



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 11, 2024 – 12:44 PM JST

PDB ID : 8WLS
BMRB ID : 36598
Title : Bcl-xL in complex with HBx BH3 delta C peptide
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Deposited on : 2023-10-01

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:

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

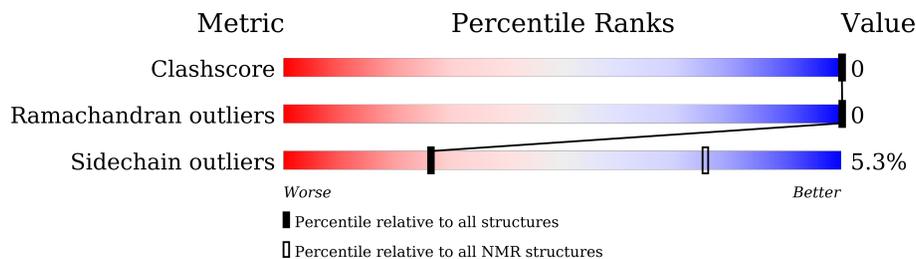
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	156	83% . 12%
2	B	25	100%

2 Ensemble composition and analysis i

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 20 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:4-A:27, A:43-A:155 (137)	0.54	10

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2815 atoms, of which 1357 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	156	2445	800	1182	211	248	4	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP Q07817
A	?	-	GLU	deletion	UNP Q07817
A	?	-	THR	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ILE	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	TRP	deletion	UNP Q07817
A	?	-	HIS	deletion	UNP Q07817
A	?	-	LEU	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ASP	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	VAL	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	THR	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	HIS	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	LEU	deletion	UNP Q07817

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ARG	deletion	UNP Q07817
A	?	-	GLU	deletion	UNP Q07817
A	?	-	VAL	deletion	UNP Q07817
A	?	-	ILE	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	MET	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817

- Molecule 2 is a protein called Protein X.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	25	370	124	175	29	39	3	0

There are 5 discrepancies between the modelled and reference sequences:

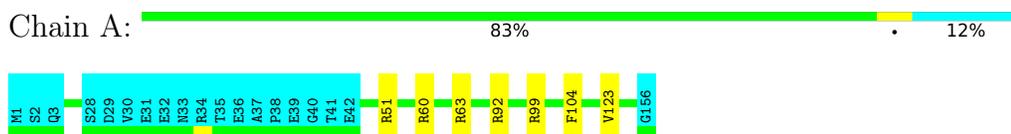
Chain	Residue	Modelled	Actual	Comment	Reference
B	301	GLY	-	cloning artifact	UNP Q9YKJ6
B	302	SER	-	cloning artifact	UNP Q9YKJ6
B	303	HIS	-	cloning artifact	UNP Q9YKJ6
B	304	MET	-	cloning artifact	UNP Q9YKJ6
B	325	GLY	-	linker	UNP Q9YKJ6

4 Residue-property plots [i](#)

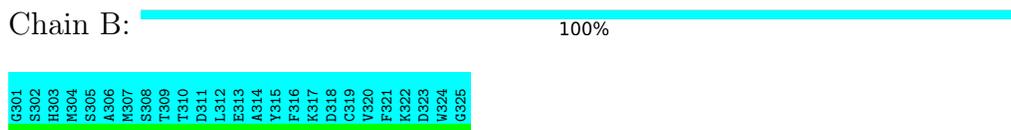
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Bcl-2-like protein 1



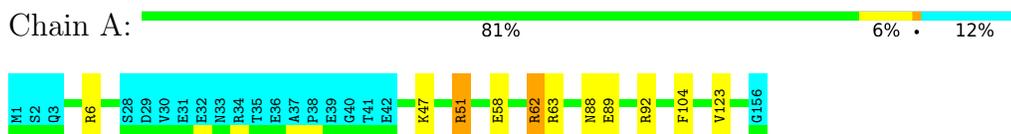
- Molecule 2: Protein X



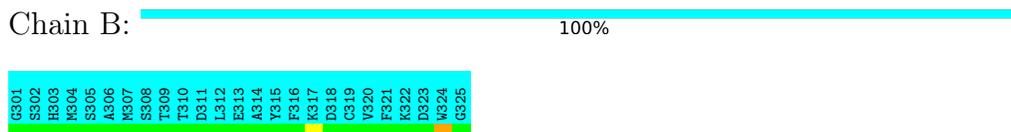
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

- Molecule 1: Bcl-2-like protein 1



- Molecule 2: Protein X



5 Refinement protocol and experimental data overview

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

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
CYANA	structure calculation	3.98
Amber	refinement	12

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	2140
Number of shifts mapped to atoms	2119
Number of unparsed shifts	0
Number of shifts with mapping errors	21
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.78±0.00	0±0/1151 (0.0± 0.0%)	1.03±0.02	4±1/1561 (0.2± 0.1%)
All	All	0.78	0/23020 (0.0%)	1.03	78/31220 (0.2%)

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	0.4±0.5
All	All	0	8

There are no bond-length outliers.

