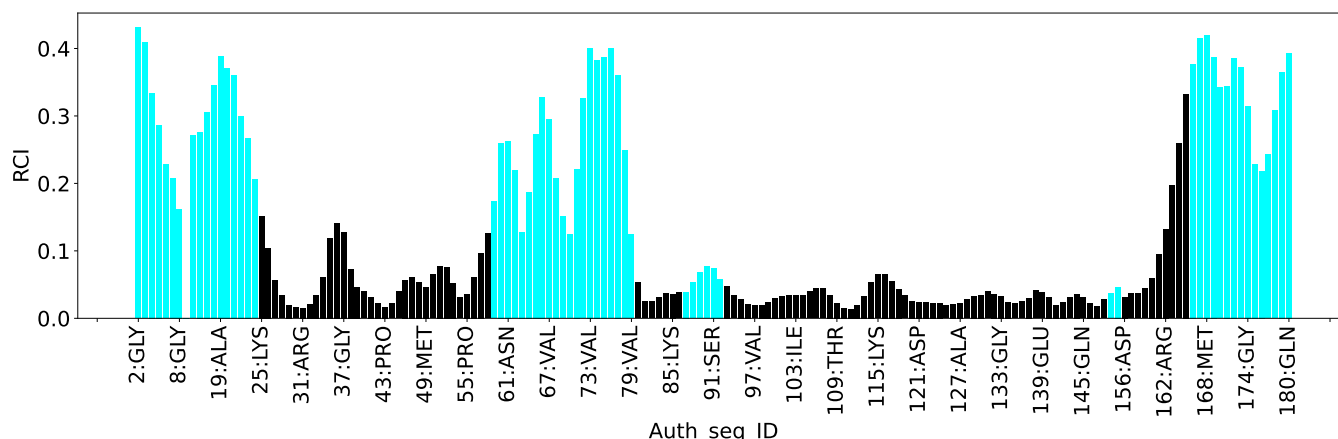
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	27	ILE	HG21	-0.79	-0.56 – 2.11	-5.8
1	A	27	ILE	HG22	-0.79	-0.56 – 2.11	-5.8
1	A	27	ILE	HG23	-0.79	-0.56 – 2.11	-5.8
1	A	39	ARG	HD2	1.85	1.97 – 4.26	-5.5

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis [i](#)

8.1 Conformationally restricting restraints [i](#)

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

Description	Value
Total distance restraints	4633
Intra-residue ($ i-j =0$)	1754
Sequential ($ i-j =1$)	1306
Medium range ($ i-j >1$ and $ i-j <5$)	454
Long range ($ i-j \geq 5$)	1119
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	174
Number of unmapped restraints	0
Number of restraints per residue	26.6
Number of long range restraints per residue ¹	6.2

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

8.2 Residual restraint violations [i](#)

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

8.2.1 Average number of distance violations per model [i](#)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	129.1	0.2
0.2-0.5 (Medium)	183.1	0.5
>0.5 (Large)	544.5	45.1

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)	14.7	8.46
10.0-20.0 (Medium)	1.9	16.94
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

