



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:43 PM UTC

PDB ID : 2N3K / pdb_00002n3k
BMRB ID : 25649
Title : Human Brd4 ET domain in complex with MLV Integrase C-term
Authors : Crowe, B.L.; Foster, M.P.
Deposited on : 2015-06-03

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

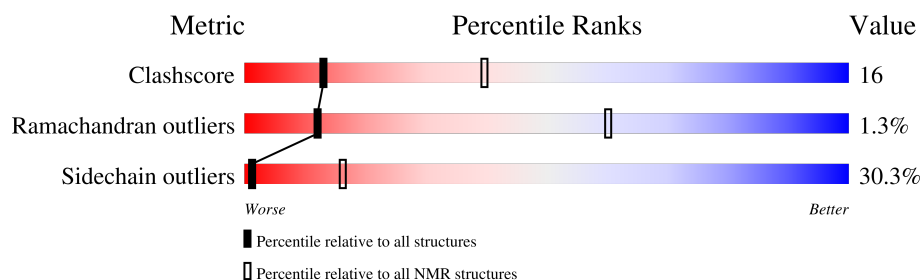
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 66%.

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	86	
2	B	17	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:607-A:641, A:649-A:673, B:389-B:405 (77)	0.52	17

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 3 clusters and 12 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1623 atoms, of which 824 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms						Trace
1	A	79	Total	C	H	N	O	S	0
			1307	401	659	113	131	3	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	595	GLY	-	expression tag	UNP O60885
A	596	ALA	-	expression tag	UNP O60885
A	597	ILE	-	expression tag	UNP O60885
A	598	ALA	-	expression tag	UNP O60885
A	599	MET	-	expression tag	UNP O60885
A	679	THR	-	expression tag	UNP O60885
A	680	ARG	-	expression tag	UNP O60885

- Molecule 2 is a protein called MLV integrase.

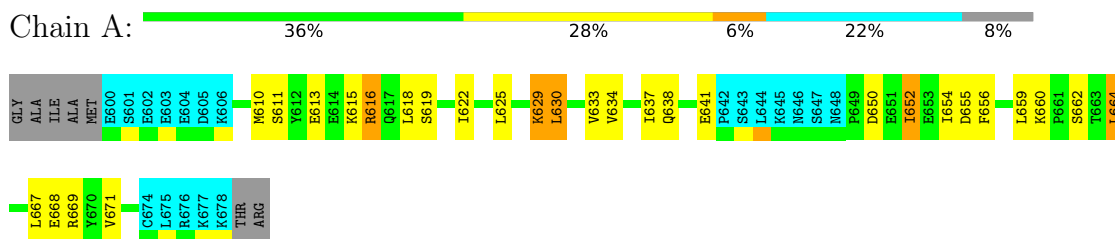
Mol	Chain	Residues	Atoms						Trace
2	B	17	Total	C	H	N	O		0
			316	94	165	34	23		

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: Bromodomain-containing protein 4



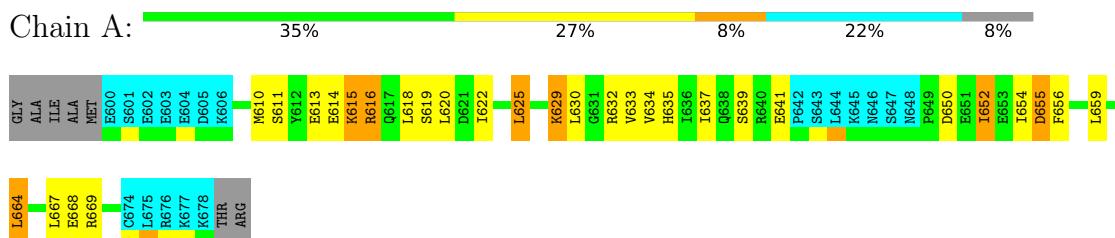
- Molecule 2: MLV integrase



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

The representative model is number 17. Colouring as in section 4.1 above.

- Molecule 1: Bromodomain-containing protein 4



- Molecule 2: MLV integrase



T389	T390	R391	Y392	Q393	R394	L395	R400	I401	R402	L403	T404	R405
------	------	------	------	------	------	------	------	------	------	------	------	------

5 Refinement protocol and experimental data overview

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

Of the 150 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
CYANA	refinement	3.97
CYANA	structure solution	3.97

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	995
Number of shifts mapped to atoms	926
Number of unparsed shifts	0
Number of shifts with mapping errors	69
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%

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	494	505	505	20±4
2	B	151	165	164	9±3
All	All	12900	13400	13380	432

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 175 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:634:VAL:HG22	2:B:403:LEU:HD23	1.01	1.31	3	2
1:A:625:LEU:HD11	1:A:671:VAL:HG23	0.98	1.33	1	2
1:A:634:VAL:HG12	2:B:403:LEU:HD23	0.97	1.29	4	3
1:A:654:ILE:HD13	2:B:403:LEU:HD23	0.93	1.40	9	2
1:A:630:LEU:HD23	1:A:634:VAL:HG11	0.79	1.55	16	8

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	60/86 (70%)	58±1 (97±2%)	2±1 (3±2%)	0±0 (0±0%)	100	100
2	B	15/17 (88%)	13±1 (84±4%)	1±1 (9±4%)	1±0 (7±2%)	2	17
All	All	1500/2060 (73%)	1418 (95%)	62 (4%)	20 (1%)	12	60

All 2 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	399	LEU	19
2	B	396	GLN	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	58/81 (72%)	41±4 (71±6%)	17±4 (29±6%)	1	18
2	B	17/17 (100%)	11±1 (65±8%)	6±1 (35±8%)	1	10
All	All	1500/1960 (77%)	1045 (70%)	455 (30%)	1	16

5 of 57 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	652	ILE	20
2	B	389	THR	20
2	B	399	LEU	20
2	B	394	ARG	18
1	A	616	ARG	17

