wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2JN0
BMRB ID	:	15079
Title	:	Solution NMR structure of the ygdR protein from Escherichia coli. Northeast Structural Genomics target ER382A.
Authors	:	Rossi, P.; Chen, C.X.; Jiang, M.; Cunningham, K.; Ma, L.; Xiao, R.; Liu, J.C.; Baran, M.; Swapna, G.V.T.; Acton, T.B.; Rost, B.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2006-12-15

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:

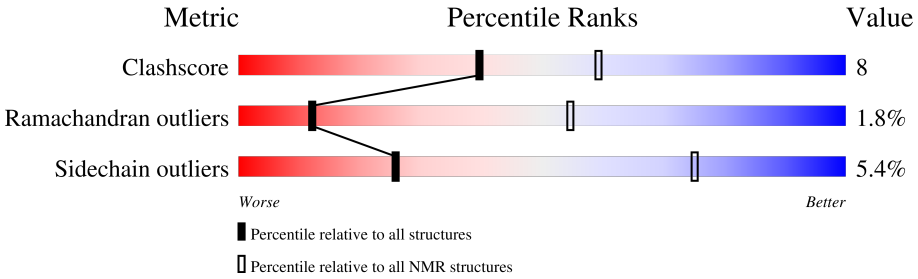
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 86%.

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	61	59% 15% 8% 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 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:6-A:50 (45)	0.77	8

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 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 768 atoms, of which 374 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical lipoprotein ygdR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	50	768	237	374	69	85	3	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P65294
A	54	LEU	-	cloning artifact	UNP P65294
A	55	GLU	-	cloning artifact	UNP P65294
A	56	HIS	-	expression tag	UNP P65294
A	57	HIS	-	expression tag	UNP P65294
A	58	HIS	-	expression tag	UNP P65294
A	59	HIS	-	expression tag	UNP P65294
A	60	HIS	-	expression tag	UNP P65294
A	61	HIS	-	expression tag	UNP P65294

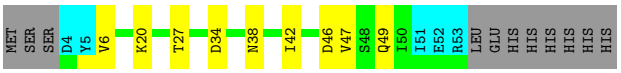
4 Residue-property plots

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: Hypothetical lipoprotein ygdR

Chain A:

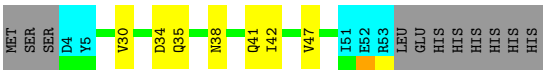


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: Hypothetical lipoprotein ygdR

Chain A:



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: *target function.*

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

Software name	Classification	Version
CNSSOLVE	refinement	1.1
X-PLOR	refinement	2.11.2
PROCHECK NMR	refinement	3.51
MolProbity	refinement	3.01
QUEEN	refinement	1.1
PSVS	refinement	1.3
AutoStructure	structure solution	2.1.1
NMRPipe	structure solution	
Sparky	structure solution	
MOLMOL	structure solution	
CNS	structure solution	
PROCHECK	structure solution	
XPLOR-NIH	structure solution	
DIANA	structure solution	
QUEEN	structure solution	1.1

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	552
Number of shifts mapped to atoms	537
Number of unparsed shifts	0
Number of shifts with mapping errors	15
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality

6.1 Standard geometry

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

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±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	19	GLY	Peptide	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	346	331	330	5±2
All	All	6920	6620	6600	104

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 8.

5 of 51 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ASP:HB3	1:A:33:HIS:HB2	0.86	1.43	12	6
1:A:43:ASN:HB3	1:A:46:ASP:HB2	0.76	1.55	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ILE:HD11	1:A:47:VAL:HB	0.70	1.64	17	5
1:A:34:ASP:HB2	1:A:38:ASN:HB2	0.67	1.65	4	8
1:A:8:ALA:HB3	1:A:49:GLN:HB3	0.65	1.69	3	2

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	45/61 (74%)	40±2 (88±3%)	4±1 (10±3%)	1±1 (2±2%)	12	54
All	All	900/1220 (74%)	796 (88%)	88 (10%)	16 (2%)	12	54

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	20	LYS	8
1	A	6	VAL	7
1	A	50	ILE	1

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	39/55 (71%)	37±1 (95±4%)	2±1 (5±4%)	26	75
All	All	780/1100 (71%)	738 (95%)	42 (5%)	26	75

5 of 19 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	34	ASP	14
1	A	22	GLU	3
1	A	44	ARG	2
1	A	46	ASP	2
1	A	41	GLN	2

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

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	552
Number of shifts mapped to atoms	537
Number of unparsed shifts	0
Number of shifts with mapping errors	15
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	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 15) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	LEU	HA	4.205	0.03	1
1	A	54	LEU	HB2	1.442	0.03	1
1	A	54	LEU	HB3	1.442	0.03	1
1	A	54	LEU	HG	1.285	0.03	1
1	A	54	LEU	HD11	0.702	0.03	2
1	A	54	LEU	HD12	0.702	0.03	2
1	A	54	LEU	HD13	0.702	0.03	2
1	A	54	LEU	HD21	0.67	0.03	2
1	A	54	LEU	HD22	0.67	0.03	2
1	A	54	LEU	HD23	0.67	0.03	2
1	A	54	LEU	CA	56.072	0.3	1
1	A	54	LEU	CB	41.969	0.3	1
1	A	54	LEU	CG	29.06	0.3	1
1	A	54	LEU	CD1	25.038	0.3	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	LEU	CD2	23.652	0.3	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	48	-0.29 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	44	0.16 ± 0.18	None needed (< 0.5 ppm)
$^{13}C'$	36	-0.03 ± 0.20	None needed (< 0.5 ppm)
^{15}N	43	-0.14 ± 0.49	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 86%, i.e. 504 atoms were assigned a chemical shift out of a possible 584. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	209/227 (92%)	89/93 (96%)	78/90 (87%)	42/44 (95%)
Sidechain	285/340 (84%)	193/218 (89%)	85/108 (79%)	7/14 (50%)
Aromatic	10/17 (59%)	5/8 (62%)	5/7 (71%)	0/2 (0%)
Overall	504/584 (86%)	287/319 (90%)	168/205 (82%)	49/60 (82%)