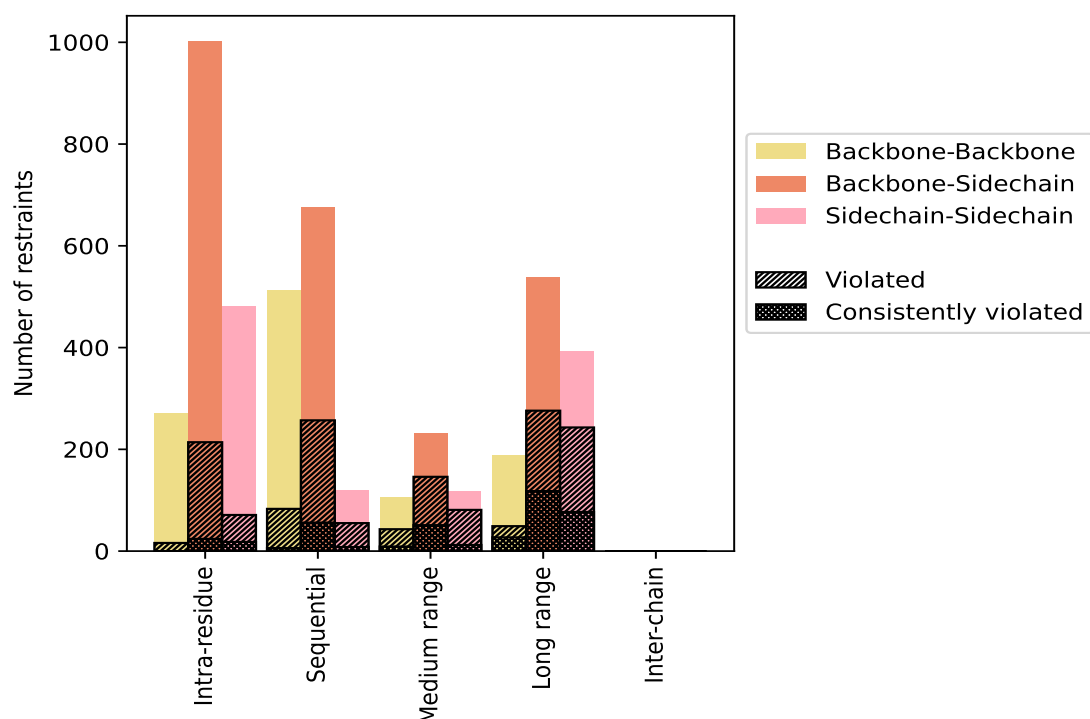
9.1 Summary of distance violations ⓘ

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	1754	37.9	301	17.2	6.5	42	2.4	0.9
Backbone-Backbone	271	5.8	16	5.9	0.3	0	0.0	0.0
Backbone-Sidechain	1002	21.6	214	21.4	4.6	24	2.4	0.5
Sidechain-Sidechain	481	10.4	71	14.8	1.5	18	3.7	0.4
Sequential (i-j =1)	1306	28.2	395	30.2	8.5	70	5.4	1.5
Backbone-Backbone	512	11.1	83	16.2	1.8	6	1.2	0.1
Backbone-Sidechain	675	14.6	257	38.1	5.5	56	8.3	1.2
Sidechain-Sidechain	119	2.6	55	46.2	1.2	8	6.7	0.2
Medium range (i-j >1 & i-j <5)	454	9.8	270	59.5	5.8	72	15.9	1.6
Backbone-Backbone	106	2.3	43	40.6	0.9	9	8.5	0.2
Backbone-Sidechain	231	5.0	146	63.2	3.2	51	22.1	1.1
Sidechain-Sidechain	117	2.5	81	69.2	1.7	12	10.3	0.3
Long range (i-j ≥5)	1119	24.2	568	50.8	12.3	222	19.8	4.8
Backbone-Backbone	189	4.1	49	25.9	1.1	27	14.3	0.6
Backbone-Sidechain	538	11.6	276	51.3	6.0	118	21.9	2.5
Sidechain-Sidechain	392	8.5	243	62.0	5.2	77	19.6	1.7
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	4633	100.0	1534	33.1	33.1	406	8.8	8.8
Backbone-Backbone	1078	23.3	191	17.7	4.1	42	3.9	0.9
Backbone-Sidechain	2446	52.8	893	36.5	19.3	249	10.2	5.4
Sidechain-Sidechain	1109	23.9	450	40.6	9.7	115	10.4	2.5

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 [i](#)



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

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	139	200	161	371	0	871	1.93	29.85	3.35	0.75
2	148	192	159	373	0	872	1.98	30.77	3.51	0.76
3	143	194	163	372	0	872	1.93	38.02	3.42	0.77
4	141	196	160	371	0	868	2.02	29.05	3.6	0.75
5	141	209	155	370	0	875	1.95	31.26	3.57	0.7
6	155	197	163	377	0	892	1.9	38.62	3.37	0.78
7	130	197	158	357	0	842	2.03	34.15	3.58	0.82
8	137	214	164	360	0	875	1.98	29.33	3.51	0.76
9	148	210	164	360	0	882	1.86	27.12	3.02	0.77
10	142	201	156	367	0	866	1.92	30.12	3.33	0.72