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 66% for the well-defined parts and 66% 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	995
Number of shifts mapped to atoms	926
Number of unparsed shifts	0
Number of shifts with mapping errors	69
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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 69) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	595	GLY	HA2	3.873	0	2
1	A	595	GLY	C	175.978	0	1
1	A	595	GLY	CA	45.158	0	1
1	A	595	GLY	N	109.419	0	1
1	A	596	ALA	H	8.085	0	1
1	A	596	ALA	HA	4.338	0	1
1	A	596	ALA	HB1	1.357	0	1
1	A	596	ALA	HB2	1.357	0	1
1	A	596	ALA	HB3	1.357	0	1
1	A	596	ALA	C	175.398	0	1
1	A	596	ALA	CA	52.43	0	1
1	A	596	ALA	CB	19.34	0	1
1	A	596	ALA	N	123.613	0	1
1	A	597	ILE	H	8.061	0	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	597	ILE	HA	4.121	0	1
1	A	597	ILE	HB	1.829	0	1
1	A	597	ILE	HD11	0.857	0	1
1	A	597	ILE	HD12	0.857	0	1
1	A	597	ILE	HD13	0.857	0	1
1	A	597	ILE	HG12	1.46	0	2
1	A	597	ILE	HG21	0.911	0	1
1	A	597	ILE	HG22	0.911	0	1
1	A	597	ILE	HG23	0.911	0	1
1	A	597	ILE	C	176.685	0	1
1	A	597	ILE	CA	60.956	0	1
1	A	597	ILE	CB	38.767	0	1
1	A	597	ILE	CD1	12.906	0	1
1	A	597	ILE	CG1	27.175	0	1
1	A	597	ILE	CG2	17.413	0	1
1	A	597	ILE	N	119.933	0	1
1	A	598	ALA	H	8.32	0	1
1	A	598	ALA	HA	4.315	0	1
1	A	598	ALA	HB1	1.355	0	1
1	A	598	ALA	HB2	1.355	0	1
1	A	598	ALA	HB3	1.355	0	1
1	A	598	ALA	C	173.773	0	1
1	A	598	ALA	CA	52.345	0	1
1	A	598	ALA	CB	19.204	0	1
1	A	598	ALA	N	128.156	0	1
1	A	599	MET	H	8.331	0	1
1	A	599	MET	HA	4.447	0	1
1	A	599	MET	HB2	2.061	0	2
1	A	599	MET	HG2	2.602	0	2
1	A	599	MET	C	175.051	0	1
1	A	599	MET	CA	55.471	0	1
1	A	599	MET	CB	33.12	0	1
1	A	599	MET	CG	31.95	0	1
1	A	599	MET	N	120.268	0	1
1	A	679	THR	H	8.204	0	1
1	A	679	THR	HA	4.327	0	1
1	A	679	THR	HB	4.245	0	1
1	A	679	THR	HG21	1.192	0	1
1	A	679	THR	HG22	1.192	0	1
1	A	679	THR	HG23	1.192	0	1
1	A	679	THR	C	177.732	0	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	679	THR	CA	61.795	0	1
1	A	679	THR	CB	69.941	0	1
1	A	679	THR	CG2	21.944	0	1
1	A	679	THR	N	115.917	0	1
1	A	680	ARG	H	7.976	0	1
1	A	680	ARG	HA	4.158	0	1
1	A	680	ARG	HB2	1.837	0	2
1	A	680	ARG	HD2	3.179	0	2
1	A	680	ARG	HG2	1.581	0	2
1	A	680	ARG	CA	57.64	0	1
1	A	680	ARG	CB	31.376	0	1
1	A	680	ARG	CD	43.456	0	1
1	A	680	ARG	CG	27.19	0	1
1	A	680	ARG	N	127.693	0	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	86	-0.76 ± 0.32	Should be checked
$^{13}\text{C}_\beta$	83	0.30 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	79	1.64 ± 0.36	Should be applied
^{15}N	81	0.65 ± 0.49	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 66%, i.e. 761 atoms were assigned a chemical shift out of a possible 1149. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	320/377 (85%)	148/151 (98%)	116/154 (75%)	56/72 (78%)
Sidechain	421/725 (58%)	284/465 (61%)	134/221 (61%)	3/39 (8%)
Aromatic	20/47 (43%)	14/23 (61%)	6/22 (27%)	0/2 (0%)
Overall	761/1149 (66%)	446/639 (70%)	256/397 (64%)	59/113 (52%)

7.1.4 Statistically unusual chemical shifts [i](#)

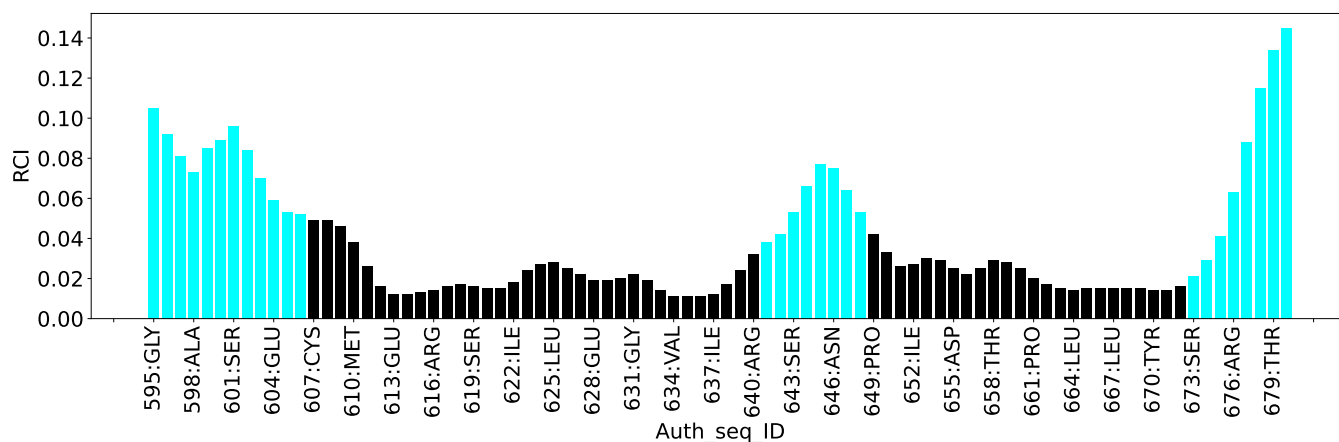
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	405	ARG	HD3	4.44	1.81 – 4.39	5.2

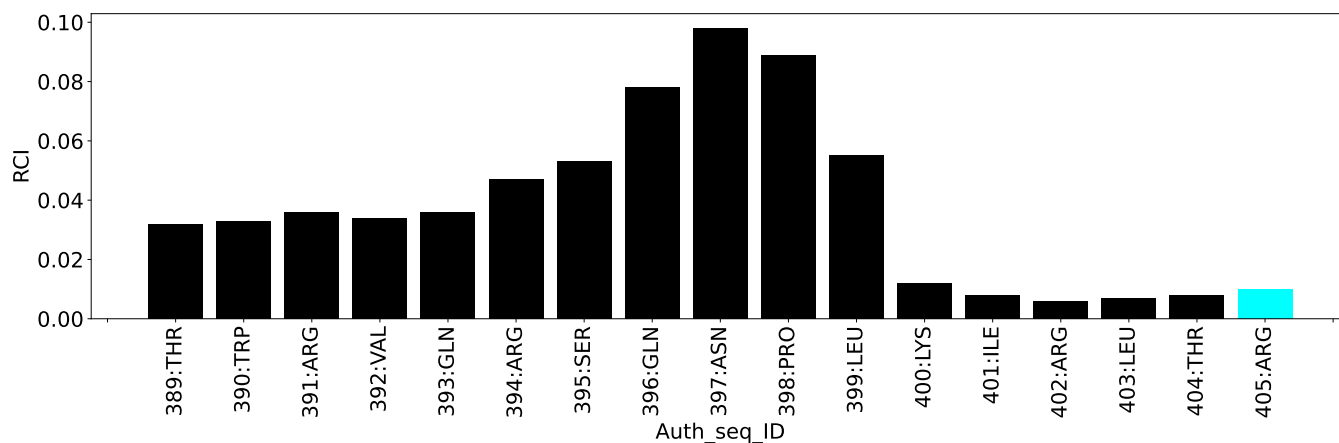
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