5 of 12 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	51	ARG	NE-CZ-NH1	9.42	125.01	120.30	10	17
1	A	99	ARG	NE-CZ-NH1	8.62	124.61	120.30	19	13
1	A	6	ARG	NE-CZ-NH1	7.72	124.16	120.30	15	7
1	A	60	ARG	NE-CZ-NH1	7.50	124.05	120.30	14	11
1	A	92	ARG	NE-CZ-NH1	7.35	123.98	120.30	14	7

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	133	TYR	Sidechain	6
1	A	60	ARG	Sidechain	1
1	A	51	ARG	Sidechain	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1121	1062	1062	0±0
2	B	0	0	0	0±0
All	All	22420	21240	21240	1

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:HD21	1:A:111:CYS:SG	0.40	2.56	17	1

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	137/156 (88%)	133±1 (97±1%)	4±1 (3±1%)	0±0 (0±0%)	100	100
2	B	0	-	-	-	-	-
All	All	2740/3620 (76%)	2665 (97%)	75 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	118/134 (88%)	112±2 (95±1%)	6±2 (5±1%)	26 75
2	B	0	-	-	-
All	All	2360/3100 (76%)	2235 (95%)	125 (5%)	26 75

5 of 29 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	104	PHE	20
1	A	123	VAL	12
1	A	47	LYS	10
1	A	88	ASN	10
1	A	72	LEU	9

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides 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 i

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping i

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	2140
Number of shifts mapped to atoms	2119
Number of unparsed shifts	0
Number of shifts with mapping errors	21
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	40

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 21) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	H	8.565	0.03	1
1	A	328	SER	C	180.314	0.3	1
1	A	329	GLY	CA	50.011	0.3	1
1	A	330	SER	CA	63.245	0.3	1
1	A	330	SER	CB	68.689	0.3	1
1	A	331	GLY	CA	50.061	0.3	1
1	A	332	SER	CB	68.747	0.3	1
1	A	332	SER	HB2	4.008	0.03	2
1	A	332	SER	HB3	4.008	0.03	2
1	A	333	GLY	CA	50.159	0.3	1
1	A	333	GLY	HA2	4.021	0.03	2
1	A	333	GLY	HA3	4.021	0.03	2
1	A	333	GLY	C	179.004	0.3	1
1	A	334	SER	N	115.712	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	334	SER	H	8.263	0.03	1
1	A	334	SER	CA	63.249	0.3	1
1	A	334	SER	HA	4.481	0.03	1
1	A	334	SER	CB	68.63	0.3	1
1	A	334	SER	HB2	3.894	0.03	2
1	A	334	SER	HB3	3.894	0.03	2
1	A	334	SER	C	179.623	0.3	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
$^{13}\text{C}_\alpha$	178	-5.25 ± 0.17	Should be checked
$^{13}\text{C}_\beta$	165	-4.42 ± 0.05	Should be checked
$^{13}\text{C}'$	164	-4.88 ± 0.14	Should be applied
^{15}N	166	0.30 ± 0.26	None needed (< 0.5 ppm)

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 89%, i.e. 1690 atoms were assigned a chemical shift out of a possible 1898. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	660/690 (96%)	268/281 (95%)	262/274 (96%)	130/135 (96%)
Sidechain	849/980 (87%)	577/635 (91%)	255/304 (84%)	17/41 (41%)
Aromatic	181/228 (79%)	94/112 (84%)	82/109 (75%)	5/7 (71%)
Overall	1690/1898 (89%)	939/1028 (91%)	599/687 (87%)	152/183 (83%)

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	325	GLY	CA	54.88	38.93 – 51.79	7.4
1	A	141	TRP	HZ3	4.23	5.05 – 8.70	-7.3