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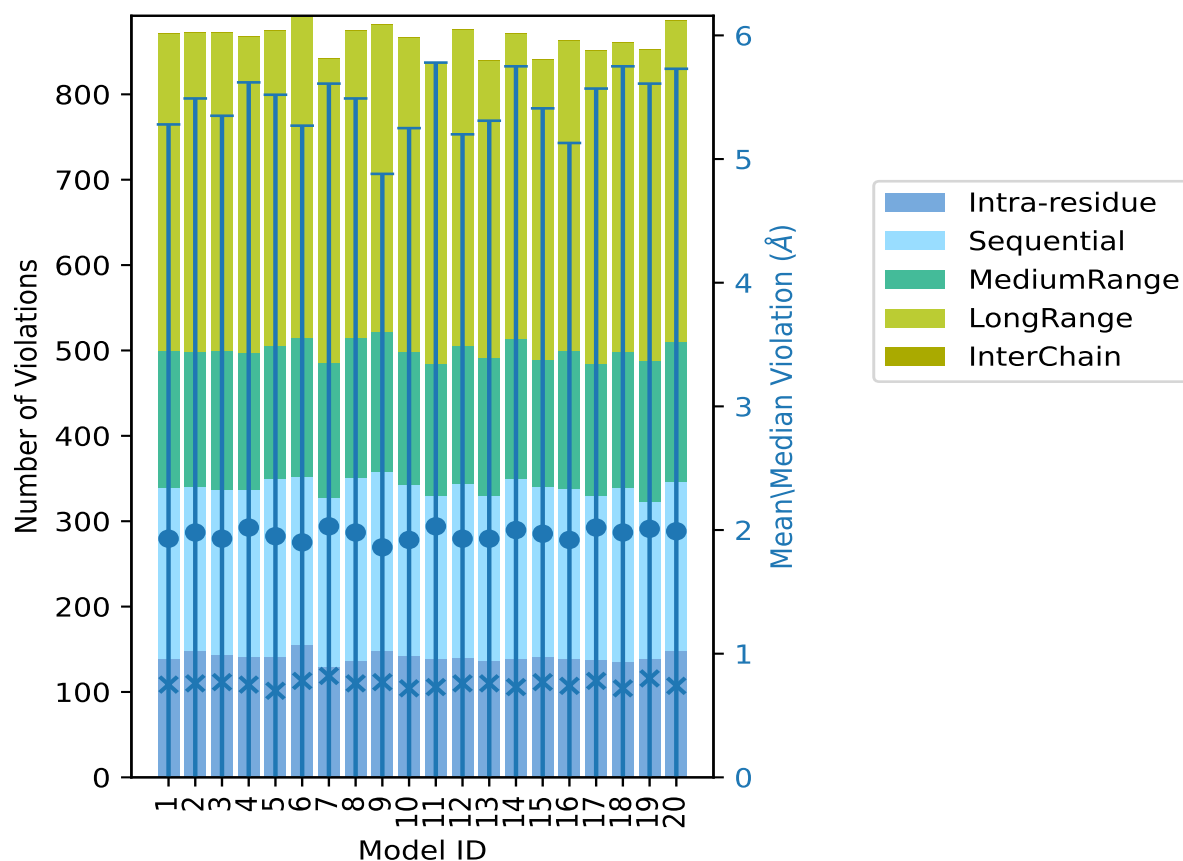
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	139	191	155	352	0	837	2.03	36.46	3.75	0.73
12	140	204	161	371	0	876	1.93	26.19	3.27	0.76
13	136	194	161	349	0	840	1.93	32.01	3.38	0.76
14	139	210	165	357	0	871	2.0	38.61	3.75	0.73
15	141	200	148	352	0	841	1.97	42.08	3.44	0.77
16	139	199	161	364	0	863	1.92	23.63	3.21	0.74
17	138	192	155	366	0	851	2.02	29.57	3.55	0.78
18	136	203	159	363	0	861	1.98	37.46	3.77	0.72
19	139	184	165	364	0	852	2.01	28.59	3.6	0.8
20	148	198	164	376	0	886	1.99	45.1	3.74	0.74

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

⁵Inter-chain restraints, ⁶Standard 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

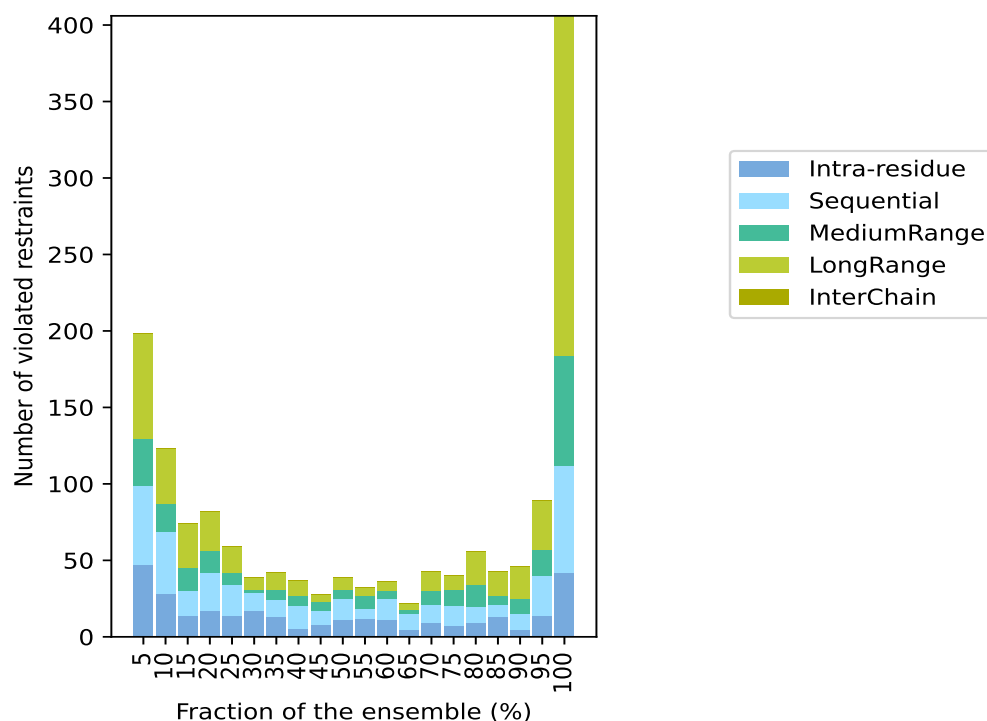
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3099(IR:1453, SQ:911, MR:184, LR:551, IC:0) restraints are 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	%
47	52	31	68	0	198	1	5.0
28	41	18	36	0	123	2	10.0
14	16	15	29	0	74	3	15.0
17	25	14	26	0	82	4	20.0
14	20	8	17	0	59	5	25.0
17	12	2	8	0	39	6	30.0
13	11	7	11	0	42	7	35.0
5	15	7	10	0	37	8	40.0
8	9	6	5	0	28	9	45.0
11	14	6	8	0	39	10	50.0
12	6	9	5	0	32	11	55.0
11	14	5	6	0	36	12	60.0
5	10	3	4	0	22	13	65.0
9	12	9	13	0	43	14	70.0
7	13	11	9	0	40	15	75.0
9	11	14	22	0	56	16	80.0
13	8	6	16	0	43	17	85.0
5	10	10	21	0	46	18	90.0
14	26	17	32	0	89	19	95.0
42	70	72	222	0	406	20	100.0