7.1.4 Statistically unusual chemical shifts

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

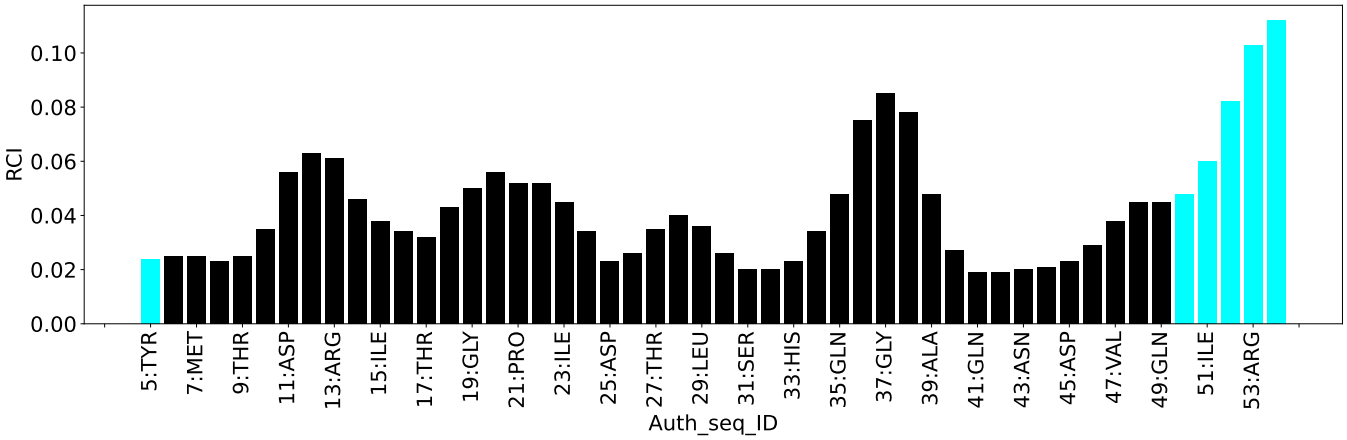
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	17	THR	HG1	5.59	0.08 – 2.19	21.1
1	A	40	MET	HB3	0.17	0.33 – 3.66	-5.5

7.1.5 Random Coil Index (RCI) plots

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication

of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	489
Intra-residue (|i-j|=0)	1
Sequential (|i-j|=1)	163
Medium range (|i-j|>1 and |i-j|<5)	89
Long range (|i-j|≥5)	216
Inter-chain	0
Hydrogen bond restraints	20
Disulfide bond restraints	0
Total dihedral-angle restraints	41
Number of unmapped restraints	0
Number of restraints per residue	8.7
Number of long range restraints per residue[1]	3.8

[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)	3.5	0.19
0.2-0.5 (Medium)	0.1	0.4
>0.5 (Large)	None	None

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)	2.1	6.89
10.0-20.0 (Medium)	None	None
>20.0 (Large)	1.0	149.28

9 Distance violation analysis (i)

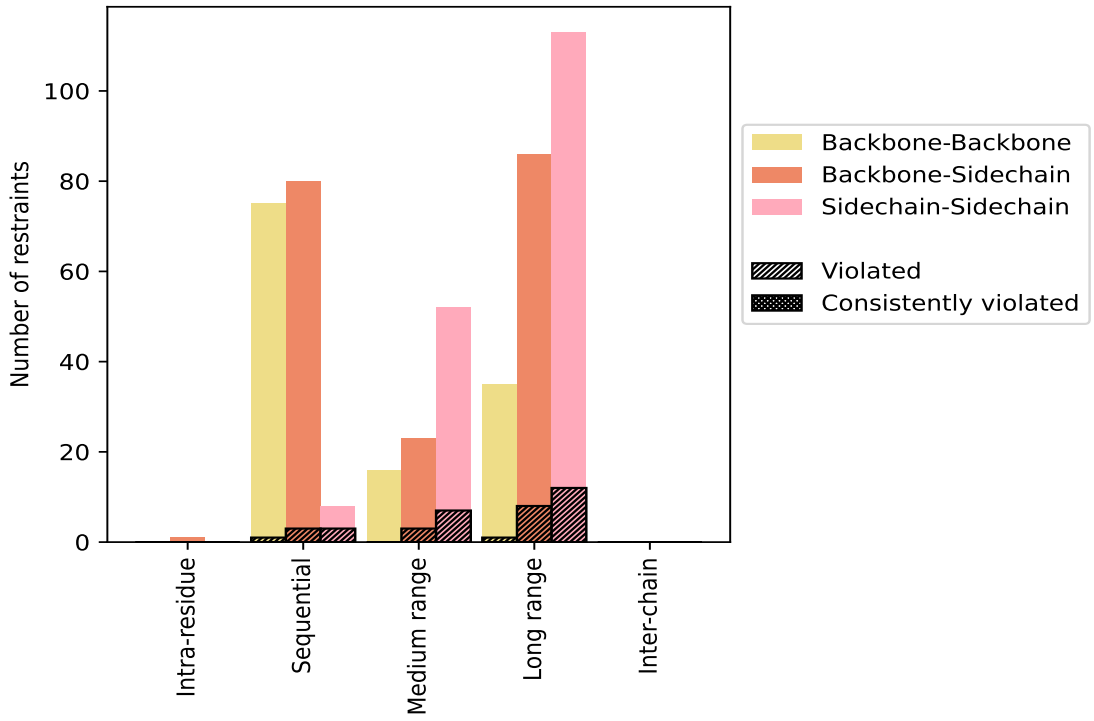
9.1 Summary of distance violations (i)