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	1103
Intra-residue ($ i-j =0$)	116
Sequential ($ i-j =1$)	255
Medium range ($ i-j >1$ and $ i-j <5$)	319
Long range ($ i-j \geq 5$)	174
Inter-chain	151
Hydrogen bond restraints	88
Disulfide bond restraints	0
Total dihedral-angle restraints	127
Number of unmapped restraints	0
Number of restraints per residue	11.9
Number of long range restraints per residue ¹	1.8

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

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)	15.9	0.2
0.2-0.5 (Medium)	4.2	0.5
>0.5 (Large)	13.2	3.25

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)	9.1	8.19
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

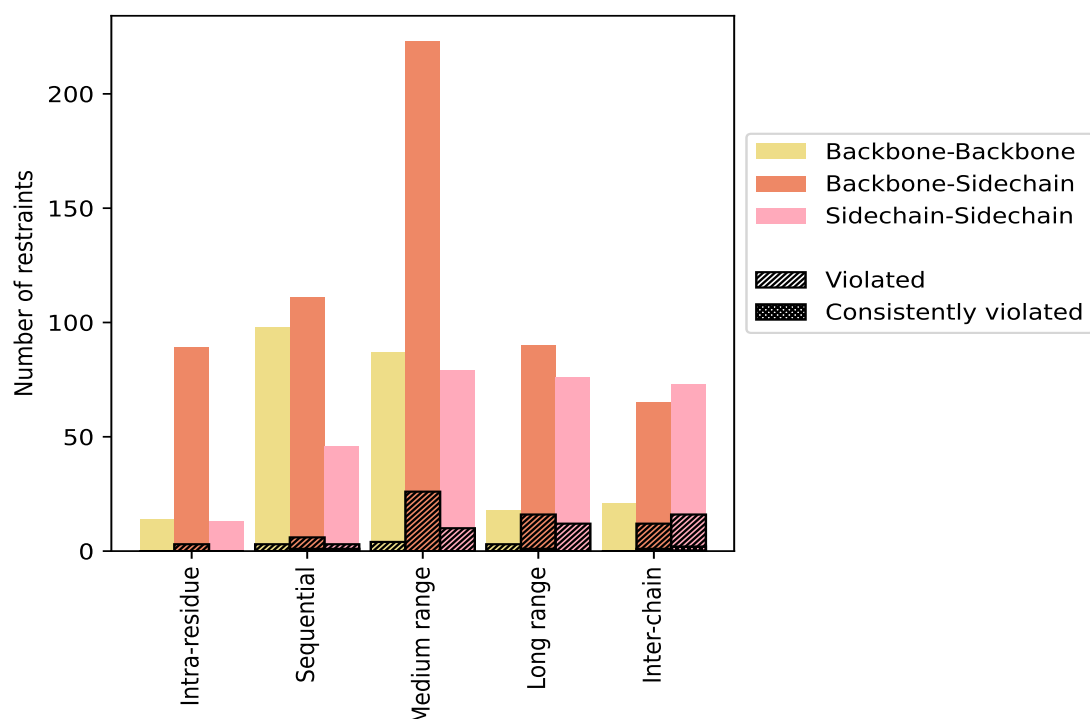
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	116	10.5	3	2.6	0.3	0	0.0	0.0
Backbone-Backbone	14	1.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	89	8.1	3	3.4	0.3	0	0.0	0.0
Sidechain-Sidechain	13	1.2	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	255	23.1	12	4.7	1.1	2	0.8	0.2
Backbone-Backbone	98	8.9	3	3.1	0.3	0	0.0	0.0
Backbone-Sidechain	111	10.1	6	5.4	0.5	1	0.9	0.1
Sidechain-Sidechain	46	4.2	3	6.5	0.3	1	2.2	0.1
Medium range ($i-j >1$ & $i-j <5$)	319	28.9	32	10.0	2.9	0	0.0	0.0
Backbone-Backbone	87	7.9	4	4.6	0.4	0	0.0	0.0
Backbone-Sidechain	153	13.9	18	11.8	1.6	0	0.0	0.0
Sidechain-Sidechain	79	7.2	10	12.7	0.9	0	0.0	0.0
Long range ($i-j \geq 5$)	174	15.8	30	17.2	2.7	1	0.6	0.1
Backbone-Backbone	18	1.6	3	16.7	0.3	0	0.0	0.0
Backbone-Sidechain	80	7.3	15	18.8	1.4	1	1.2	0.1
Sidechain-Sidechain	76	6.9	12	15.8	1.1	0	0.0	0.0
Inter-chain	151	13.7	26	17.2	2.4	3	2.0	0.3
Backbone-Backbone	21	1.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	57	5.2	10	17.5	0.9	1	1.8	0.1
Sidechain-Sidechain	73	6.6	16	21.9	1.5	2	2.7	0.2
Hydrogen bond	88	8.0	11	12.5	1.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1103	100.0	114	10.3	10.3	6	0.5	0.5
Backbone-Backbone	238	21.6	10	4.2	0.9	0	0.0	0.0
Backbone-Sidechain	578	52.4	63	10.9	5.7	3	0.5	0.3
Sidechain-Sidechain	287	26.0	41	14.3	3.7	3	1.0	0.3

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 disulfid 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	0	7	7	10	8	32	0.57	2.39	0.59	0.22
2	0	4	7	6	17	34	0.67	2.45	0.7	0.18
3	0	5	6	12	8	31	0.53	2.25	0.59	0.17
4	1	5	8	10	11	35	0.58	2.35	0.59	0.33
5	1	5	8	6	14	34	0.76	2.87	0.76	0.38
6	1	5	9	7	13	35	0.69	2.3	0.7	0.27
7	0	6	15	6	16	43	0.6	2.35	0.64	0.21
8	1	7	10	8	5	31	0.5	2.91	0.62	0.16
9	0	8	10	5	13	36	0.62	2.81	0.71	0.18
10	1	8	7	7	8	31	0.53	2.8	0.61	0.15

Continued on next page...

