wwPDB NMR Structure Validation Summary Report

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BMRB ID	:	30791
Title	:	Solution NMR structure and dynamics of human Brd3 ET in complex with MLV IN CTD
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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:

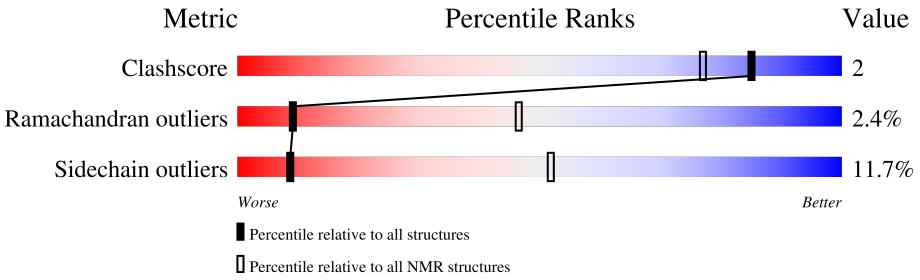
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 79%.

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	89	18% . 79%
2	B	96	67% 6% 27%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:69-A:87, B:223-B:292 (89)	0.85	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 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3005 atoms, of which 1498 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Integrase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1442	451	725	147	118	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP Q8UN00
A	2	HIS	-	expression tag	UNP Q8UN00
A	3	HIS	-	expression tag	UNP Q8UN00
A	4	HIS	-	expression tag	UNP Q8UN00
A	5	HIS	-	expression tag	UNP Q8UN00
A	6	HIS	-	expression tag	UNP Q8UN00
A	7	SER	-	expression tag	UNP Q8UN00
A	8	HIS	-	expression tag	UNP Q8UN00
A	9	MET	-	expression tag	UNP Q8UN00

- Molecule 2 is a protein called Bromodomain-containing protein 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	96	1563	484	773	146	157	3	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	201	HIS	-	expression tag	UNP Q15059
B	202	HIS	-	expression tag	UNP Q15059
B	203	HIS	-	expression tag	UNP Q15059
B	204	HIS	-	expression tag	UNP Q15059
B	205	HIS	-	expression tag	UNP Q15059
B	206	HIS	-	expression tag	UNP Q15059
B	207	SER	-	expression tag	UNP Q15059
B	208	HIS	-	expression tag	UNP Q15059
B	209	MET	-	expression tag	UNP Q15059

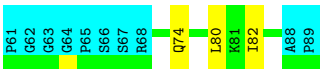
4 Residue-property plots

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.

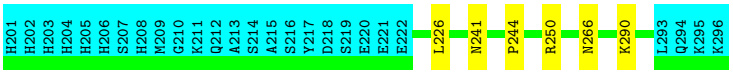
• Molecule 1: Integrase

Chain A:



• Molecule 2: Bromodomain-containing protein 3

Chain B:

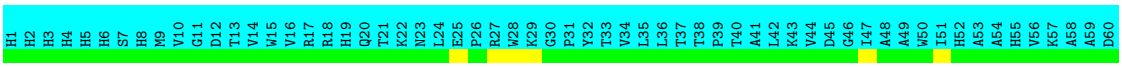


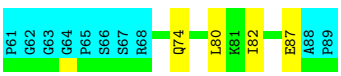
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

• Molecule 1: Integrase

Chain A:





• Molecule 2: Bromodomain-containing protein 3

Chain B:


H201
H202
H203
H204
H205
H206
S207
H208
M209
G210
K211
Q212
A213
S214
A215
S216
Y217
D218
S219
E220
E221
E222
G225
L226
E232
L236
I240
N241
P244
G245
E246
R250
L262
R263
N266
P267
D273
L277
R287
Y288
V289
L293
Q294
K295
K296

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
ASDP	geometry optimization	2.3
ASDP	structure calculation	2.3
CYANA	structure calculation	3.98.13
CNS	refinement	

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	1889
Number of shifts mapped to atoms	1889
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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	168	182	182	1±1
2	B	573	576	575	3±2
All	All	14820	15160	15140	67

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 2.

5 of 44 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:236:LEU:HD11	2:B:282:LEU:HD12	0.55	1.78	13	4
2:B:227:PRO:HG3	2:B:283:ARG:HD3	0.53	1.80	15	1
1:A:73:VAL:HG21	2:B:247:LYS:NZ	0.52	2.20	2	1
2:B:243:LEU:HB2	2:B:247:LYS:HB3	0.51	1.83	5	1
2:B:260:PRO:HB2	2:B:263:ARG:HD2	0.50	1.84	14	1

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	19/89 (21%)	17±1 (91±5%)	2±1 (8±5%)	0±0 (1±2%)	18 66
2	B	70/96 (73%)	64±1 (91±2%)	4±1 (6±2%)	2±1 (3±1%)	8 42
All	All	1780/3700 (48%)	1626 (91%)	111 (6%)	43 (2%)	9 46

5 of 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	244	PRO	19
2	B	266	ASN	12
2	B	225	GLY	7
1	A	79	PRO	3
1	A	80	LEU	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	19/75 (25%)	15±1 (78±5%)	4±1 (22±5%)	3 31
2	B	67/90 (74%)	61±1 (91±2%)	6±1 (9±2%)	13 60
All	All	1720/3300 (52%)	1519 (88%)	201 (12%)	9 52

5 of 27 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	74	GLN	20
1	A	80	LEU	20
2	B	226	LEU	20
1	A	82	ILE	19
2	B	241	ASN	17

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 79% for the well-defined parts and 72% 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	1889
Number of shifts mapped to atoms	1889
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	164	-0.20 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	156	-0.14 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	150	0.25 ± 0.43	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 79%, i.e. 1043 atoms were assigned a chemical shift out of a possible 1312. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	346/436 (79%)	175/175 (100%)	89/178 (50%)	82/83 (99%)
Sidechain	659/828 (80%)	446/530 (84%)	206/253 (81%)	7/45 (16%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	38/48 (79%)	19/23 (83%)	18/22 (82%)	1/3 (33%)
Overall	1043/1312 (79%)	640/728 (88%)	313/453 (69%)	90/131 (69%)