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)	1	0.2	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	1	0.2	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
Sequential (|i-j|=1)	163	33.3	7	4.3	1.4	0	0.0	0.0
Backbone-Backbone	75	15.3	1	1.3	0.2	0	0.0	0.0
Backbone-Sidechain	80	16.4	3	3.8	0.6	0	0.0	0.0
Sidechain-Sidechain	8	1.6	3	37.5	0.6	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	89	18.2	9	10.1	1.8	0	0.0	0.0
Backbone-Backbone	16	3.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	21	4.3	2	9.5	0.4	0	0.0	0.0
Sidechain-Sidechain	52	10.6	7	13.5	1.4	0	0.0	0.0
Long range (|i-j|≥5)	216	44.2	21	9.7	4.3	0	0.0	0.0
Backbone-Backbone	35	7.2	1	2.9	0.2	0	0.0	0.0
Backbone-Sidechain	68	13.9	8	11.8	1.6	0	0.0	0.0
Sidechain-Sidechain	113	23.1	12	10.6	2.5	0	0.0	0.0
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	20	4.1	1	5.0	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	489	100.0	38	7.8	7.8	0	0.0	0.0
Backbone-Backbone	126	25.8	2	1.6	0.4	0	0.0	0.0
Backbone-Sidechain	190	38.9	14	7.4	2.9	0	0.0	0.0
Sidechain-Sidechain	173	35.4	22	12.7	4.5	0	0.0	0.0

[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	0	0	1	4	0	5	0.12	0.13	0.01	0.12
2	0	1	0	2	0	3	0.13	0.14	0.01	0.14
3	0	1	1	2	0	4	0.15	0.18	0.02	0.15
4	0	2	1	2	0	5	0.13	0.17	0.02	0.13
5	0	1	0	2	0	3	0.13	0.15	0.01	0.13
6	0	1	0	1	0	2	0.12	0.12	0.0	0.12
7	0	1	1	1	0	3	0.15	0.16	0.01	0.14
8	0	1	0	1	0	2	0.11	0.11	0.0	0.11
9	0	2	0	1	0	3	0.13	0.17	0.03	0.12
10	0	1	1	3	0	5	0.12	0.17	0.02	0.11
11	0	0	1	2	0	3	0.13	0.15	0.02	0.14

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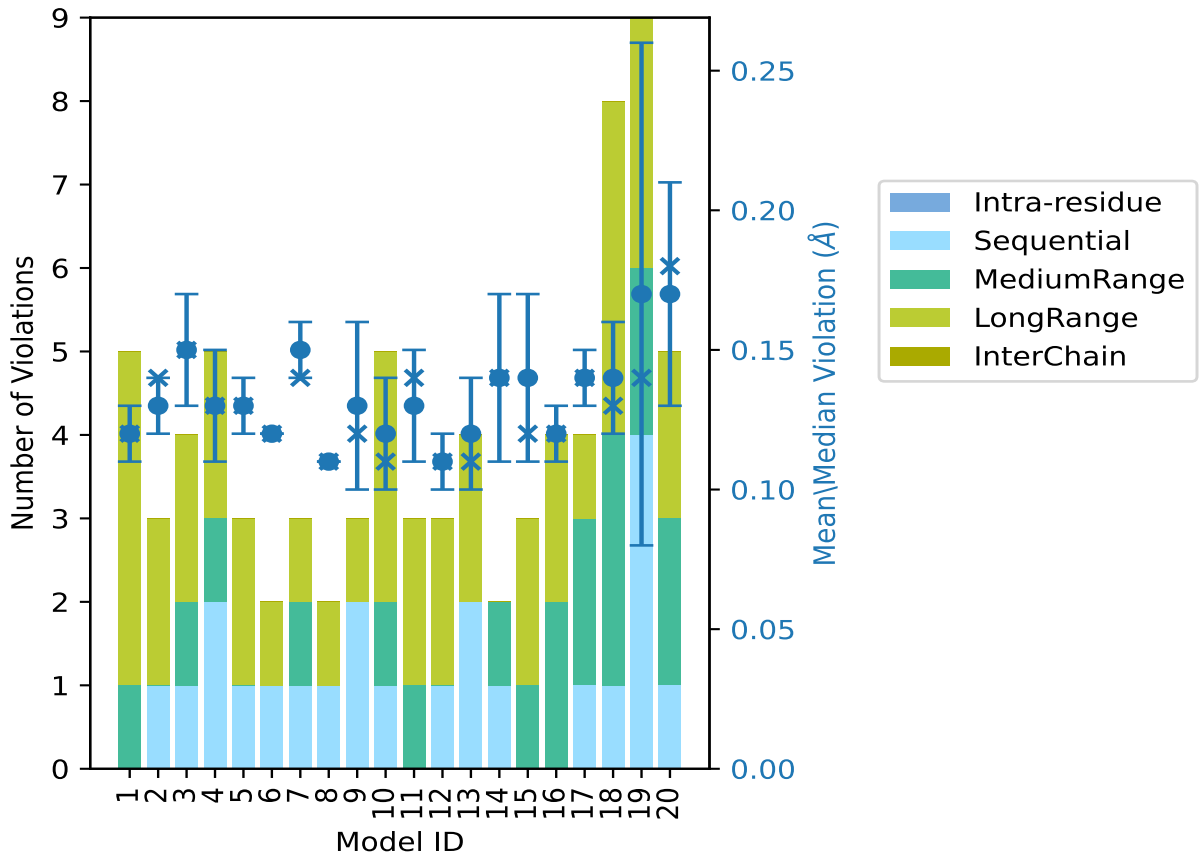
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	1	0	2	0	3	0.11	0.12	0.01	0.11
13	0	2	0	2	0	4	0.12	0.15	0.02	0.11
14	0	1	1	0	0	2	0.14	0.17	0.03	0.14
15	0	0	1	2	0	3	0.14	0.18	0.03	0.12
16	0	0	2	2	0	4	0.12	0.13	0.01	0.12
17	0	1	2	1	0	4	0.14	0.16	0.01	0.14
18	0	1	3	4	0	8	0.14	0.18	0.02	0.13
19	0	4	2	3	0	9	0.17	0.4	0.09	0.14
20	0	1	2	2	0	5	0.17	0.24	0.04	0.18