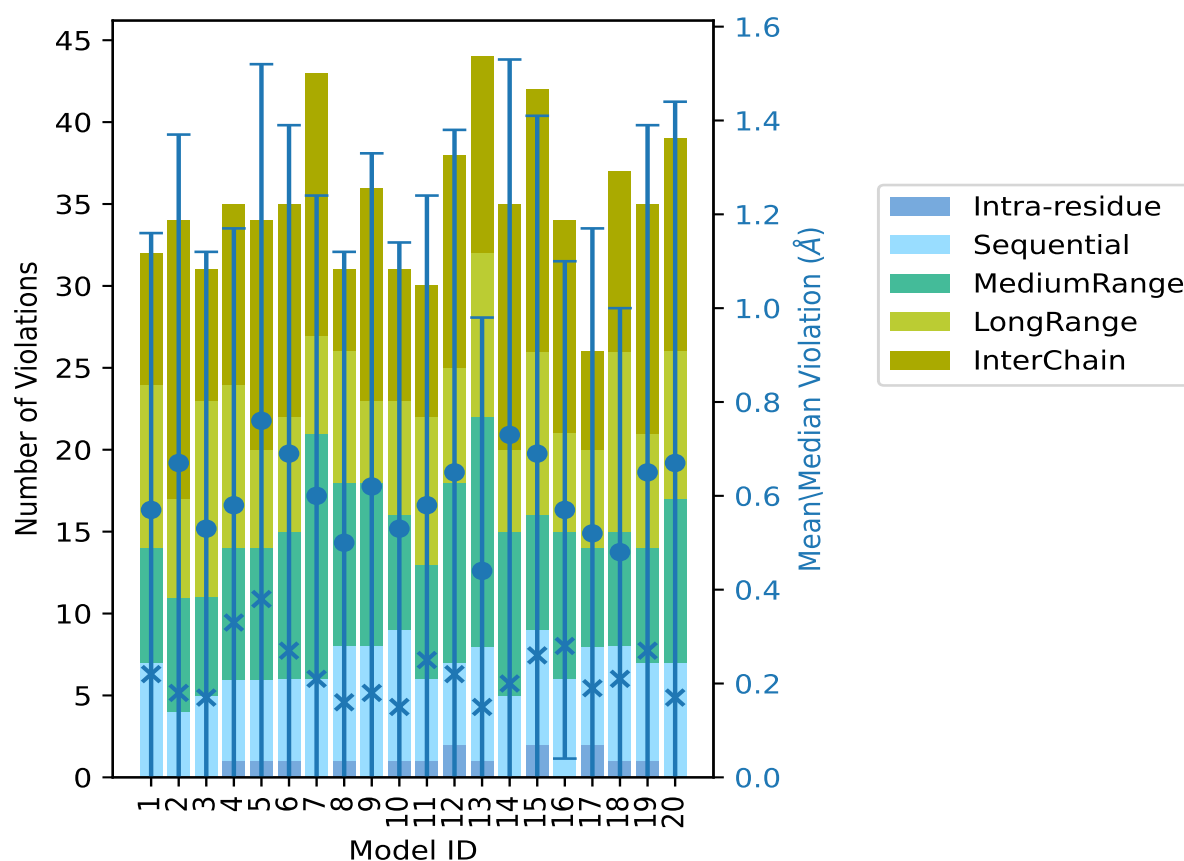
Continued from previous page...

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	1	5	7	9	8	30	0.58	3.25	0.66	0.25
12	2	5	11	7	13	38	0.65	3.01	0.73	0.22
13	1	7	14	10	12	44	0.44	2.2	0.54	0.15
14	0	5	10	5	15	35	0.73	2.86	0.8	0.2
15	2	7	7	10	16	42	0.69	2.56	0.72	0.26
16	0	6	9	6	13	34	0.57	2.35	0.53	0.28
17	2	6	6	6	6	26	0.52	2.9	0.65	0.19
18	1	7	7	11	11	37	0.48	2.37	0.52	0.21
19	1	6	7	7	14	35	0.65	3.17	0.74	0.27
20	0	7	10	9	13	39	0.67	3.02	0.77	0.17

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

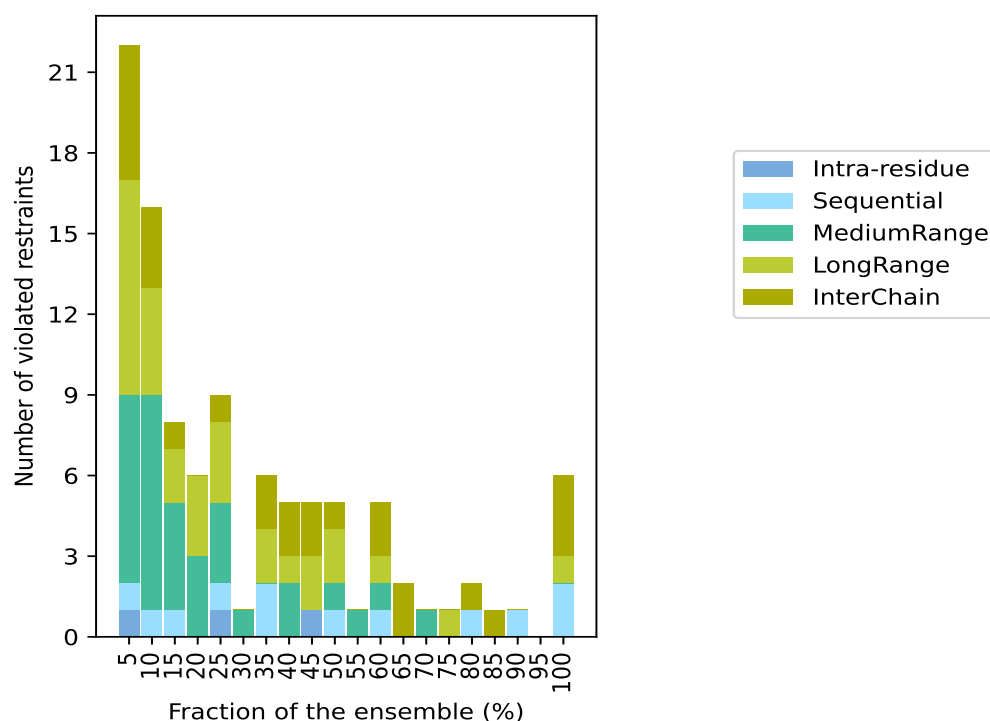
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 912(IR:113, SQ:243, MR:287, LR:144, IC:125) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	1	7	8	5	22	1	5.0
0	1	8	4	3	16	2	10.0
0	1	4	2	1	8	3	15.0
0	0	3	3	0	6	4	20.0
1	1	3	3	1	9	5	25.0
0	0	1	0	0	1	6	30.0
0	2	0	2	2	6	7	35.0
0	0	2	1	2	5	8	40.0
1	0	0	2	2	5	9	45.0
0	1	1	2	1	5	10	50.0
0	0	1	0	0	1	11	55.0
0	1	1	1	2	5	12	60.0
0	0	0	0	2	2	13	65.0
0	0	1	0	0	1	14	70.0
0	0	0	1	0	1	15	75.0
0	1	0	0	1	2	16	80.0
0	0	0	0	1	1	17	85.0
0	1	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	2	0	1	3	6	20	100.0