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

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

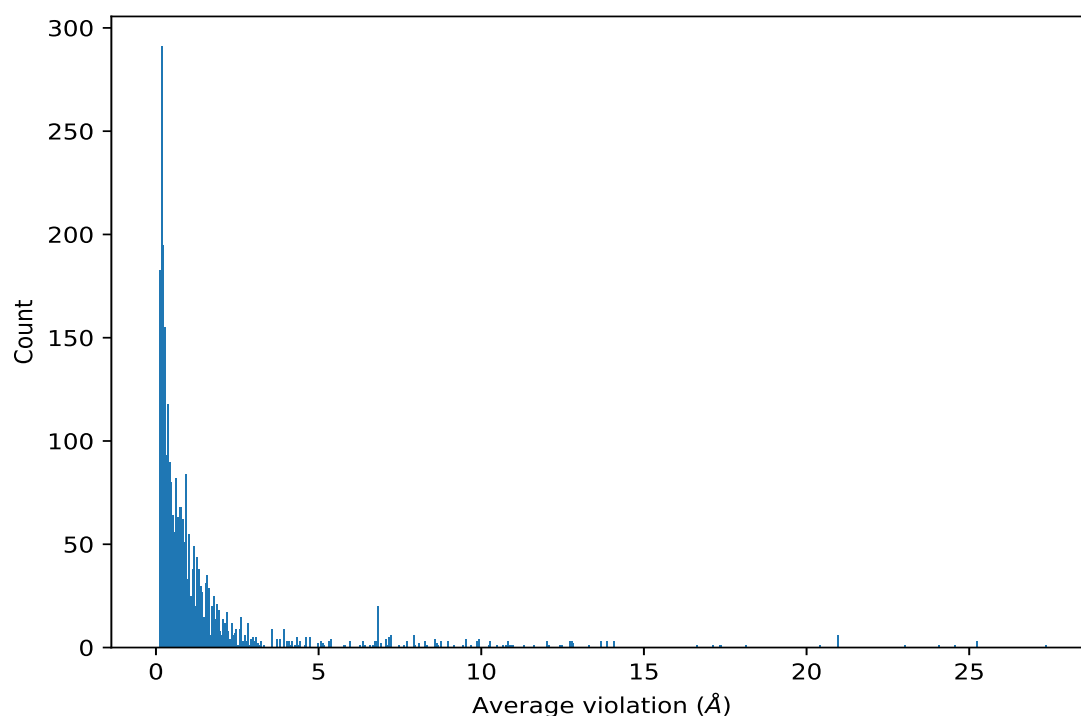
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,88)	1:17:A:ALA:HA	1:98:A:PRO:HB3	20	27.36	10.52	27.7
(4,68)	1:35:A:VAL:HG11	1:81:A:THR:HA	20	25.21	6.75	26.19
(4,68)	1:35:A:VAL:HG12	1:81:A:THR:HA	20	25.21	6.75	26.19
(4,68)	1:35:A:VAL:HG13	1:81:A:THR:HA	20	25.21	6.75	26.19
(4,23)	1:87:A:GLY:HA3	1:75:A:GLN:H	20	24.57	3.87	25.54
(4,89)	1:17:A:ALA:HA	1:32:A:ASP:HB3	20	24.05	4.37	23.54
(4,20)	1:69:A:ILE:H	1:133:A:GLY:HA2	20	23.03	6.33	24.07
(4,95)	1:120:A:PHE:HB2	1:35:A:VAL:HG11	20	20.96	6.38	19.57
(4,95)	1:120:A:PHE:HB2	1:35:A:VAL:HG12	20	20.96	6.38	19.57
(4,95)	1:120:A:PHE:HB2	1:35:A:VAL:HG13	20	20.96	6.38	19.57
(4,95)	1:120:A:PHE:HB3	1:35:A:VAL:HG11	20	20.96	6.38	19.57
(4,95)	1:120:A:PHE:HB3	1:35:A:VAL:HG12	20	20.96	6.38	19.57
(4,95)	1:120:A:PHE:HB3	1:35:A:VAL:HG13	20	20.96	6.38	19.57
(4,21)	1:75:A:GLN:H	1:133:A:GLY:HA2	20	20.42	4.81	20.98
(4,19)	1:69:A:ILE:H	1:52:A:PRO:HD2	20	18.11	3.74	18.87
(4,22)	1:75:A:GLN:H	1:122:A:PRO:HD2	20	17.36	3.88	16.98