7.1.4 Statistically unusual chemical shifts (i)

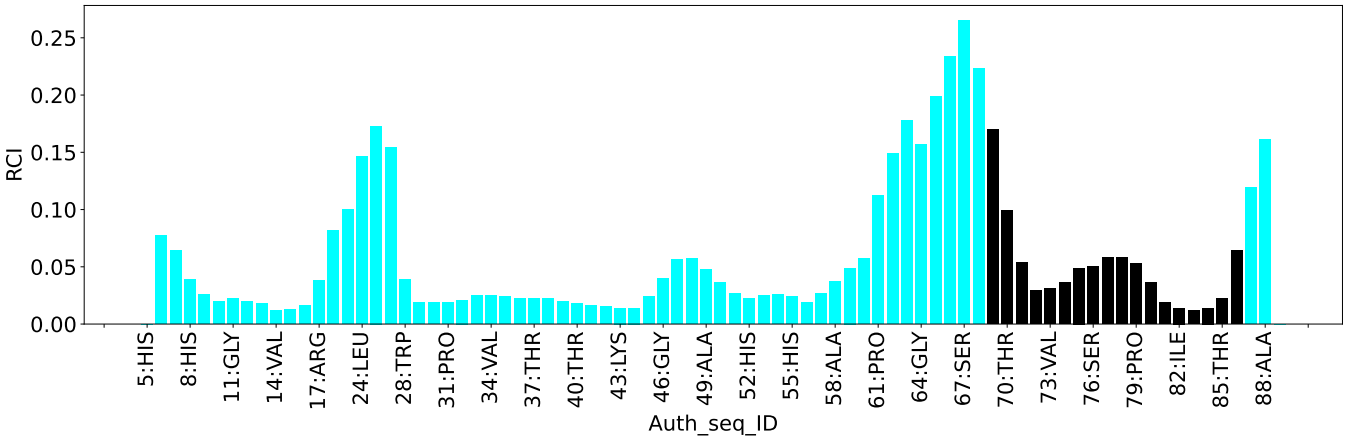
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	57	LYS	HE2	1.75	1.95 – 3.88	-6.0
1	A	43	LYS	HE3	1.75	1.92 – 3.89	-5.9
1	A	43	LYS	HB3	0.30	0.46 – 3.04	-5.6

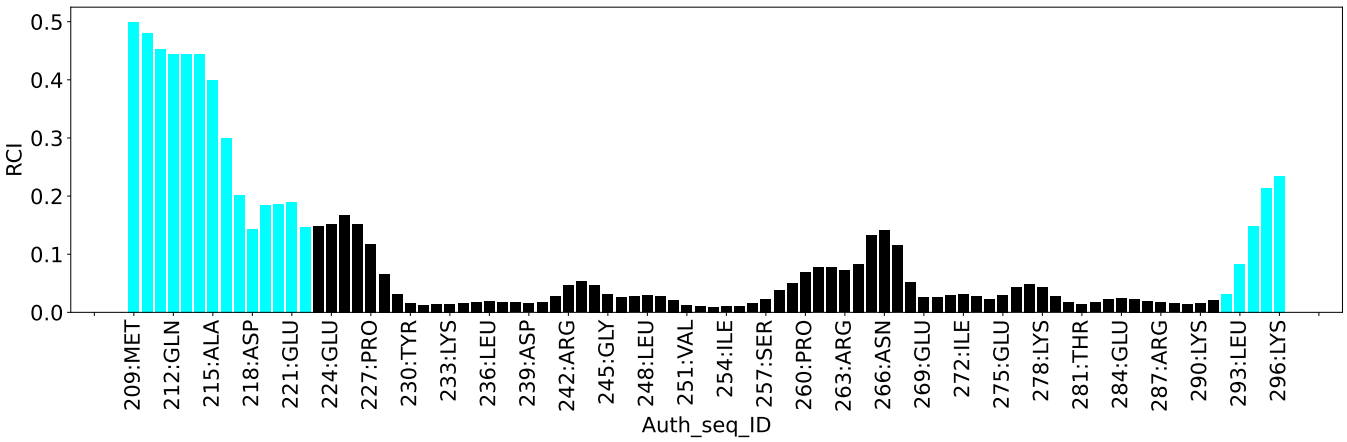
7.1.5 Random Coil Index (RCI) plots (i)

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:



Random coil index (RCI) for chain B:


RCI
0.5
0.4
0.3
0.2
0.1
0.0
209:MET
212:GLN
215:ALA
218:ASP
221:GLU
224:GLU
227:PRO
230:TYR
233:LYS
236:LEU
239:ASP
242:ARG
245:GLY
248:LEU
251:VAL
254:ILE
257:SER
260:PRO
263:ARG
266:ASN
269:GLU
272:ILE
275:GLU
278:LYS
281:THR
284:GLU
287:ARG
290:LYS
293:LEU
296:LYS
Auth_seq_ID

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	3999
Intra-residue (|i-j|=0)	980
Sequential (|i-j|=1)	1076
Medium range (|i-j|>1 and |i-j|<5)	591
Long range (|i-j|≥5)	1011
Inter-chain	237
Hydrogen bond restraints	104
Disulfide bond restraints	0
Total dihedral-angle restraints	212
Number of unmapped restraints	0
Number of restraints per residue	22.8
Number of long range restraints per residue[1]	5.6

[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)	3.4	0.2
0.2-0.5 (Medium)	0.1	0.43
>0.5 (Large)	0.1	0.86

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)	15.5	9.9
10.0-20.0 (Medium)	0.4	11.9
>20.0 (Large)	None	None