[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

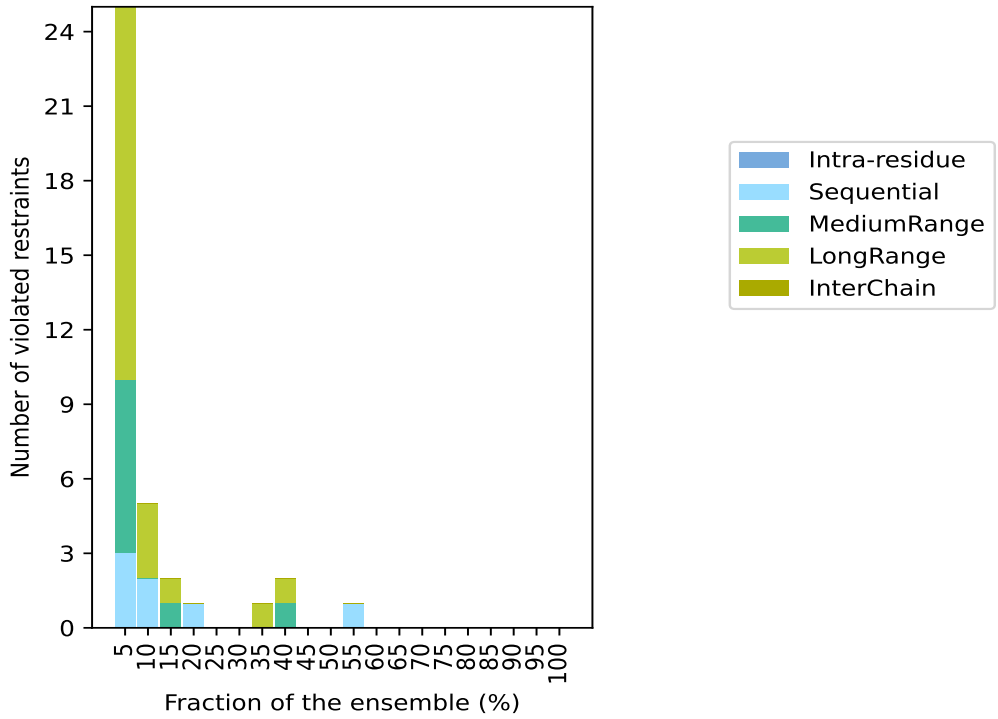
9.3 Distance violation statistics for the ensemble (i)

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, 432(IR:1, SQ:156, MR:80, LR:195, 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]	%
0	3	7	15	0	25	1	5.0
0	2	0	3	0	5	2	10.0
0	0	1	1	0	2	3	15.0
0	1	0	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	1	0	1	7	35.0
0	0	1	1	0	2	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	1	0	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	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

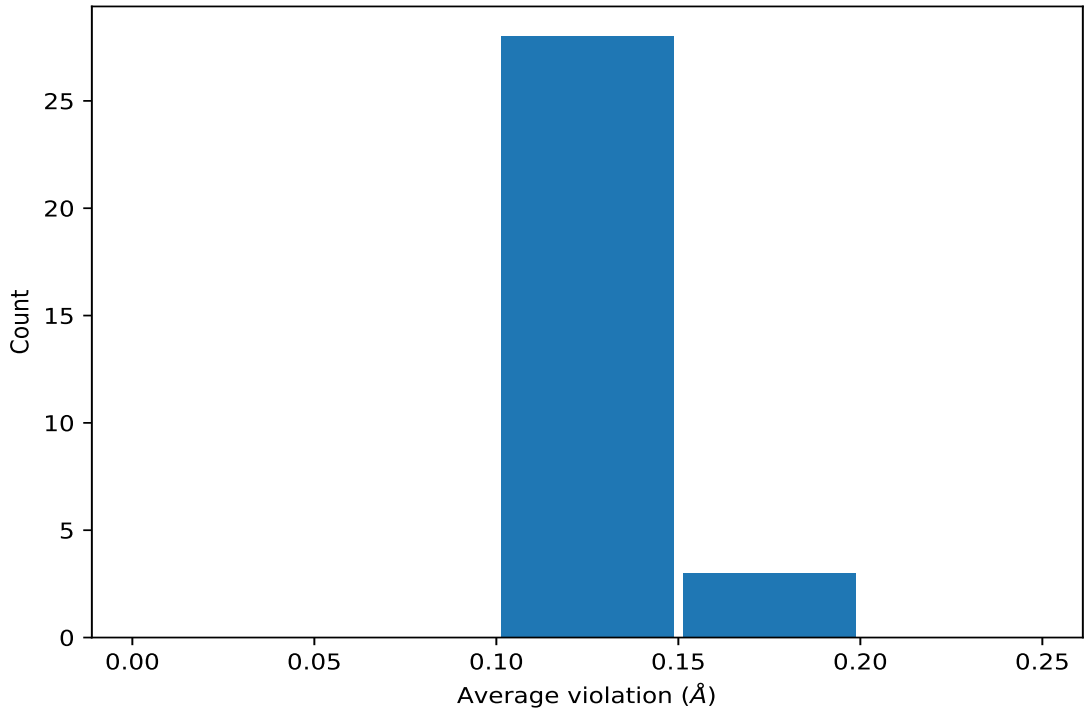
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (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)
(1,426)	1:42:A:ILE:HD11	1:43:A:ASN:HB2	11	0.14	0.02	0.14
(1,426)	1:42:A:ILE:HD12	1:43:A:ASN:HB2	11	0.14	0.02	0.14
(1,426)	1:42:A:ILE:HD13	1:43:A:ASN:HB2	11	0.14	0.02	0.14
(1,137)	1:17:A:THR:HG21	1:42:A:ILE:HG21	8	0.14	0.02	0.13
(1,137)	1:17:A:THR:HG21	1:42:A:ILE:HG22	8	0.14	0.02	0.13
(1,137)	1:17:A:THR:HG21	1:42:A:ILE:HG23	8	0.14	0.02	0.13
(1,137)	1:17:A:THR:HG22	1:42:A:ILE:HG21	8	0.14	0.02	0.13
(1,137)	1:17:A:THR:HG22	1:42:A:ILE:HG22	8	0.14	0.02	0.13
(1,137)	1:17:A:THR:HG22	1:42:A:ILE:HG23	8	0.14	0.02	0.13
(1,137)	1:17:A:THR:HG23	1:42:A:ILE:HG21	8	0.14	0.02	0.13
(1,137)	1:17:A:THR:HG23	1:42:A:ILE:HG22	8	0.14	0.02	0.13
(1,137)	1:17:A:THR:HG23	1:42:A:ILE:HG23	8	0.14	0.02	0.13
(1,129)	1:17:A:THR:HB	1:20:A:LYS:H	8	0.13	0.02	0.13
(1,320)	1:32:A:TYR:HE1	1:40:A:MET:HG2	7	0.14	0.02	0.14
(1,320)	1:32:A:TYR:HE2	1:40:A:MET:HG2	7	0.14	0.02	0.14
(1,427)	1:42:A:ILE:HD11	1:43:A:ASN:HB3	4	0.13	0.02	0.13