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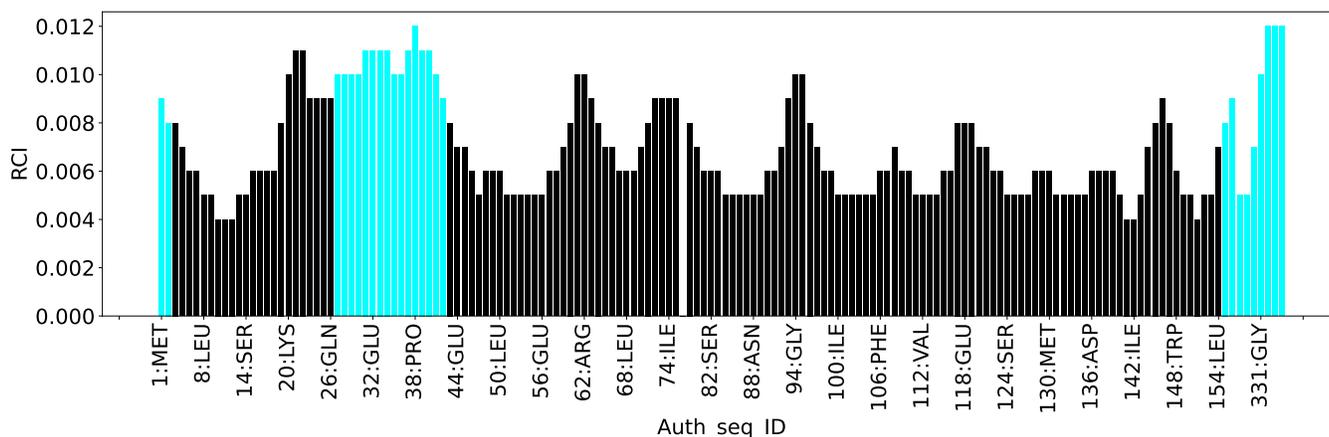
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	47	LYS	CE	47.95	37.57 – 46.21	7.0
1	A	51	ARG	CD	48.87	38.57 – 47.75	6.2
1	A	125	ARG	CD	48.61	38.57 – 47.75	5.9
1	A	117	LYS	CE	47.00	37.57 – 46.21	5.9
1	A	145	ASN	HB2	1.00	1.27 – 4.34	-5.9
1	A	20	LYS	CE	46.91	37.57 – 46.21	5.8
1	B	317	LYS	CE	46.86	37.57 – 46.21	5.8
1	A	16	LYS	CE	46.83	37.57 – 46.21	5.7
1	A	83	PHE	CE2	137.49	124.80 – 136.72	5.7
1	A	107	GLY	CA	52.60	38.93 – 51.79	5.6
1	A	108	GLY	CA	52.54	38.93 – 51.79	5.6
1	B	322	LYS	CE	46.71	37.57 – 46.21	5.6
1	A	35	THR	C	184.01	166.08 – 183.07	5.6
1	A	134	LEU	CG	32.76	21.37 – 32.19	5.5
1	A	140	PRO	CG	33.24	21.69 – 32.72	5.5
1	A	95	VAL	HB	0.31	0.43 – 3.54	-5.4
1	A	98	GLY	CA	52.19	38.93 – 51.79	5.3
1	A	17	LEU	CG	32.48	21.37 – 32.19	5.3
1	A	60	ARG	CD	47.99	38.57 – 47.75	5.3
1	A	75	THR	CG2	27.31	16.06 – 27.03	5.3
1	A	62	ARG	CD	47.98	38.57 – 47.75	5.2
1	A	34	ARG	CD	47.96	38.57 – 47.75	5.2
1	A	92	ARG	CD	47.96	38.57 – 47.75	5.2
1	A	27	PHE	CE2	136.96	124.80 – 136.72	5.2
1	A	95	VAL	HG21	-0.63	-0.58 – 2.19	-5.2
1	A	95	VAL	HG22	-0.63	-0.58 – 2.19	-5.2
1	A	95	VAL	HG23	-0.63	-0.58 – 2.19	-5.2
1	A	76	PRO	CD	55.75	45.11 – 55.58	5.2
1	A	83	PHE	CE1	137.49	124.17 – 137.29	5.2
1	A	63	ARG	CD	47.87	38.57 – 47.75	5.1
1	A	6	ARG	CD	47.86	38.57 – 47.75	5.1
1	A	140	PRO	CA	71.03	55.85 – 70.84	5.1
1	A	81	GLN	CG	39.33	28.36 – 39.21	5.1
1	A	69	THR	CG2	27.12	16.06 – 27.03	5.1
1	A	54	GLY	CA	51.89	38.93 – 51.79	5.1
1	A	150	THR	CG2	27.12	16.06 – 27.03	5.1
1	A	152	VAL	CG2	28.96	13.71 – 28.88	5.0
1	A	18	SER	C	183.19	166.15 – 183.14	5.0