9 Distance violation analysis (i)

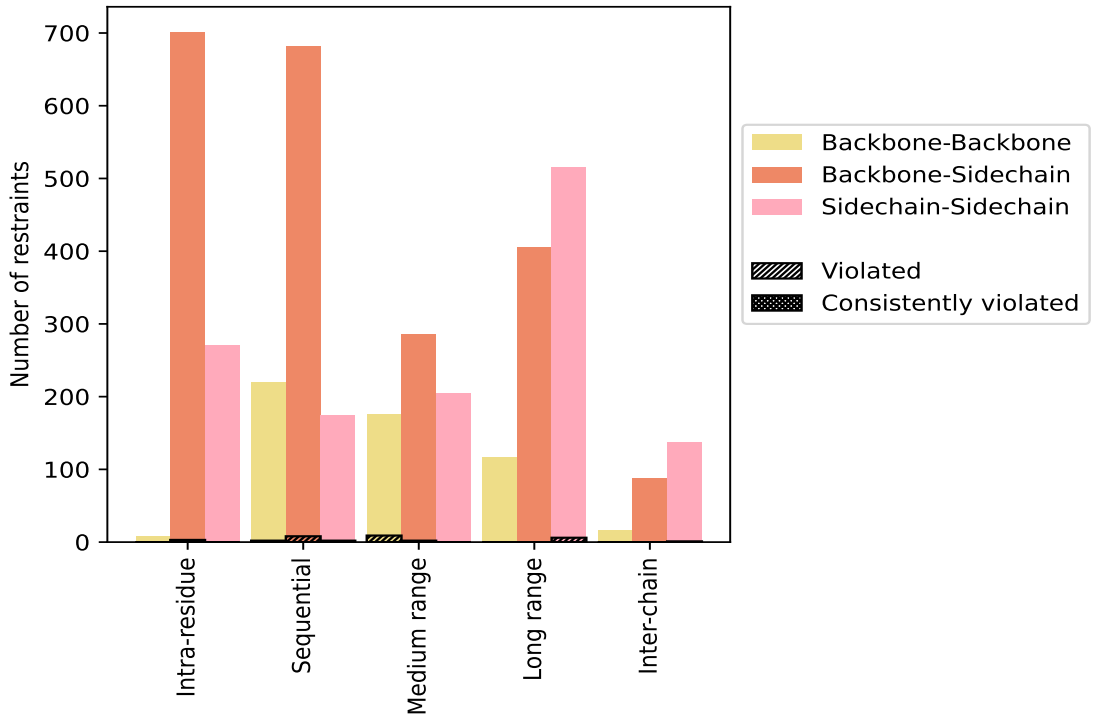
9.1 Summary of distance violations (i)

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)	980	24.5	3	0.3	0.1	0	0.0	0.0
Backbone-Backbone	8	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	701	17.5	3	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	271	6.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1076	26.9	12	1.1	0.3	0	0.0	0.0
Backbone-Backbone	220	5.5	2	0.9	0.1	0	0.0	0.0
Backbone-Sidechain	682	17.1	8	1.2	0.2	0	0.0	0.0
Sidechain-Sidechain	174	4.4	2	1.1	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	591	14.8	2	0.3	0.1	0	0.0	0.0
Backbone-Backbone	101	2.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	286	7.2	2	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	204	5.1	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	1011	25.3	6	0.6	0.2	0	0.0	0.0
Backbone-Backbone	91	2.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	405	10.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	515	12.9	6	1.2	0.2	0	0.0	0.0
Inter-chain	237	5.9	1	0.4	0.0	0	0.0	0.0
Backbone-Backbone	12	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	88	2.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	137	3.4	1	0.7	0.0	0	0.0	0.0
Hydrogen bond	104	2.6	9	8.7	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3999	100.0	33	0.8	0.8	0	0.0	0.0
Backbone-Backbone	536	13.4	11	2.1	0.3	0	0.0	0.0
Backbone-Sidechain	2162	54.1	13	0.6	0.3	0	0.0	0.0
Sidechain-Sidechain	1301	32.5	9	0.7	0.2	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	1	0	1	0	1	3	0.13	0.14	0.01	0.12
2	0	1	1	0	0	2	0.12	0.12	0.0	0.12
3	0	1	1	1	0	3	0.13	0.15	0.02	0.14
4	0	1	1	0	0	2	0.13	0.15	0.02	0.13
5	1	1	1	1	0	4	0.18	0.32	0.08	0.14
6	0	1	1	0	0	2	0.52	0.86	0.34	0.52
7	0	1	1	1	0	3	0.12	0.14	0.01	0.12
8	0	4	1	0	0	5	0.18	0.43	0.12	0.12
9	0	1	3	0	0	4	0.12	0.14	0.01	0.12
10	0	2	1	1	0	4	0.13	0.19	0.03	0.12
11	0	1	2	0	0	3	0.13	0.16	0.02	0.12

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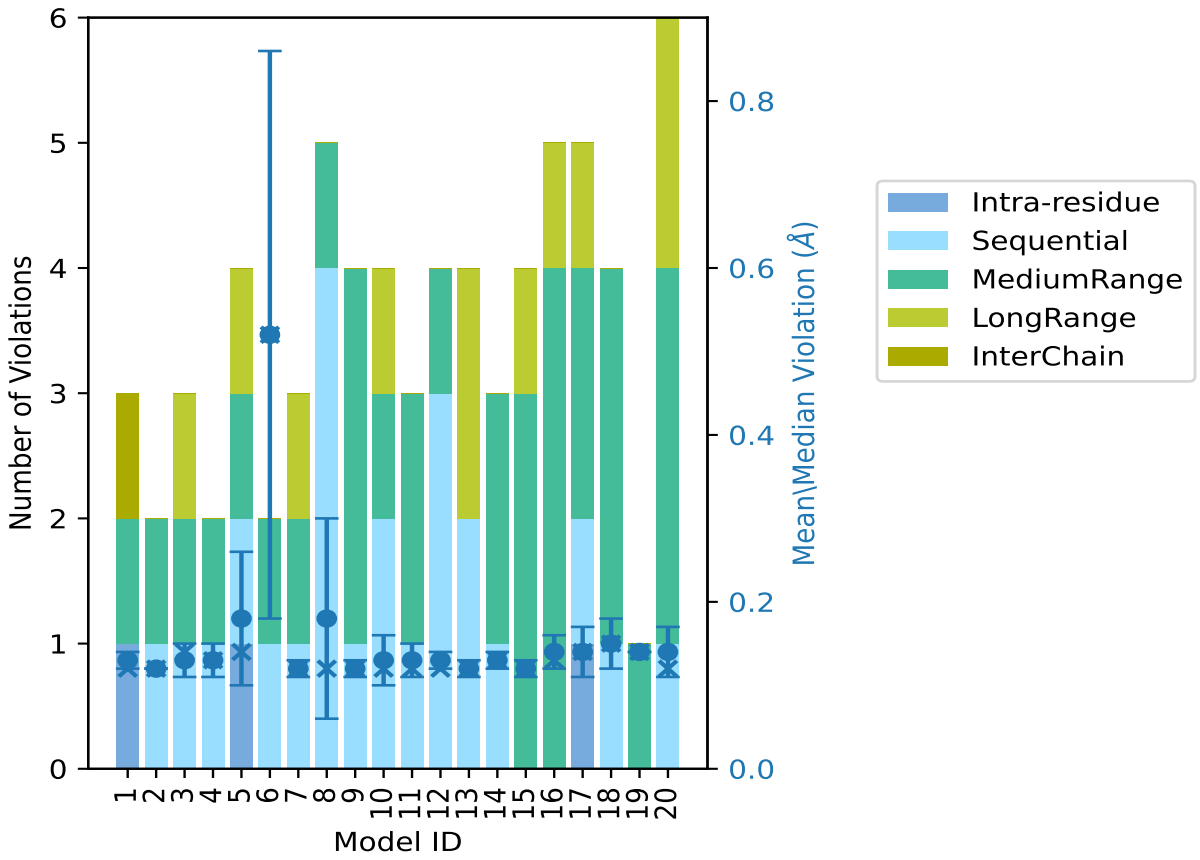
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	3	1	0	0	4	0.13	0.15	0.01	0.12
13	0	2	0	2	0	4	0.12	0.13	0.01	0.12
14	0	1	2	0	0	3	0.13	0.14	0.01	0.13
15	0	0	3	1	0	4	0.12	0.13	0.01	0.12
16	0	0	4	1	0	5	0.14	0.18	0.02	0.13
17	1	1	2	1	0	5	0.14	0.18	0.03	0.14
18	0	1	3	0	0	4	0.15	0.19	0.03	0.15
19	0	0	1	0	0	1	0.14	0.14	0.0	0.14
20	0	1	3	2	0	6	0.14	0.2	0.03	0.12