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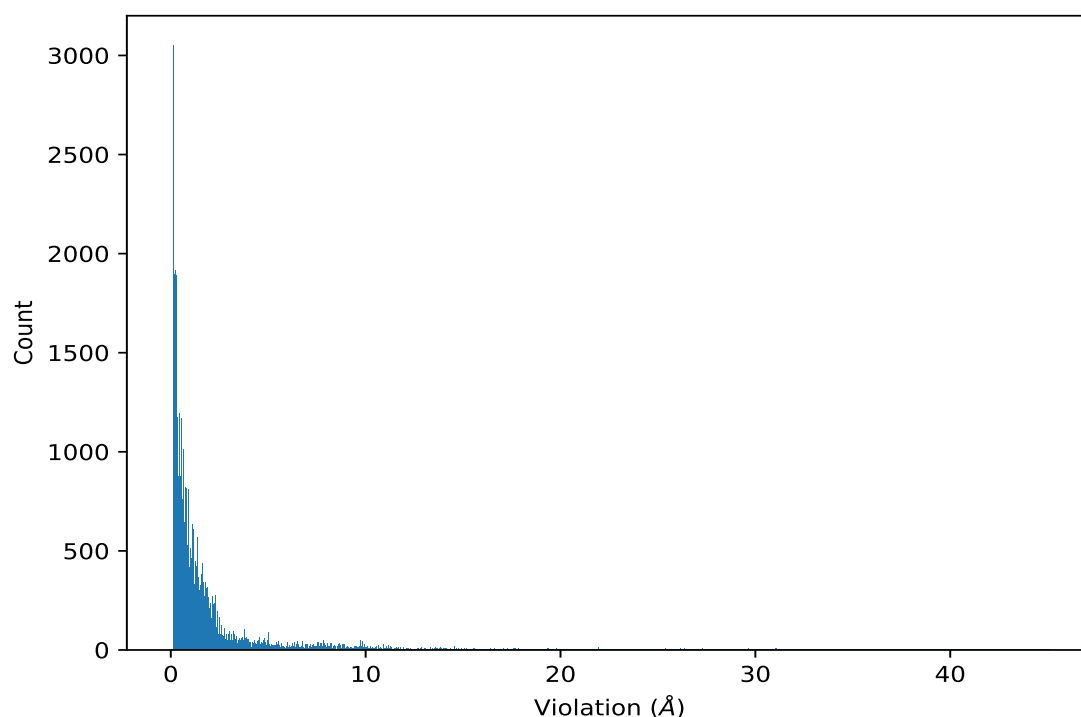
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,57)	1:68:A:ARG:HA	1:172:A:THR:HB	20	17.34	3.08	17.56

¹Number of violated models, ²Standard 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)
(4,88)	1:17:A:ALA:HA	1:98:A:PRO:HB3	20	45.1
(4,88)	1:17:A:ALA:HA	1:98:A:PRO:HB3	15	42.08
(4,88)	1:17:A:ALA:HA	1:98:A:PRO:HB3	6	38.62
(4,68)	1:35:A:VAL:HG11	1:81:A:THR:HA	14	38.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,68)	1:35:A:VAL:HG12	1:81:A:THR:HA	14	38.61
(4,68)	1:35:A:VAL:HG13	1:81:A:THR:HA	14	38.61
(4,88)	1:17:A:ALA:HA	1:98:A:PRO:HB3	3	38.02
(4,68)	1:35:A:VAL:HG11	1:81:A:THR:HA	18	37.46
(4,68)	1:35:A:VAL:HG12	1:81:A:THR:HA	18	37.46
(4,68)	1:35:A:VAL:HG13	1:81:A:THR:HA	18	37.46
(4,88)	1:17:A:ALA:HA	1:98:A:PRO:HB3	11	36.46
(4,88)	1:17:A:ALA:HA	1:98:A:PRO:HB3	7	34.15
(4,20)	1:69:A:ILE:H	1:133:A:GLY:HA2	20	34.0
(4,88)	1:17:A:ALA:HA	1:98:A:PRO:HB3	18	33.97