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	3127
Intra-residue ($ i-j =0$)	763
Sequential ($ i-j =1$)	666
Medium range ($ i-j >1$ and $ i-j <5$)	1022
Long range ($ i-j \geq 5$)	512
Inter-chain	20
Hydrogen bond restraints	144
Disulfide bond restraints	0
Total dihedral-angle restraints	355
Number of unmapped restraints	0
Number of restraints per residue	19.2
Number of long range restraints per residue ¹	2.8

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)	12.9	0.2
0.2-0.5 (Medium)	11.8	0.5
>0.5 (Large)	14.7	2.6

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)	42.6	10.0
10.0-20.0 (Medium)	15.2	19.99
>20.0 (Large)	12.2	135.21

9 Distance violation analysis [i](#)

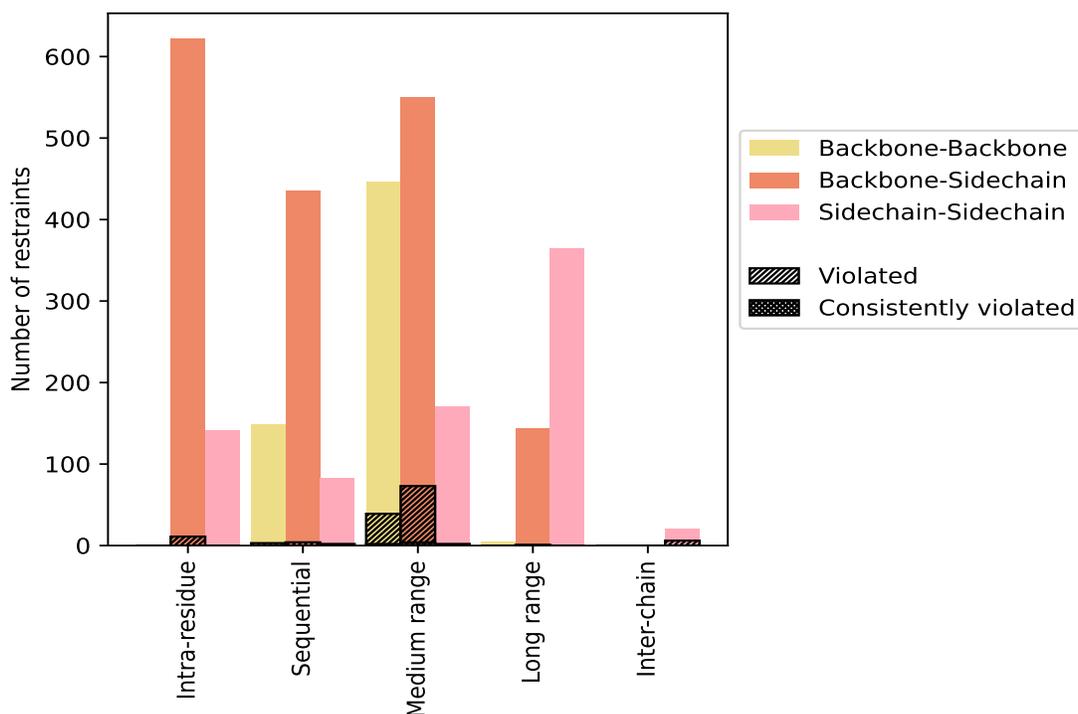
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	763	24.4	11	1.4	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	622	19.9	11	1.8	0.4	0	0.0	0.0
Sidechain-Sidechain	141	4.5	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	666	21.3	9	1.4	0.3	0	0.0	0.0
Backbone-Backbone	148	4.7	3	2.0	0.1	0	0.0	0.0
Backbone-Sidechain	435	13.9	4	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	83	2.7	2	2.4	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	1022	32.7	46	4.5	1.5	2	0.2	0.1
Backbone-Backbone	446	14.3	39	8.7	1.2	2	0.4	0.1
Backbone-Sidechain	406	13.0	5	1.2	0.2	0	0.0	0.0
Sidechain-Sidechain	170	5.4	2	1.2	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	512	16.4	1	0.2	0.0	0	0.0	0.0
Backbone-Backbone	5	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	143	4.6	1	0.7	0.0	0	0.0	0.0
Sidechain-Sidechain	364	11.6	0	0.0	0.0	0	0.0	0.0
Inter-chain	20	0.6	6	30.0	0.2	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	20	0.6	6	30.0	0.2	0	0.0	0.0
Hydrogen bond	144	4.6	68	47.2	2.2	4	2.8	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3127	100.0	141	4.5	4.5	6	0.2	0.2
Backbone-Backbone	599	19.2	42	7.0	1.3	2	0.3	0.1
Backbone-Sidechain	1750	56.0	89	5.1	2.8	4	0.2	0.1
Sidechain-Sidechain	778	24.9	10	1.3	0.3	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 [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	2	35	0	0	37	0.59	1.87	0.51	0.4
2	0	2	39	0	0	41	0.56	2.29	0.51	0.43
3	2	1	30	0	0	33	0.51	2.05	0.51	0.26
4	0	1	42	0	0	43	0.53	1.82	0.46	0.34
5	2	2	42	0	0	46	0.48	1.93	0.49	0.26
6	5	1	35	0	0	41	0.56	1.82	0.46	0.39
7	2	1	51	0	0	54	0.48	1.61	0.38	0.32
8	3	0	30	0	0	33	0.52	1.88	0.53	0.27
9	4	0	31	0	0	35	0.66	2.03	0.58	0.42
10	2	1	34	0	0	37	0.62	2.6	0.62	0.28
11	1	0	23	0	2	26	0.58	1.75	0.44	0.46