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

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

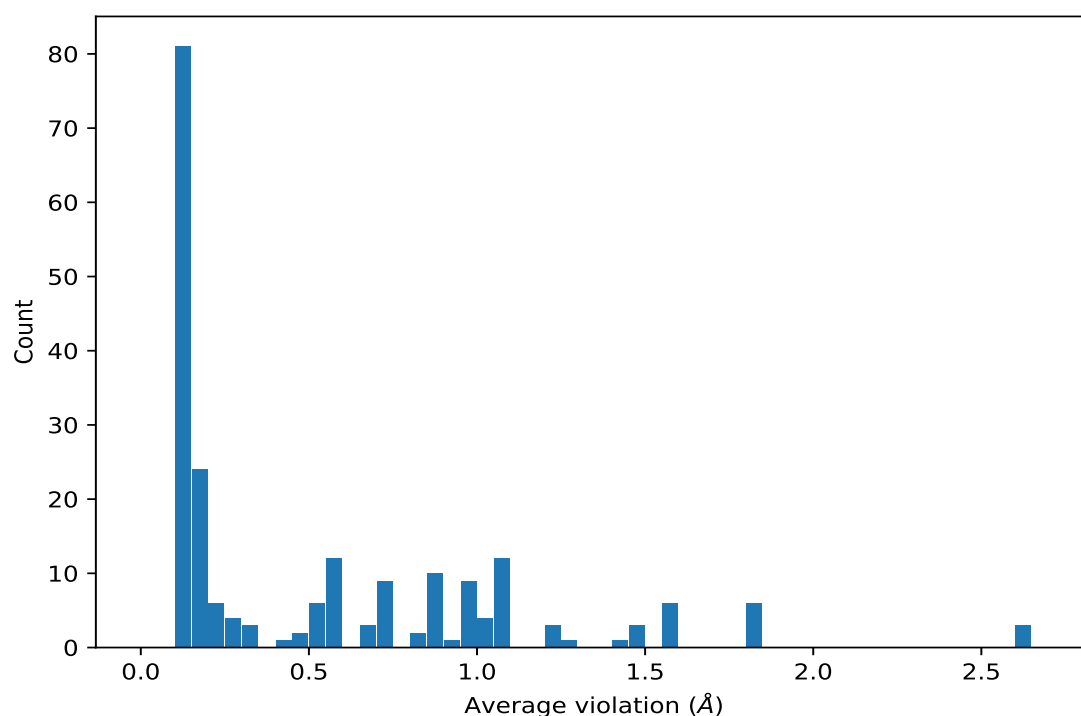
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	20	2.65	0.33	2.63
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD12	20	2.65	0.33	2.63
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD13	20	2.65	0.33	2.63
(1,947)	1:652:A:ILE:HG12	2:403:B:LEU:HD11	20	1.83	0.36	1.78
(1,947)	1:652:A:ILE:HG12	2:403:B:LEU:HD12	20	1.83	0.36	1.78
(1,947)	1:652:A:ILE:HG12	2:403:B:LEU:HD13	20	1.83	0.36	1.78
(1,947)	1:652:A:ILE:HG13	2:403:B:LEU:HD11	20	1.83	0.36	1.78
(1,947)	1:652:A:ILE:HG13	2:403:B:LEU:HD12	20	1.83	0.36	1.78
(1,947)	1:652:A:ILE:HG13	2:403:B:LEU:HD13	20	1.83	0.36	1.78
(1,904)	1:634:A:VAL:HA	2:403:B:LEU:HD12	20	1.58	0.52	1.74
(1,904)	1:634:A:VAL:HA	2:403:B:LEU:HD11	20	1.58	0.52	1.74
(1,904)	1:634:A:VAL:H	2:403:B:LEU:HD12	20	1.58	0.52	1.74
(1,904)	1:634:A:VAL:HA	2:403:B:LEU:HD13	20	1.58	0.52	1.74
(1,904)	1:634:A:VAL:H	2:403:B:LEU:HD11	20	1.58	0.52	1.74
(1,904)	1:634:A:VAL:H	2:403:B:LEU:HD13	20	1.58	0.52	1.74
(1,730)	2:389:B:THR:HG21	2:390:B:TRP:HD1	20	1.44	0.24	1.48

Continued on next page...

Continued from previous page...