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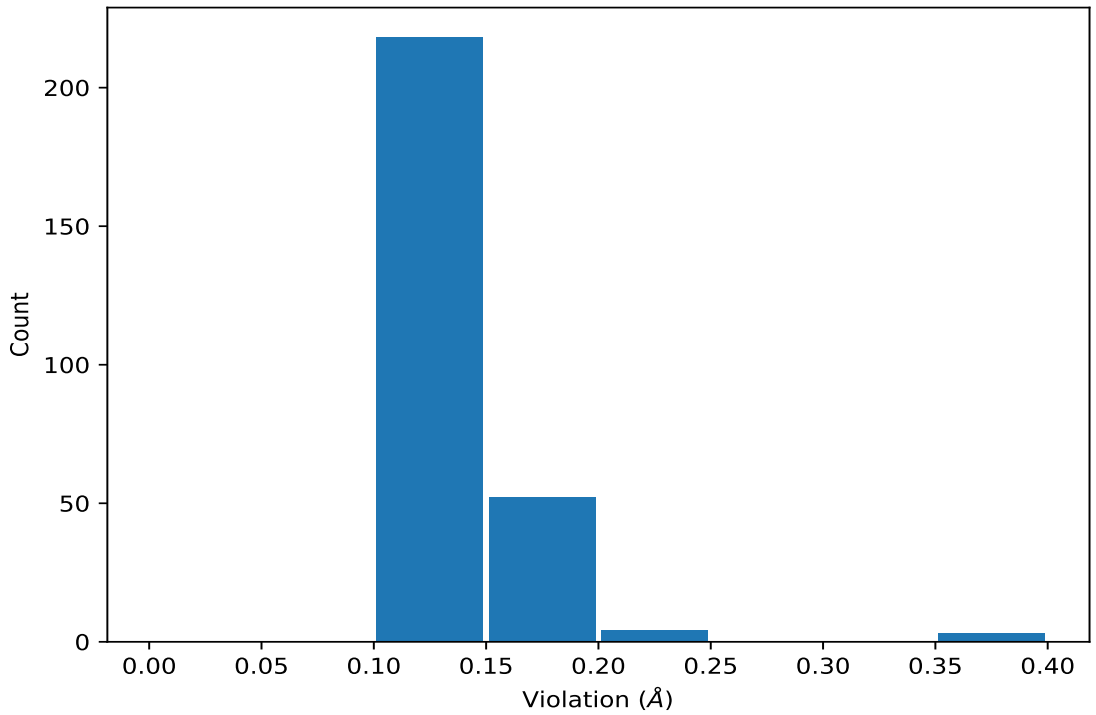
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,427)	1:42:A:ILE:HD12	1:43:A:ASN:HB3	4	0.13	0.02	0.13
(1,427)	1:42:A:ILE:HD13	1:43:A:ASN:HB3	4	0.13	0.02	0.13
(1,238)	1:27:A:THR:HB	1:29:A:LEU:HD21	3	0.15	0.02	0.13
(1,238)	1:27:A:THR:HB	1:29:A:LEU:HD22	3	0.15	0.02	0.13
(1,238)	1:27:A:THR:HB	1:29:A:LEU:HD23	3	0.15	0.02	0.13
(1,302)	1:31:A:SER:HB2	1:41:A:GLN:HA	3	0.11	0.01	0.1
(1,222)	1:26:A:ASP:H	1:27:A:THR:HG21	2	0.16	0.02	0.16
(1,222)	1:26:A:ASP:H	1:27:A:THR:HG22	2	0.16	0.02	0.16
(1,222)	1:26:A:ASP:H	1:27:A:THR:HG23	2	0.16	0.02	0.16
(1,64)	1:9:A:THR:HB	1:48:A:SER:HB3	2	0.12	0.0	0.12
(1,468)	1:6:A:VAL:H	1:17:A:THR:HG1	2	0.11	0.0	0.11