[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

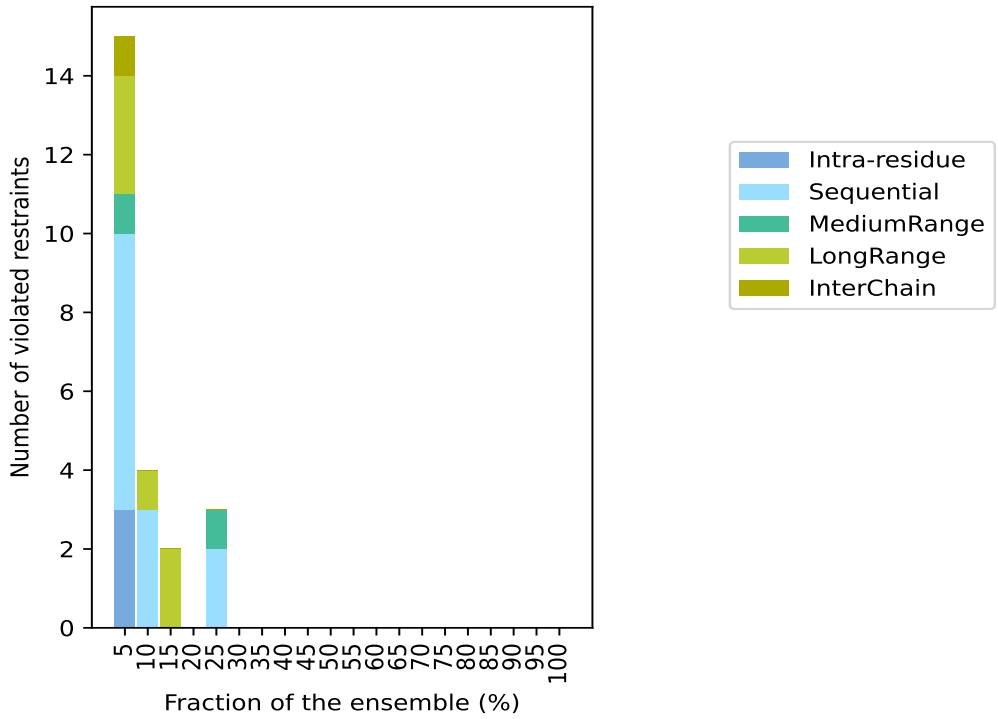
9.3 Distance violation statistics for the ensemble (i)

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, 3871(IR:977, SQ:1064, MR:589, LR:1005, IC:236) 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]	%
3	7	1	3	1	15	1	5.0
0	3	0	1	0	4	2	10.0
0	0	0	2	0	2	3	15.0
0	0	0	0	0	0	4	20.0
0	2	1	0	0	3	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
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

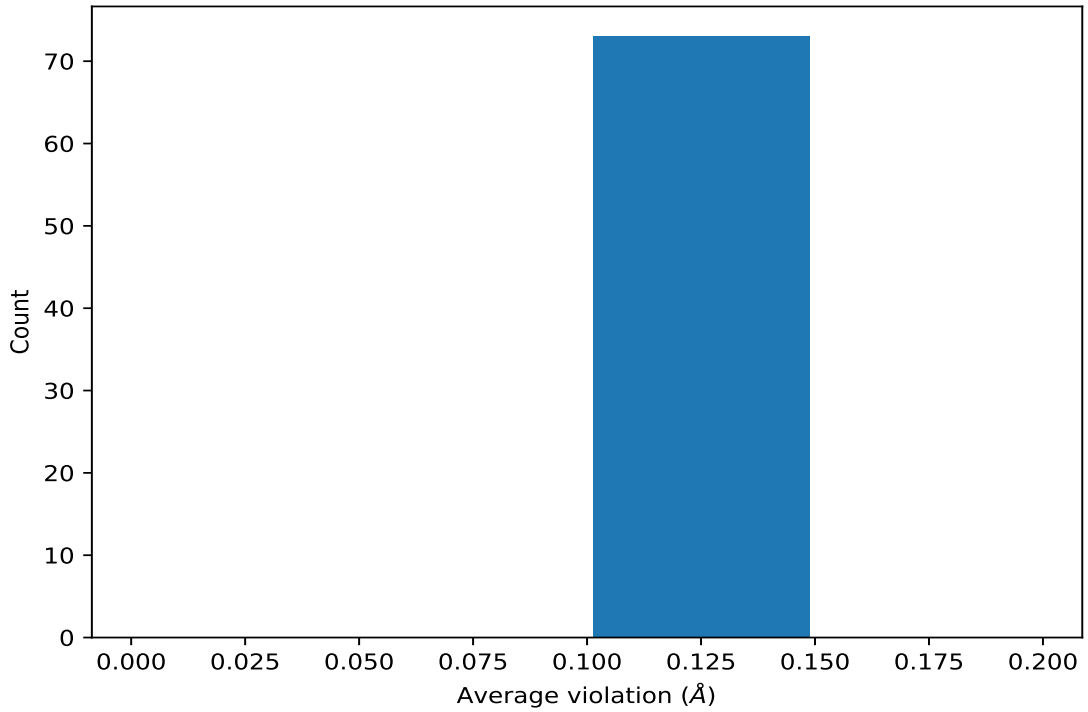
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(2,78)	2:B:255:ILE:O	2:B:259:GLU:N	7	0.14	0.03	0.12
(2,13)	1:A:38:THR:O	1:A:40:THR:H	7	0.12	0.01	0.12
(1,1100)	2:B:255:ILE:HG21	2:B:256:GLN:HE21	5	0.14	0.03	0.15
(1,1100)	2:B:255:ILE:HG22	2:B:256:GLN:HE21	5	0.14	0.03	0.15
(1,1100)	2:B:255:ILE:HG23	2:B:256:GLN:HE21	5	0.14	0.03	0.15
(1,2424)	2:B:238:LEU:HD21	2:B:240:ILE:H	5	0.14	0.02	0.14
(1,2424)	2:B:238:LEU:HD22	2:B:240:ILE:H	5	0.14	0.02	0.14
(1,2424)	2:B:238:LEU:HD23	2:B:240:ILE:H	5	0.14	0.02	0.14
(1,3427)	2:B:220:GLU:HG2	2:B:221:GLU:H	5	0.12	0.01	0.11
(1,3427)	2:B:220:GLU:HG3	2:B:221:GLU:H	5	0.12	0.01	0.11
(2,14)	1:A:38:THR:O	1:A:40:THR:N	4	0.13	0.01	0.13
(1,2044)	1:A:51:ILE:HG21	1:A:56:VAL:HG11	3	0.13	0.01	0.13
(1,2044)	1:A:51:ILE:HG21	1:A:56:VAL:HG12	3	0.13	0.01	0.13
(1,2044)	1:A:51:ILE:HG21	1:A:56:VAL:HG13	3	0.13	0.01	0.13
(1,2044)	1:A:51:ILE:HG22	1:A:56:VAL:HG11	3	0.13	0.01	0.13
(1,2044)	1:A:51:ILE:HG22	1:A:56:VAL:HG12	3	0.13	0.01	0.13