10 Dihedral-angle violation analysis [i](#)

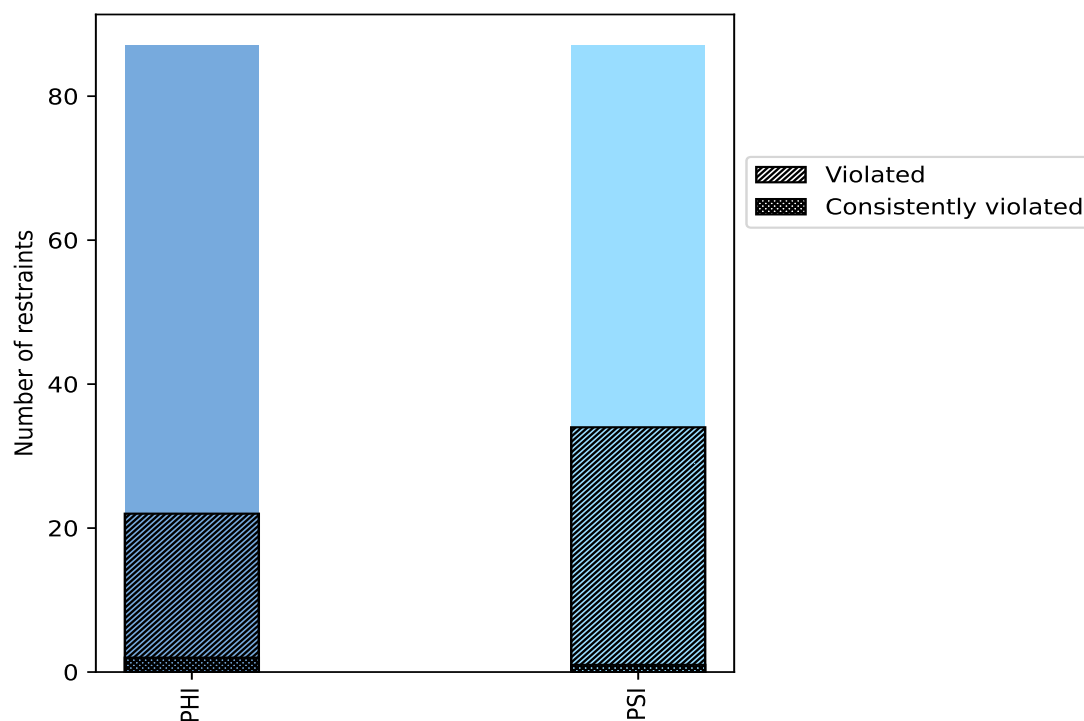
10.1 Summary of dihedral-angle violations [i](#)

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	50.0	22	25.3	12.6	2	2.3	1.1
PSI	87	50.0	34	39.1	19.5	1	1.1	0.6
Total	174	100.0	56	32.2	32.2	3	1.7	1.7

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 [i](#)



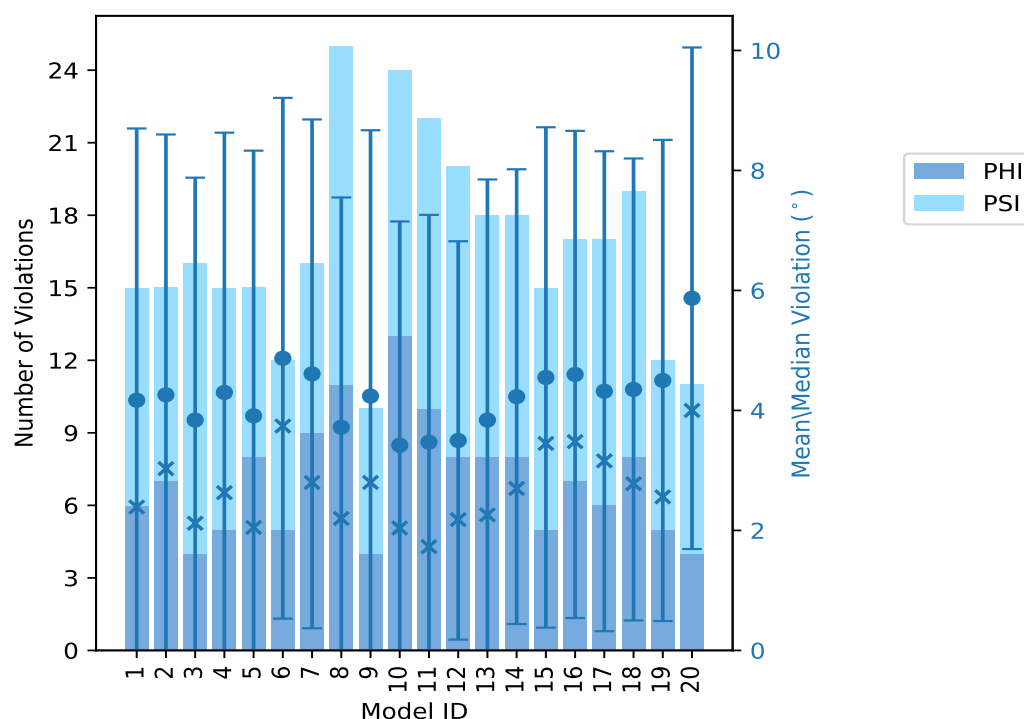
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	6	9	15	4.17	15.54	4.53	2.39
2	7	8	15	4.26	15.22	4.34	3.03
3	4	12	16	3.84	15.1	4.04	2.12
4	5	10	15	4.3	15.01	4.33	2.63
5	8	7	15	3.91	15.47	4.42	2.05
6	5	7	12	4.87	14.95	4.34	3.74
7	9	7	16	4.61	15.97	4.24	2.8
8	11	14	25	3.72	16.11	3.83	2.2
9	4	6	10	4.24	16.94	4.43	2.8
10	13	11	24	3.42	15.37	3.73	2.04
11	10	12	22	3.47	15.66	3.79	1.73
12	8	12	20	3.5	16.36	3.32	2.18
13	8	10	18	3.84	14.96	4.01	2.26
14	8	10	18	4.23	14.81	3.79	2.7
15	5	10	15	4.55	15.28	4.17	3.45
16	7	10	17	4.6	14.99	4.06	3.48
17	6	11	17	4.32	15.1	4.0	3.16
18	8	11	19	4.35	14.72	3.85	2.78
19	5	7	12	4.5	13.88	4.01	2.56
20	4	7	11	5.87	13.62	4.18	4.0