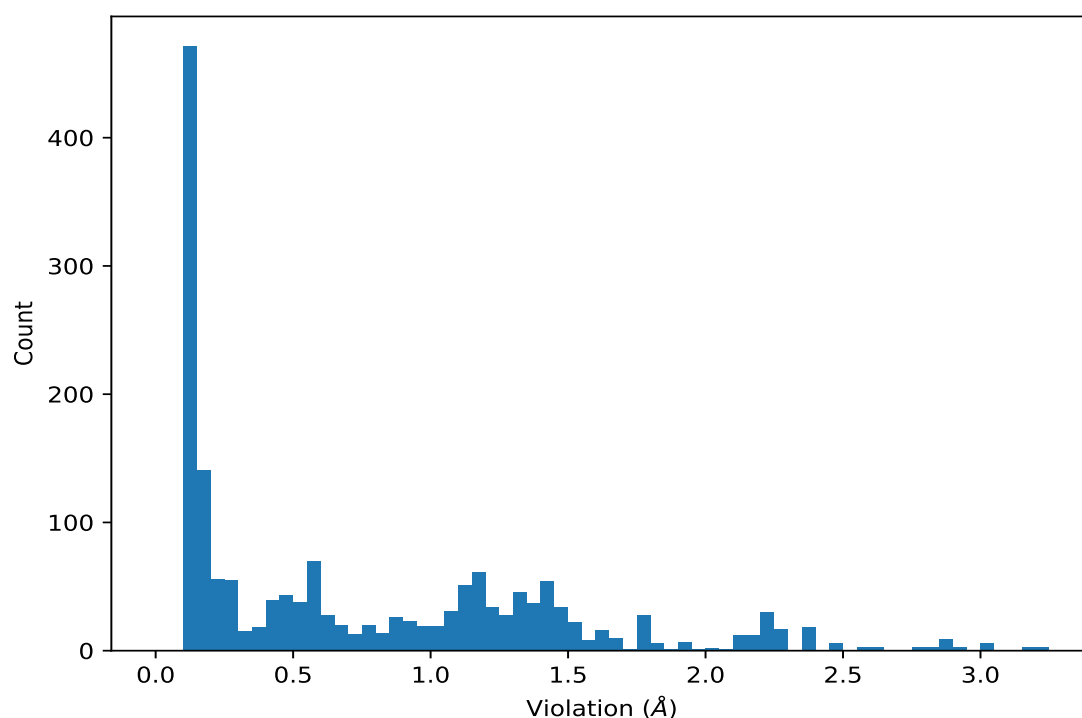
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,944)	1:652:A:ILE:HB	2:403:B:LEU:HD11	20	1.21	0.24	1.14
(1,944)	1:652:A:ILE:HB	2:403:B:LEU:HD12	20	1.21	0.24	1.14
(1,944)	1:652:A:ILE:HB	2:403:B:LEU:HD13	20	1.21	0.24	1.14
(1,729)	2:389:B:THR:HG21	2:390:B:TRP:H	20	0.81	0.14	0.84
(2,27)	1:628:A:GLU:O	1:632:A:ARG:H	19	0.15	0.02	0.15
(1,343)	1:635:A:HIS:HB2	1:636:A:ILE:HD13	18	0.45	0.12	0.46
(1,343)	1:635:A:HIS:HB3	1:636:A:ILE:HD13	18	0.45	0.12	0.46
(1,950)	1:652:A:ILE:HD11	2:403:B:LEU:HD11	17	0.89	0.46	1.09
(1,950)	1:652:A:ILE:HD11	2:403:B:LEU:HD12	17	0.89	0.46	1.09
(1,950)	1:652:A:ILE:HD11	2:403:B:LEU:HD13	17	0.89	0.46	1.09
(1,950)	1:652:A:ILE:HD12	2:403:B:LEU:HD11	17	0.89	0.46	1.09
(1,950)	1:652:A:ILE:HD12	2:403:B:LEU:HD12	17	0.89	0.46	1.09
(1,950)	1:652:A:ILE:HD12	2:403:B:LEU:HD13	17	0.89	0.46	1.09
(1,950)	1:652:A:ILE:HD13	2:403:B:LEU:HD11	17	0.89	0.46	1.09
(1,950)	1:652:A:ILE:HD13	2:403:B:LEU:HD12	17	0.89	0.46	1.09
(1,950)	1:652:A:ILE:HD13	2:403:B:LEU:HD13	17	0.89	0.46	1.09
(1,978)	1:654:A:ILE:HA	2:403:B:LEU:HD11	16	1.49	0.78	1.66

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)
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	11	3.25
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD12	11	3.25
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD13	11	3.25
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	19	3.17
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD12	19	3.17
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD13	19	3.17
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	20	3.02
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD12	20	3.02
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD13	20	3.02
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	12	3.01
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD12	12	3.01
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD13	12	3.01
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	8	2.91
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD12	8	2.91
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD13	8	2.91
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	17	2.9
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD12	17	2.9

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD13	17	2.9
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	5	2.87
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD12	5	2.87
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD13	5	2.87
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	14	2.86
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD12	14	2.86
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD13	14	2.86
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	9	2.81
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD12	9	2.81
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD13	9	2.81
(1,801)	2:394:B:ARG:HA	2:401:B:ILE:HD11	10	2.8

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

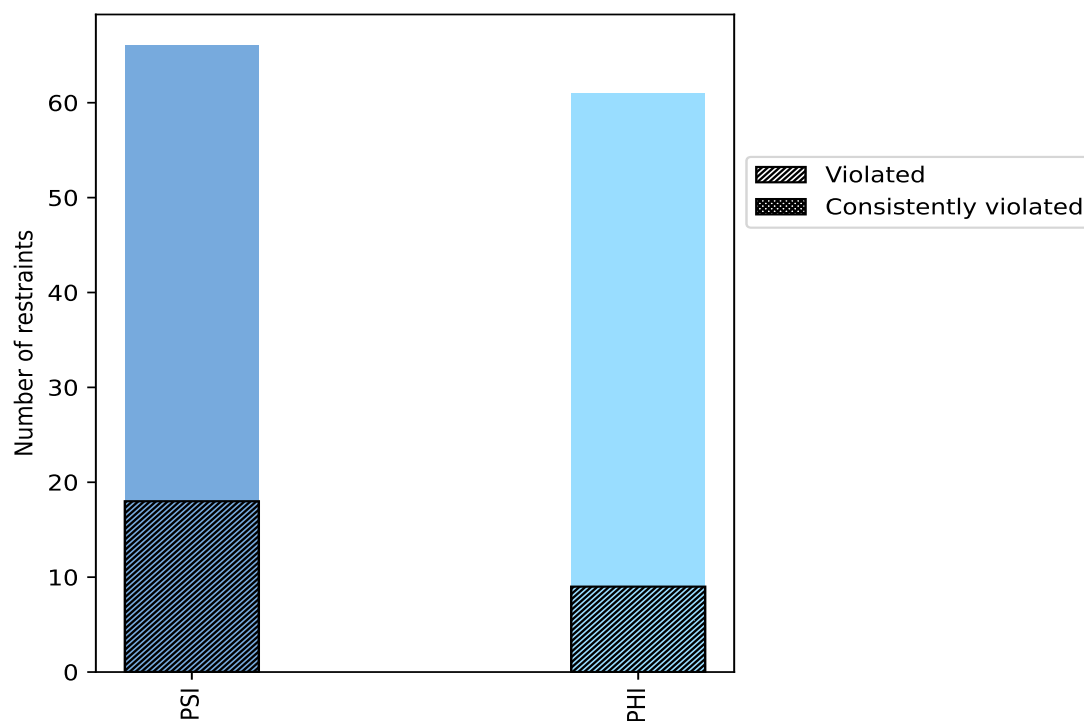
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	66	52.0	18	27.3	14.2	0	0.0	0.0
PHI	61	48.0	9	14.8	7.1	0	0.0	0.0
Total	127	100.0	27	21.3	21.3	0	0.0	0.0