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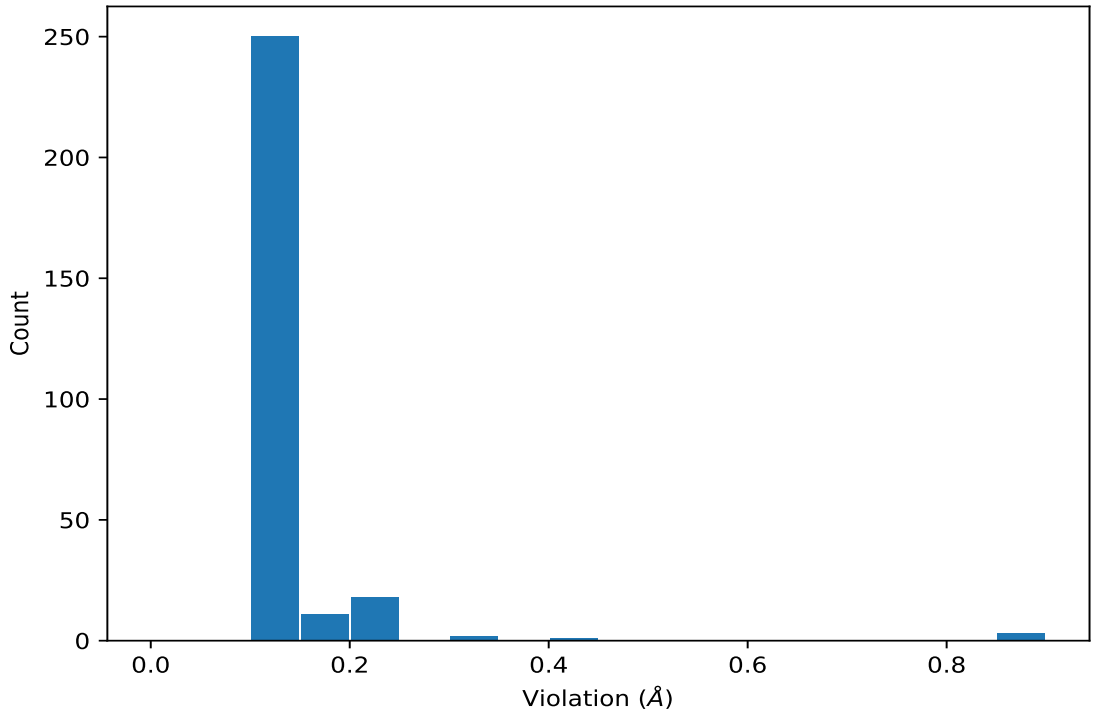
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2044)	1:A:51:ILE:HG22	1:A:56:VAL:HG13	3	0.13	0.01	0.13
(1,2044)	1:A:51:ILE:HG23	1:A:56:VAL:HG11	3	0.13	0.01	0.13
(1,2044)	1:A:51:ILE:HG23	1:A:56:VAL:HG12	3	0.13	0.01	0.13
(1,2044)	1:A:51:ILE:HG23	1:A:56:VAL:HG13	3	0.13	0.01	0.13
(2,57)	2:B:245:GLY:O	2:B:249:GLY:H	3	0.13	0.02	0.12
(1,3631)	2:B:252:VAL:HG11	2:B:270:ILE:HD11	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG11	2:B:270:ILE:HD12	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG11	2:B:270:ILE:HD13	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG12	2:B:270:ILE:HD11	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG12	2:B:270:ILE:HD12	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG12	2:B:270:ILE:HD13	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG13	2:B:270:ILE:HD11	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG13	2:B:270:ILE:HD12	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG13	2:B:270:ILE:HD13	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG21	2:B:270:ILE:HD11	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG21	2:B:270:ILE:HD12	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG21	2:B:270:ILE:HD13	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG22	2:B:270:ILE:HD11	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG22	2:B:270:ILE:HD12	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG22	2:B:270:ILE:HD13	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG23	2:B:270:ILE:HD11	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG23	2:B:270:ILE:HD12	3	0.12	0.0	0.12
(1,3631)	2:B:252:VAL:HG23	2:B:270:ILE:HD13	3	0.12	0.0	0.12
(1,3028)	1:A:42:LEU:HD21	1:A:56:VAL:HG11	2	0.14	0.01	0.14