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
3	13	16	1	5.0
4	4	8	2	10.0
4	1	5	3	15.0
2	3	5	4	20.0
0	0	0	5	25.0
2	2	4	6	30.0
1	1	2	7	35.0
0	2	2	8	40.0
0	0	0	9	45.0
2	0	2	10	50.0
0	3	3	11	55.0

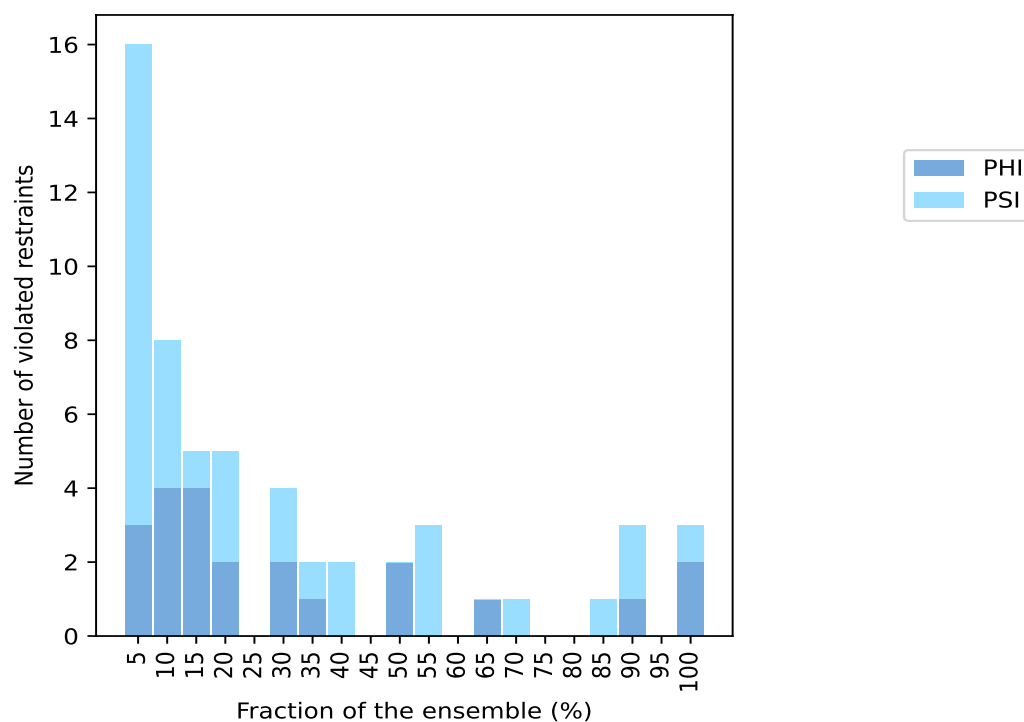
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
1	0	1	13	65.0
0	1	1	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	1	1	17	85.0
1	2	3	18	90.0
0	0	0	19	95.0
2	1	3	20	100.0