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



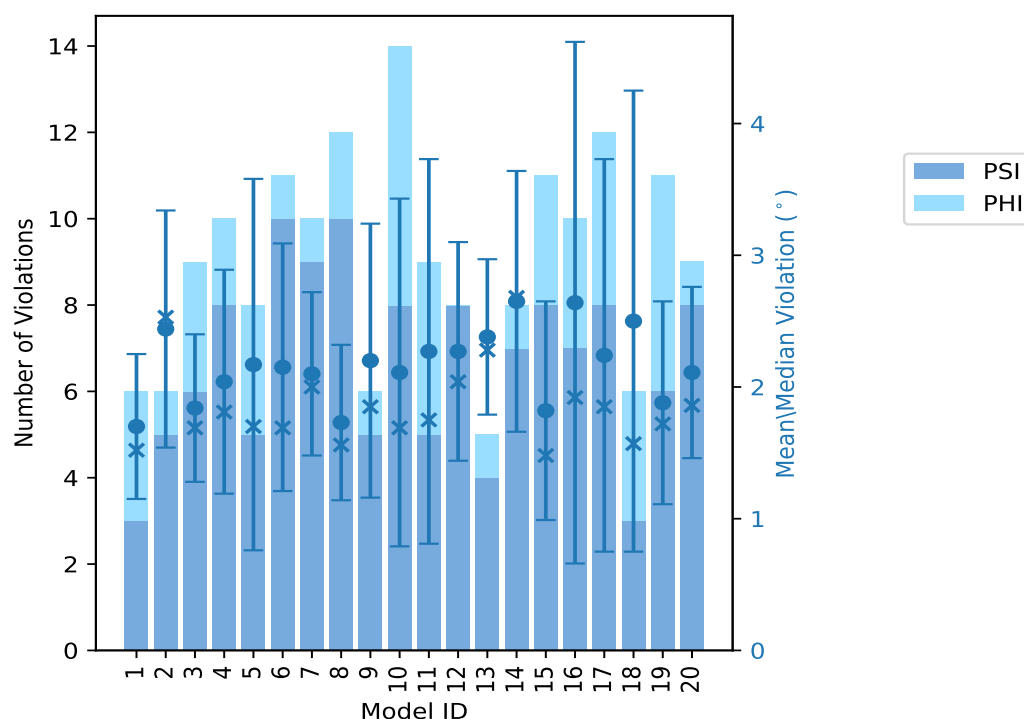
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	3	3	6	1.7	2.81	0.55	1.52
2	5	1	6	2.44	3.57	0.9	2.53
3	6	3	9	1.84	3.05	0.56	1.69
4	8	2	10	2.04	3.56	0.85	1.81
5	5	3	8	2.17	5.73	1.41	1.7
6	10	1	11	2.15	4.23	0.94	1.69
7	9	1	10	2.1	2.93	0.62	2.0
8	10	2	12	1.73	3.3	0.59	1.56
9	5	1	6	2.2	4.24	1.04	1.85
10	8	6	14	2.11	6.47	1.32	1.69
11	5	4	9	2.27	5.95	1.46	1.75
12	8	0	8	2.27	3.92	0.83	2.04
13	4	1	5	2.38	3.34	0.59	2.28
14	7	1	8	2.65	4.42	0.99	2.68
15	8	3	11	1.82	3.32	0.83	1.48
16	7	3	10	2.64	8.19	1.98	1.92
17	8	4	12	2.24	6.31	1.49	1.85
18	3	3	6	2.5	6.09	1.75	1.57
19	6	5	11	1.88	3.66	0.77	1.72
20	8	1	9	2.11	2.94	0.65	1.86

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

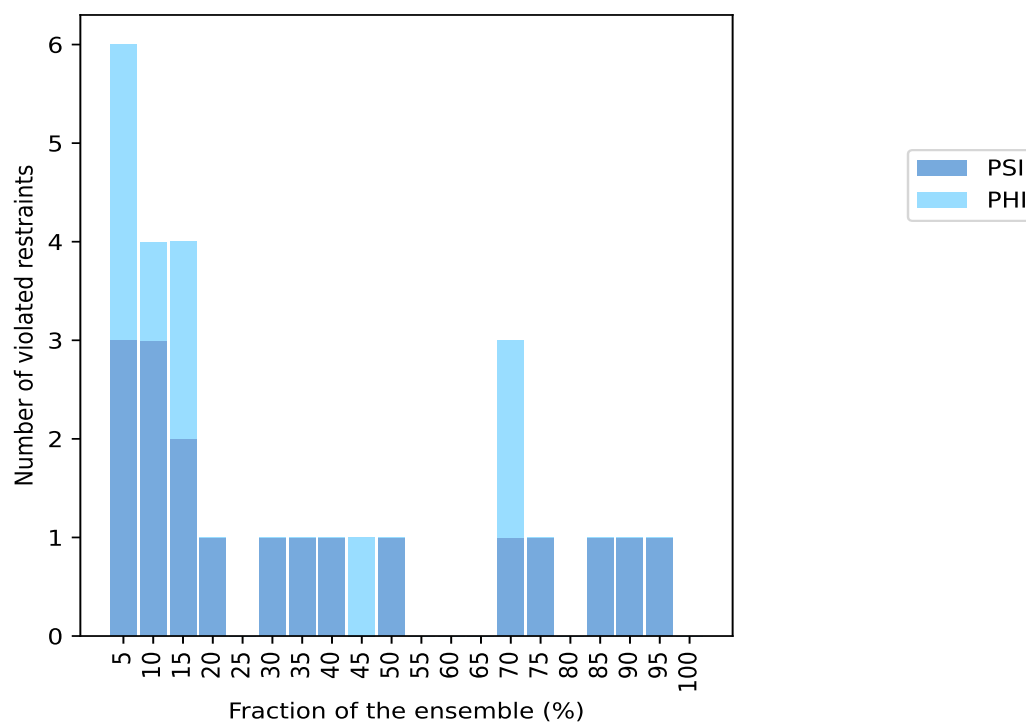
Continued on next page...

Continued from previous page...

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	2	3	14	70.0
1	0	1	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
1	0	1	18	90.0
1	0	1	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