[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)
(1,1756)	2:B:275:GLU:H	2:B:276:THR:HG21	6	0.86
(1,1756)	2:B:275:GLU:H	2:B:276:THR:HG22	6	0.86
(1,1756)	2:B:275:GLU:H	2:B:276:THR:HG23	6	0.86
(1,314)	2:B:295:LYS:HA	2:B:296:LYS:H	8	0.43
(1,1531)	2:B:296:LYS:HA	2:B:296:LYS:HD2	5	0.32
(1,1531)	2:B:296:LYS:HA	2:B:296:LYS:HD3	5	0.32
(1,3547)	2:B:240:ILE:HD11	2:B:289:VAL:HG11	20	0.2
(1,3547)	2:B:240:ILE:HD11	2:B:289:VAL:HG12	20	0.2
(1,3547)	2:B:240:ILE:HD11	2:B:289:VAL:HG13	20	0.2
(1,3547)	2:B:240:ILE:HD11	2:B:289:VAL:HG21	20	0.2
(1,3547)	2:B:240:ILE:HD11	2:B:289:VAL:HG22	20	0.2
(1,3547)	2:B:240:ILE:HD11	2:B:289:VAL:HG23	20	0.2
(1,3547)	2:B:240:ILE:HD12	2:B:289:VAL:HG11	20	0.2
(1,3547)	2:B:240:ILE:HD12	2:B:289:VAL:HG12	20	0.2
(1,3547)	2:B:240:ILE:HD12	2:B:289:VAL:HG13	20	0.2
(1,3547)	2:B:240:ILE:HD12	2:B:289:VAL:HG21	20	0.2
(1,3547)	2:B:240:ILE:HD12	2:B:289:VAL:HG22	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3547)	2:B:240:ILE:HD12	2:B:289:VAL:HG23	20	0.2
(1,3547)	2:B:240:ILE:HD13	2:B:289:VAL:HG11	20	0.2
(1,3547)	2:B:240:ILE:HD13	2:B:289:VAL:HG12	20	0.2
(1,3547)	2:B:240:ILE:HD13	2:B:289:VAL:HG13	20	0.2
(1,3547)	2:B:240:ILE:HD13	2:B:289:VAL:HG21	20	0.2
(1,3547)	2:B:240:ILE:HD13	2:B:289:VAL:HG22	20	0.2
(1,3547)	2:B:240:ILE:HD13	2:B:289:VAL:HG23	20	0.2
(2,43)	2:B:234:ARG:O	2:B:238:LEU:H	18	0.19
(1,1100)	2:B:255:ILE:HG21	2:B:256:GLN:HE21	10	0.19
(1,1100)	2:B:255:ILE:HG22	2:B:256:GLN:HE21	10	0.19
(1,1100)	2:B:255:ILE:HG23	2:B:256:GLN:HE21	10	0.19
(2,78)	2:B:255:ILE:O	2:B:259:GLU:N	16	0.18
(1,2424)	2:B:238:LEU:HD21	2:B:240:ILE:H	6	0.18
(1,2424)	2:B:238:LEU:HD22	2:B:240:ILE:H	6	0.18
(1,2424)	2:B:238:LEU:HD23	2:B:240:ILE:H	6	0.18
(1,1433)	2:B:266:ASN:HA	2:B:266:ASN:HD21	17	0.18
(2,78)	2:B:255:ILE:O	2:B:259:GLU:N	11	0.16

10 Dihedral-angle violation analysis

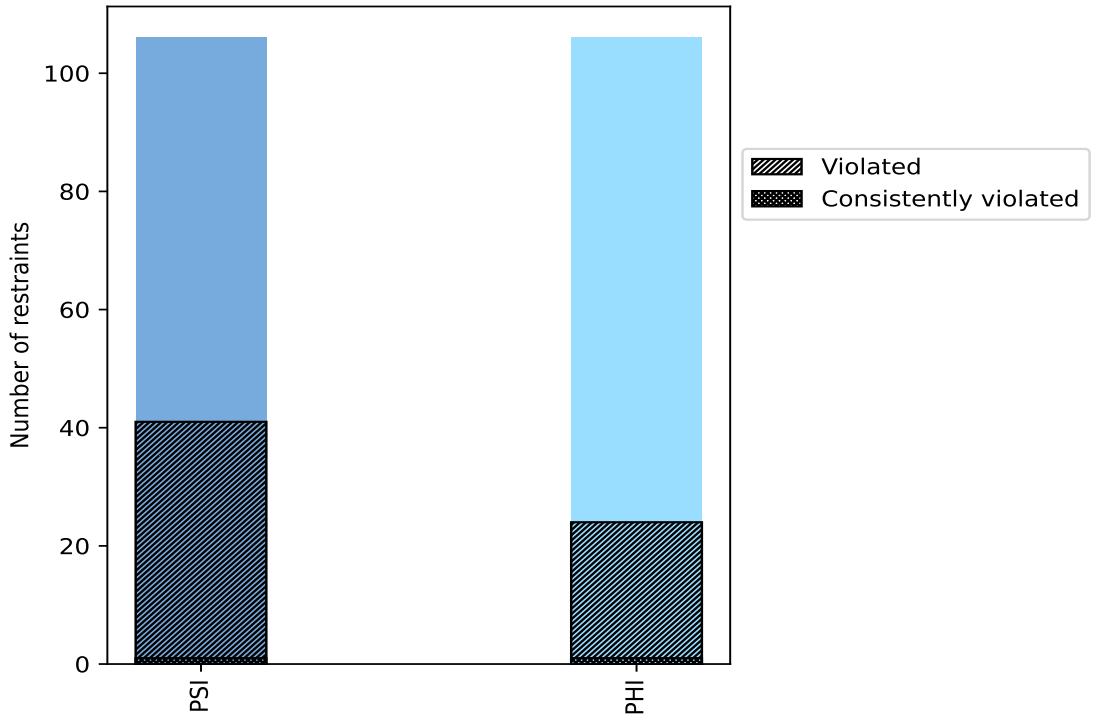
10.1 Summary of dihedral-angle violations

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	106	50.0	41	38.7	19.3	1	0.9	0.5
PHI	106	50.0	24	22.6	11.3	1	0.9	0.5
Total	212	100.0	65	30.7	30.7	2	0.9	0.9