[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)
(1,228)	1:26:A:ASP:HB2	1:27:A:THR:HG21	19	0.4
(1,228)	1:26:A:ASP:HB2	1:27:A:THR:HG22	19	0.4
(1,228)	1:26:A:ASP:HB2	1:27:A:THR:HG23	19	0.4
(1,92)	1:13:A:ARG:HG3	1:14:A:MET:H	20	0.24
(1,204)	1:24:A:ASP:HB2	1:27:A:THR:HG21	19	0.21
(1,204)	1:24:A:ASP:HB2	1:27:A:THR:HG22	19	0.21
(1,204)	1:24:A:ASP:HB2	1:27:A:THR:HG23	19	0.21
(1,79)	1:11:A:ASP:HB2	1:13:A:ARG:HG3	19	0.19
(1,79)	1:11:A:ASP:HB3	1:13:A:ARG:HG3	19	0.19
(1,59)	1:9:A:THR:HB	1:13:A:ARG:HG2	20	0.19
(1,320)	1:32:A:TYR:HE1	1:40:A:MET:HG2	3	0.18
(1,320)	1:32:A:TYR:HE2	1:40:A:MET:HG2	3	0.18
(1,275)	1:30:A:VAL:H	1:42:A:ILE:HD11	15	0.18
(1,275)	1:30:A:VAL:H	1:42:A:ILE:HD12	15	0.18
(1,275)	1:30:A:VAL:H	1:42:A:ILE:HD13	15	0.18
(1,238)	1:27:A:THR:HB	1:29:A:LEU:HD21	18	0.18
(1,238)	1:27:A:THR:HB	1:29:A:LEU:HD22	18	0.18
(1,238)	1:27:A:THR:HB	1:29:A:LEU:HD23	18	0.18
(1,129)	1:17:A:THR:HB	1:20:A:LYS:H	20	0.18
(1,426)	1:42:A:ILE:HD11	1:43:A:ASN:HB2	14	0.17

10 Dihedral-angle violation analysis

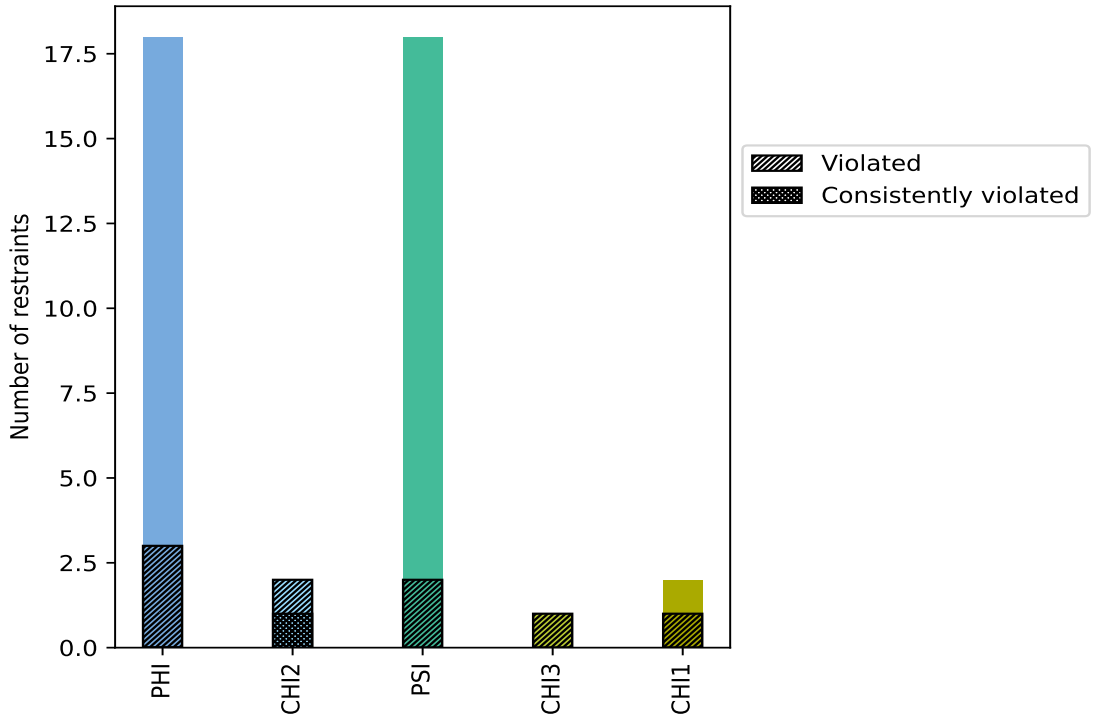
10.1 Summary of dihedral-angle violations

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	18	43.9	3	16.7	7.3	0	0.0	0.0
CHI2	2	4.9	2	100.0	4.9	1	50.0	2.4
PSI	18	43.9	2	11.1	4.9	0	0.0	0.0
CHI3	1	2.4	1	100.0	2.4	0	0.0	0.0
CHI1	2	4.9	1	50.0	2.4	0	0.0	0.0
Total	41	100.0	9	22.0	22.0	1	2.4	2.4