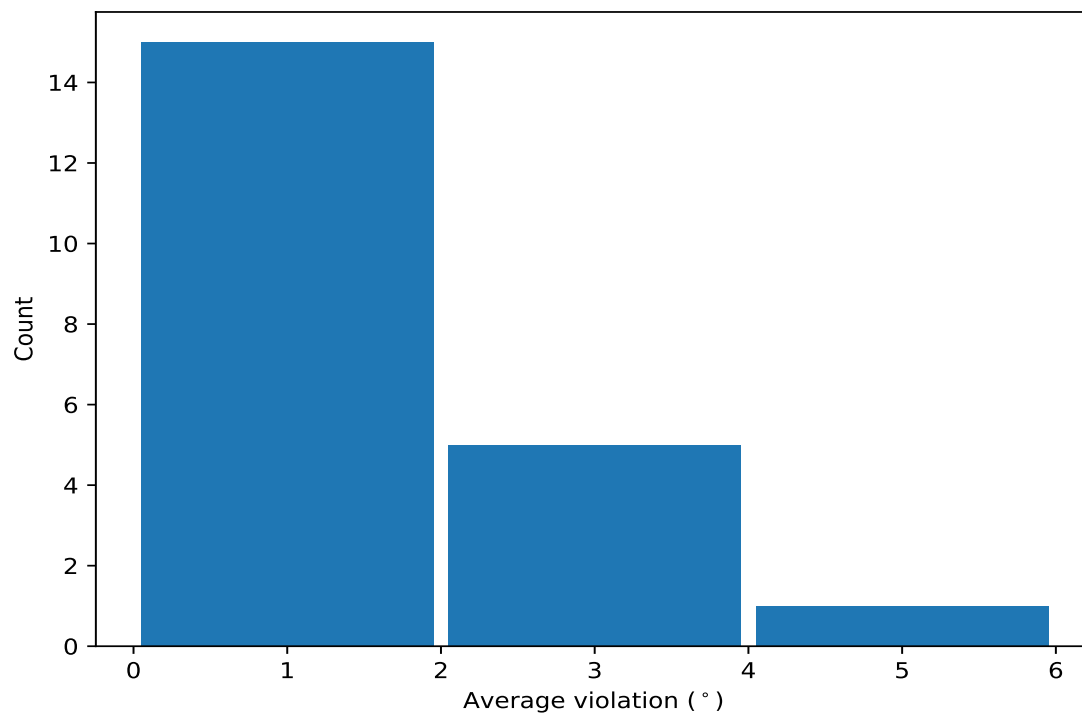


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

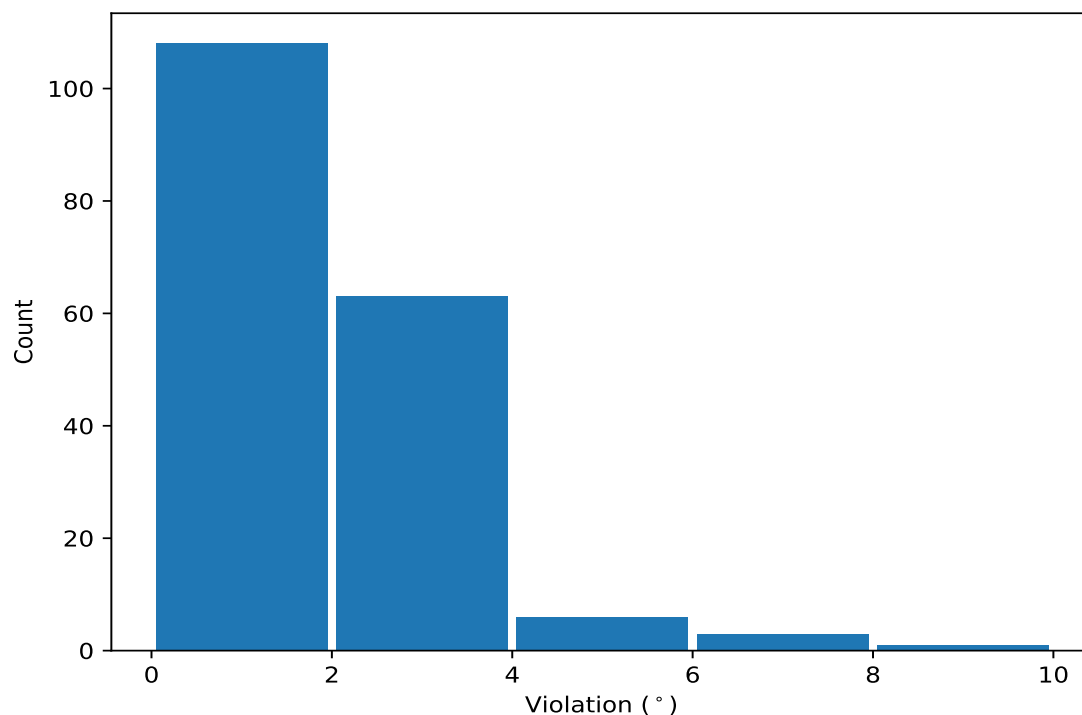
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,42)	1:628:A:GLU:N	1:628:A:GLU:CA	1:628:A:GLU:C	1:629:A:LYS:N	19	2.67	0.82	2.62
(1,39)	1:625:A:LEU:N	1:625:A:LEU:CA	1:625:A:LEU:C	1:626:A:PRO:N	18	2.77	0.83	2.64
(1,80)	1:653:A:GLU:N	1:653:A:GLU:CA	1:653:A:GLU:C	1:654:A:ILE:N	17	2.35	0.65	2.2
(1,62)	1:640:A:ARG:N	1:640:A:ARG:CA	1:640:A:ARG:C	1:641:A:GLU:N	15	2.23	0.88	2.21
(1,75)	1:650:A:ASP:C	1:651:A:GLU:N	1:651:A:GLU:CA	1:651:A:GLU:C	14	4.49	1.81	3.34
(1,91)	1:658:A:THR:C	1:659:A:LEU:N	1:659:A:LEU:CA	1:659:A:LEU:C	14	1.55	0.33	1.62
(1,123)	1:675:A:LEU:N	1:675:A:LEU:CA	1:675:A:LEU:C	1:676:A:ARG:N	14	1.36	0.31	1.21
(1,82)	1:654:A:ILE:N	1:654:A:ILE:CA	1:654:A:ILE:C	1:655:A:ASP:N	10	1.42	0.31	1.34
(1,77)	1:651:A:GLU:C	1:652:A:ILE:N	1:652:A:ILE:CA	1:652:A:ILE:C	9	1.73	0.29	1.78
(1,15)	1:613:A:GLU:N	1:613:A:GLU:CA	1:613:A:GLU:C	1:614:A:GLU:N	8	1.79	0.46	1.7

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 (°)
(1,75)	1:650:A:ASP:C	1:651:A:GLU:N	1:651:A:GLU:CA	1:651:A:GLU:C	16	8.19
(1,75)	1:650:A:ASP:C	1:651:A:GLU:N	1:651:A:GLU:CA	1:651:A:GLU:C	10	6.47
(1,75)	1:650:A:ASP:C	1:651:A:GLU:N	1:651:A:GLU:CA	1:651:A:GLU:C	17	6.31
(1,75)	1:650:A:ASP:C	1:651:A:GLU:N	1:651:A:GLU:CA	1:651:A:GLU:C	18	6.09
(1,75)	1:650:A:ASP:C	1:651:A:GLU:N	1:651:A:GLU:CA	1:651:A:GLU:C	11	5.95
(1,75)	1:650:A:ASP:C	1:651:A:GLU:N	1:651:A:GLU:CA	1:651:A:GLU:C	5	5.73
(1,42)	1:628:A:GLU:N	1:628:A:GLU:CA	1:628:A:GLU:C	1:629:A:LYS:N	14	4.42
(1,39)	1:625:A:LEU:N	1:625:A:LEU:CA	1:625:A:LEU:C	1:626:A:PRO:N	9	4.24
(1,62)	1:640:A:ARG:N	1:640:A:ARG:CA	1:640:A:ARG:C	1:641:A:GLU:N	6	4.23
(1,39)	1:625:A:LEU:N	1:625:A:LEU:CA	1:625:A:LEU:C	1:626:A:PRO:N	17	4.05