[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



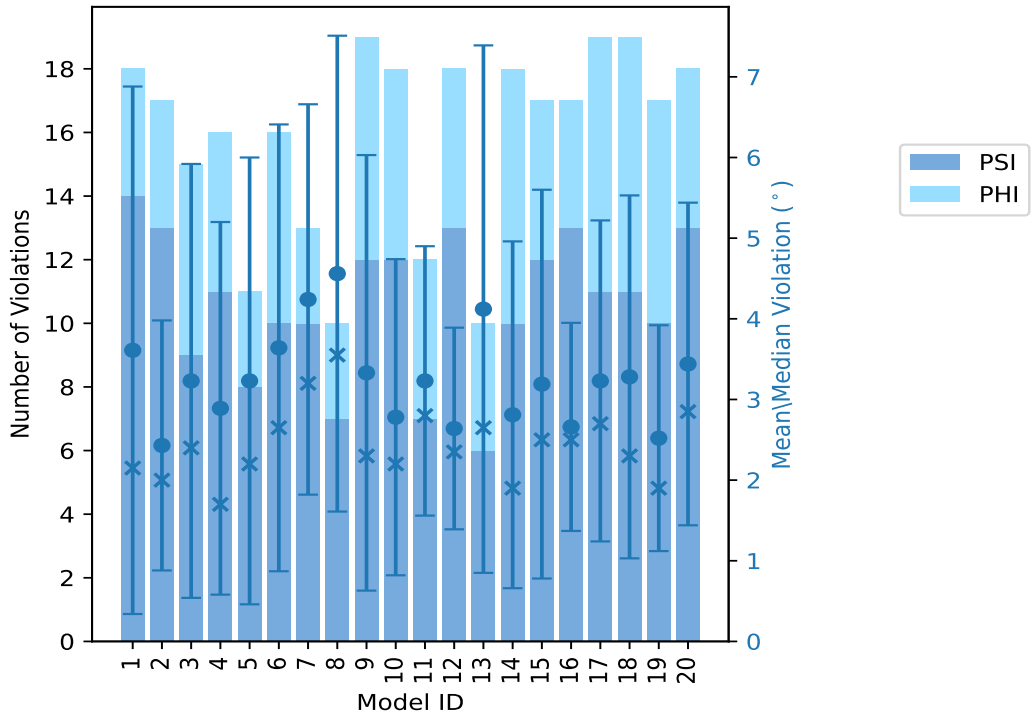
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	14	4	18	3.61	11.9	3.27	2.15
2	13	4	17	2.43	7.5	1.55	2.0
3	9	6	15	3.23	11.0	2.69	2.4
4	11	5	16	2.89	8.3	2.31	1.7
5	8	3	11	3.23	9.1	2.77	2.2
6	10	6	16	3.64	10.6	2.77	2.65
7	10	3	13	4.24	9.4	2.42	3.2
8	7	3	10	4.56	11.2	2.95	3.55
9	12	7	19	3.33	10.4	2.7	2.3
10	12	6	18	2.78	8.5	1.96	2.2
11	7	5	12	3.23	6.5	1.67	2.8
12	13	5	18	2.64	5.0	1.25	2.35
13	6	4	10	4.12	11.0	3.27	2.65
14	10	8	18	2.81	8.9	2.15	1.9
15	12	5	17	3.19	9.9	2.41	2.5
16	13	4	17	2.66	6.2	1.29	2.5
17	11	8	19	3.23	8.4	1.99	2.7
18	11	8	19	3.28	8.6	2.25	2.3
19	10	7	17	2.52	6.3	1.4	1.9
20	13	5	18	3.44	9.1	2.0	2.85

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]	%
9	6	15	1	5.0
9	5	14	2	10.0
1	5	6	3	15.0
5	1	6	4	20.0
4	1	5	5	25.0
3	1	4	6	30.0
0	0	0	7	35.0
2	2	4	8	40.0
1	0	1	9	45.0
2	1	3	10	50.0
1	0	1	11	55.0

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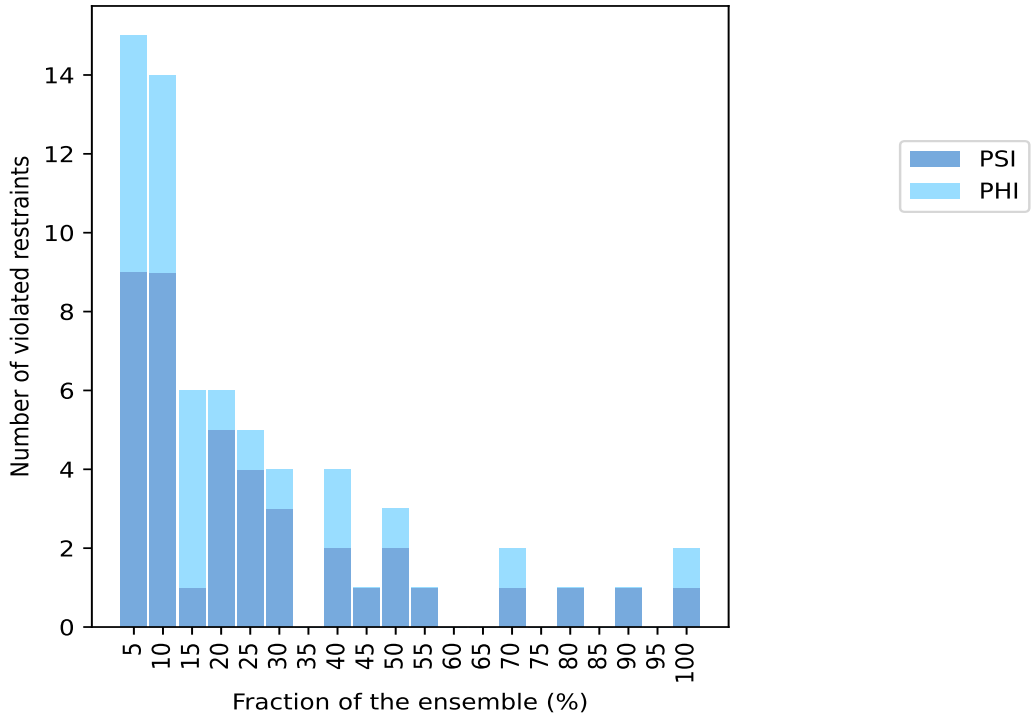
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
1	1	2	14	70.0
0	0	0	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
1	0	1	18	90.0
0	0	0	19	95.0
1	1	2	20	100.0