[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



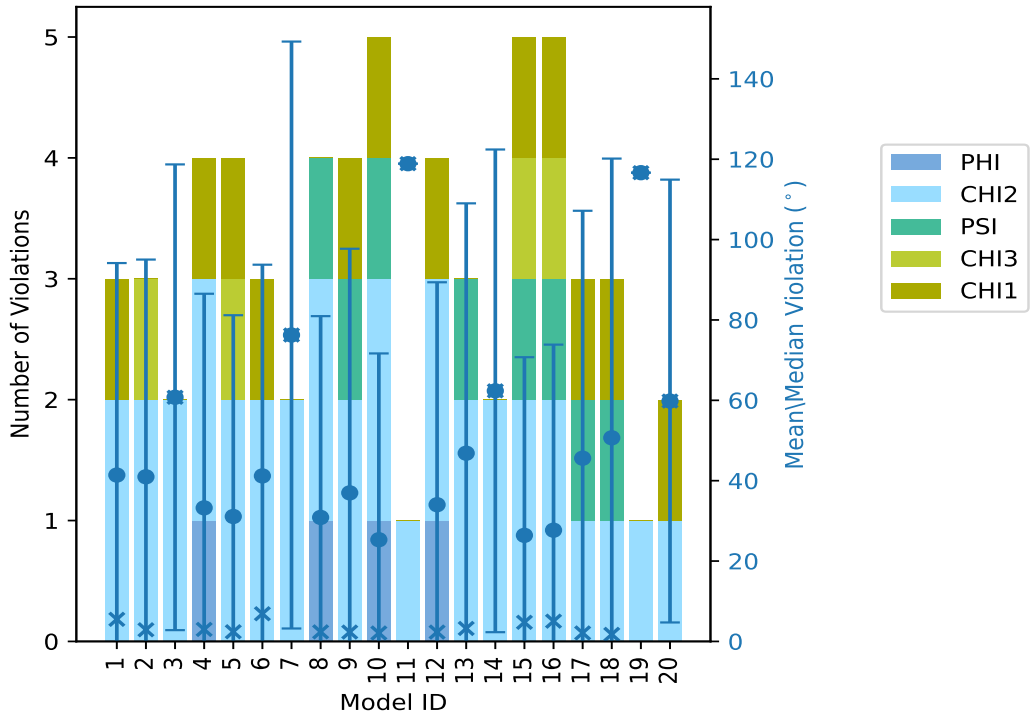
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	CHI2	PSI	CHI3	CHI1	Total				
1	0	2	0	0	1	3	41.4	115.99	52.76	5.5
2	0	2	0	1	0	3	40.97	117.42	54.06	2.9
3	0	2	0	0	0	2	60.76	118.71	57.95	60.76
4	1	2	0	0	1	4	33.24	125.52	53.28	2.99
5	0	2	0	1	1	4	31.09	117.84	50.09	2.41
6	0	2	0	0	1	3	41.19	115.44	52.56	6.89
7	0	2	0	0	0	2	76.25	149.28	73.03	76.25
8	1	2	1	0	0	4	30.86	117.6	50.09	2.38
9	0	2	1	0	1	4	36.97	142.19	60.75	2.33
10	1	2	1	0	1	5	25.31	118.01	46.36	2.1
11	0	1	0	0	0	1	118.89	118.89	0.0	118.89
12	1	2	0	0	1	4	34.02	129.9	55.36	2.33
13	0	2	1	0	0	3	46.84	134.77	62.18	3.23
14	0	2	0	0	0	2	62.36	122.42	60.06	62.36
15	0	2	1	1	1	5	26.4	115.05	44.33	4.76
16	0	2	1	1	1	5	27.68	120.03	46.18	5.04
17	0	1	1	0	1	3	45.6	132.67	61.57	2.11
18	0	1	1	0	1	3	50.67	148.94	69.49	1.76
19	0	1	0	0	0	1	116.65	116.65	0.0	116.65
20	0	1	0	0	1	2	59.82	114.91	55.1	59.82

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	CHI2	PSI	CHI3	CHI1	Total	Count[1]	%
2	0	0	0	0	2	1	5.0
1	0	0	0	0	1	2	10.0
0	0	1	0	0	1	3	15.0
0	0	0	1	0	1	4	20.0
0	0	1	0	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0

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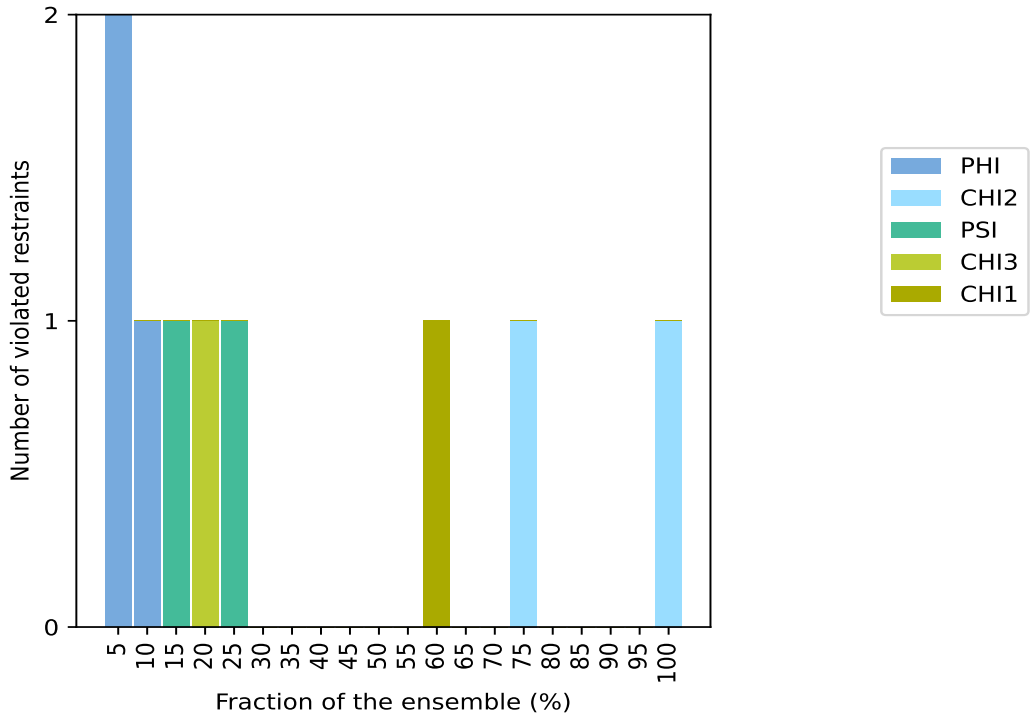
Number of violated restraints						Fraction of the ensemble	
PHI	CHI2	PSI	CHI3	CHI1	Total	Count[1]	%
0	0	0	0	1	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	1	0	0	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	1	0	0	0	1	20	100.0