¹ Number of models with violations

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

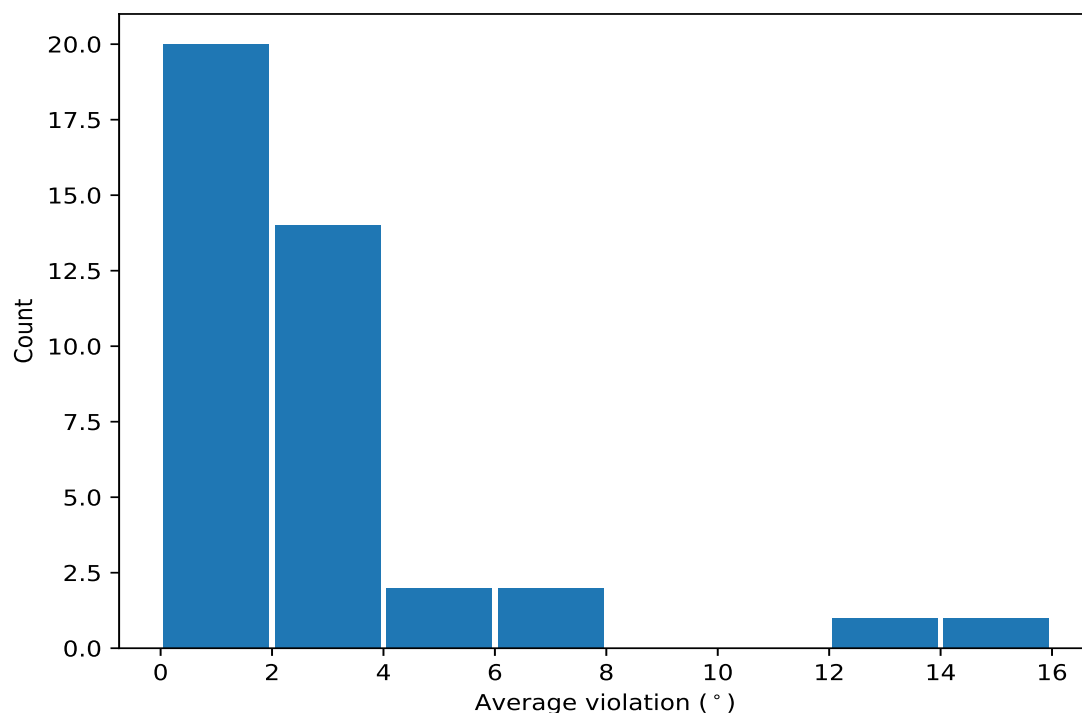


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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 [i](#)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

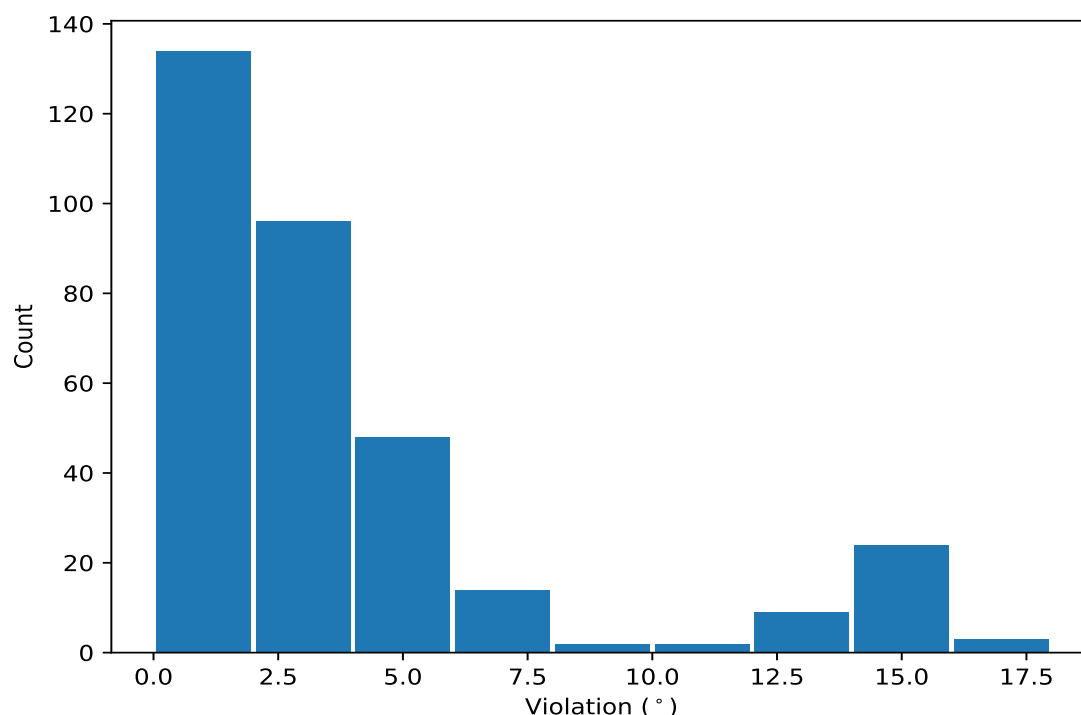
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	20	15.23	0.76	15.16
(1,127)	1:128:A:GLY:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	20	12.82	2.82	13.6
(1,125)	1:127:A:ALA:C	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	20	4.42	1.06	4.48
(1,123)	1:126:A:LYS:C	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	18	3.87	0.96	3.8
(1,40)	1:56:A:VAL:N	1:56:A:VAL:CA	1:56:A:VAL:C	1:57:A:TYR:N	18	3.03	1.25	2.85
(1,70)	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1:97:A:VAL:N	18	2.44	0.78	2.49
(1,128)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:THR:N	17	2.2	0.73	2.05
(1,68)	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	1:96:A:LEU:N	14	2.11	0.8	2.12
(1,19)	1:40:A:PHE:C	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	13	1.64	0.46	1.47
(1,60)	1:91:A:SER:N	1:91:A:SER:CA	1:91:A:SER:C	1:92:A:THR:N	11	6.46	1.32	6.92

¹ Number of violated models, ²Standard 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 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 (°)
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	9	16.94
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	12	16.36
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	8	16.11
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	7	15.97
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	11	15.66
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	1	15.54
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	5	15.47
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	10	15.37
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	15	15.28
(1,126)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	2	15.22