[1] Number of models with violations

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

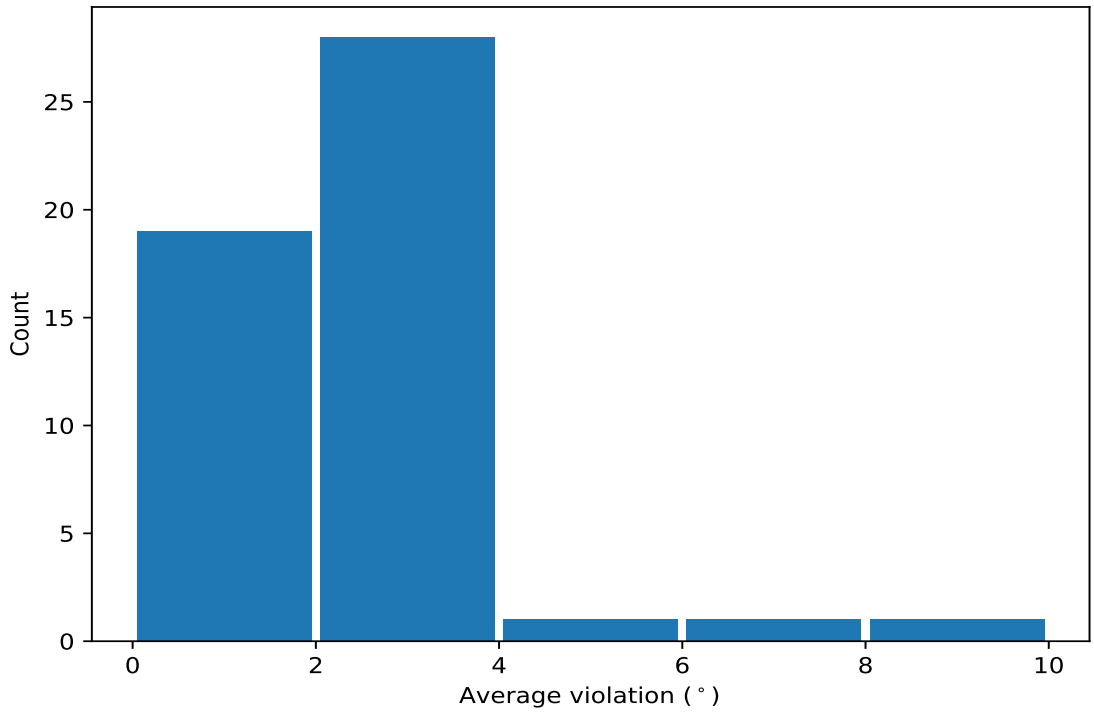


10.4 Most violated dihedral-angle restraints in the ensemble

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.

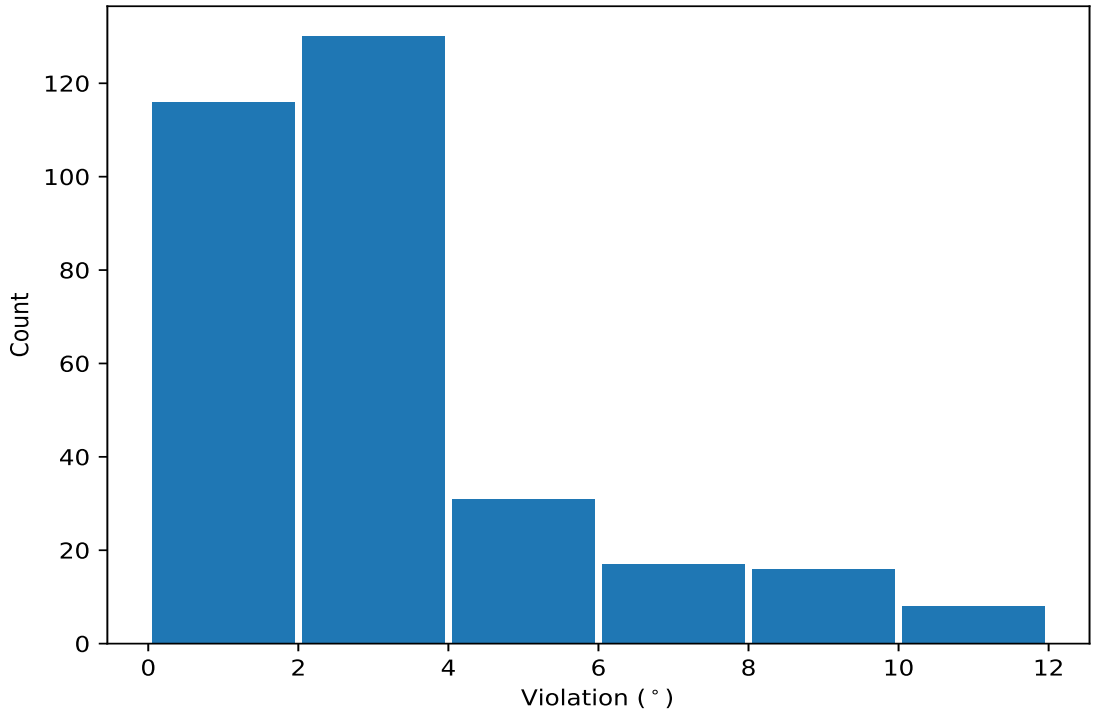
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	20	8.74	2.08	8.9
(1,3)	1:A:7:SER:C	1:A:8:HIS:N	1:A:8:HIS:CA	1:A:8:HIS:C	20	7.18	2.0	7.3
(1,172)	2:B:272:ILE:N	2:B:272:ILE:CA	2:B:272:ILE:C	2:B:273:ASP:N	18	3.14	1.49	2.75
(1,46)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:LEU:N	16	2.43	0.81	2.55
(1,174)	2:B:273:ASP:N	2:B:273:ASP:CA	2:B:273:ASP:C	2:B:274:PHE:N	14	2.71	0.99	2.5
(1,19)	1:A:15:TRP:C	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	14	2.47	1.02	2.45
(1,74)	1:A:70:THR:N	1:A:70:THR:CA	1:A:70:THR:C	1:A:71:TRP:N	11	2.82	0.8	2.9
(1,212)	2:B:293:LEU:N	2:B:293:LEU:CA	2:B:293:LEU:C	2:B:294:GLN:N	10	3.04	1.2	2.65
(1,31)	1:A:31:PRO:C	1:A:32:TYR:N	1:A:32:TYR:CA	1:A:32:TYR:C	10	2.97	1.23	2.4
(1,88)	1:A:78:ASN:N	1:A:78:ASN:CA	1:A:78:ASN:C	1:A:79:PRO:N	10	2.39	0.95	2.15

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

The following table provides the list of violationsfor the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	1	11.9
(1,140)	2:B:246:GLU:N	2:B:246:GLU:CA	2:B:246:GLU:C	2:B:247:LYS:N	1	11.6
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	8	11.2
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	3	11.0
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	13	11.0
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	6	10.6
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	9	10.4
(1,3)	1:A:7:SER:C	1:A:8:HIS:N	1:A:8:HIS:CA	1:A:8:HIS:C	9	10.2
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	15	9.9
(1,2)	1:A:7:SER:N	1:A:7:SER:CA	1:A:7:SER:C	1:A:8:HIS:N	7	9.4