[1] Number of models with violations

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

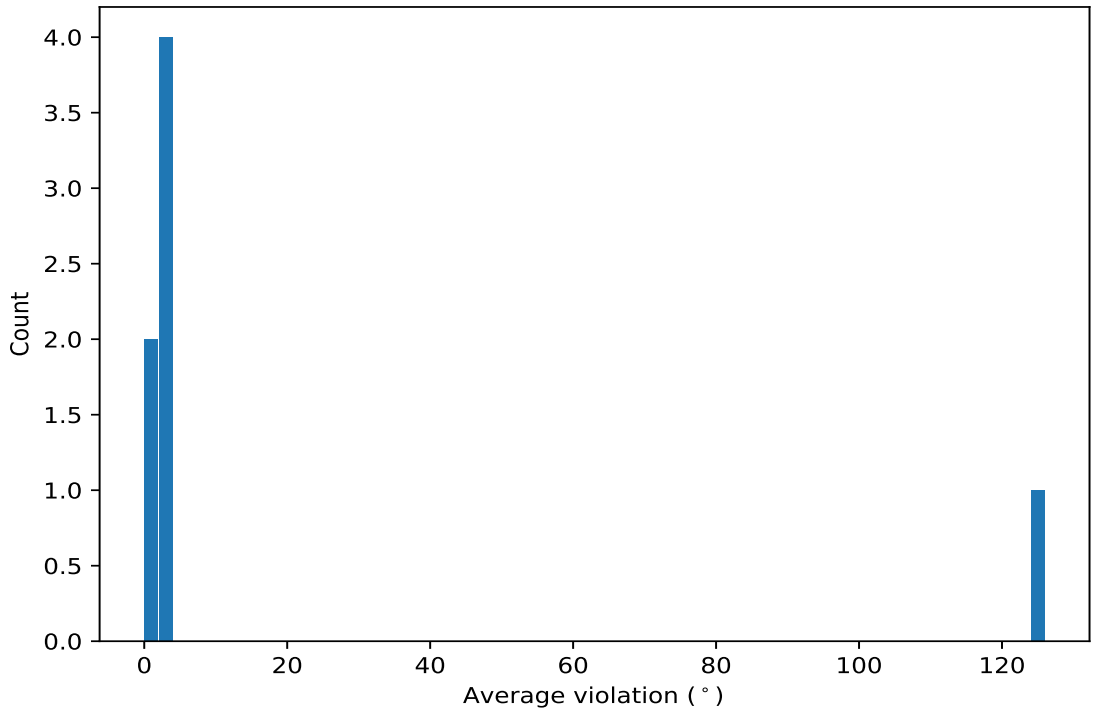


10.4 Most violated dihedral-angle restraints in the ensemble

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 (i)

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

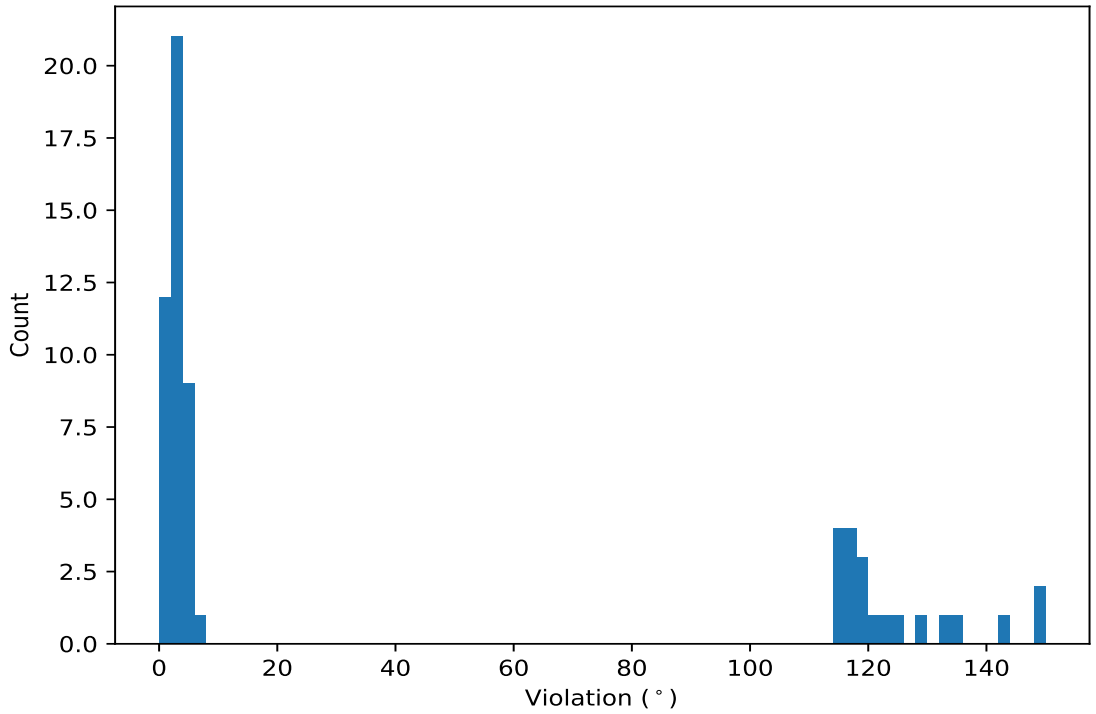
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	20	124.61	10.95	118.8
(1,8)	1:10:A:LYS:CA	1:10:A:LYS:CB	1:10:A:LYS:CG	1:10:A:LYS:CD	15	2.88	1.03	2.7
(1,10)	1:34:A:ASP:N	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	12	3.8	1.62	3.65
(1,41)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:ASN:N	5	1.43	0.43	1.16
(1,9)	1:10:A:LYS:CB	1:10:A:LYS:CG	1:10:A:LYS:CD	1:10:A:LYS:CE	4	3.5	1.27	3.78
(1,6)	1:9:A:THR:N	1:9:A:THR:CA	1:9:A:THR:C	1:10:A:LYS:N	3	2.73	0.41	2.51
(1,18)	1:15:A:ILE:C	1:16:A:LEU:N	1:16:A:LEU:CA	1:16:A:LEU:C	2	1.5	0.03	1.5

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints

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 (°)
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	7	149.28
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	18	148.94
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	9	142.19
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	13	134.77
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	17	132.67
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	12	129.9
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	4	125.52
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	14	122.42
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	16	120.03
(1,11)	1:34:A:ASP:CA	1:34:A:ASP:CB	1:34:A:ASP:CG	1:34:A:ASP:OD1	11	118.89