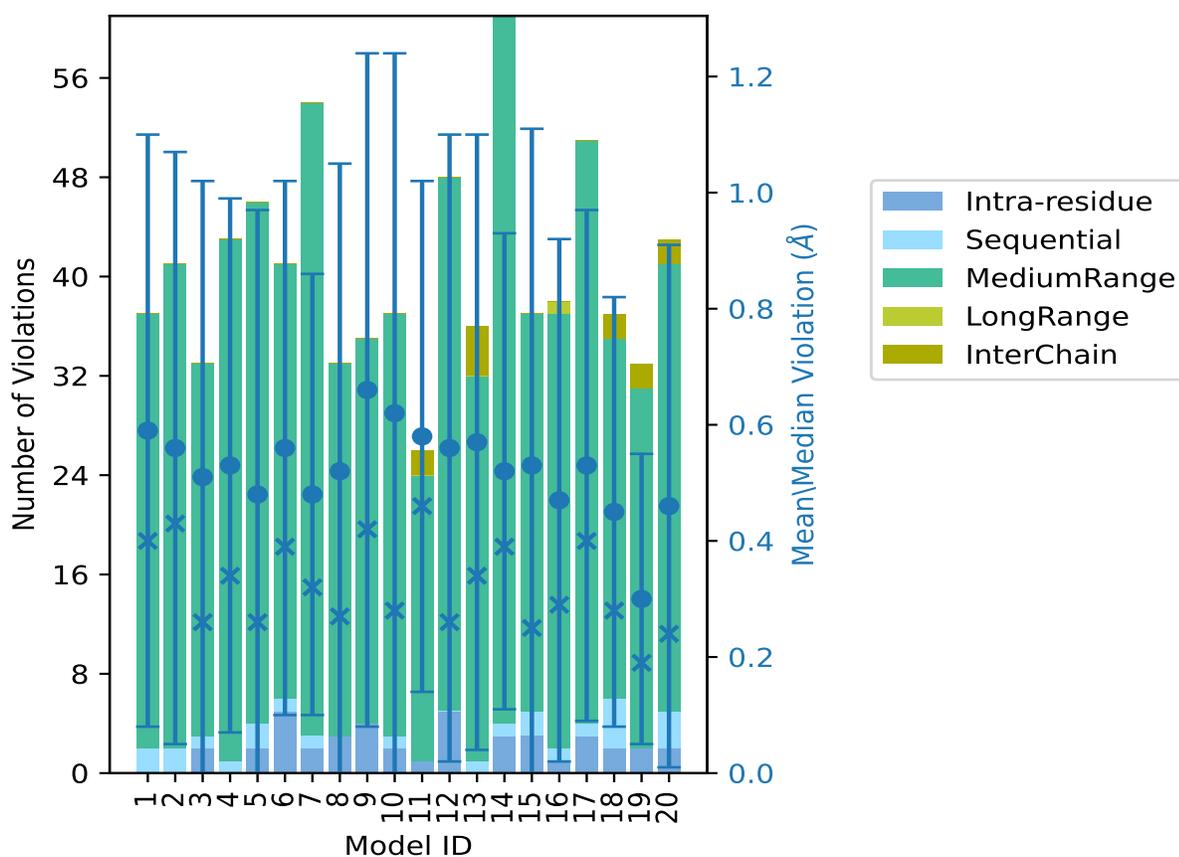
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
12	5	0	43	0	0	48	0.56	2.27	0.54	0.26
13	0	1	31	0	4	36	0.57	2.14	0.53	0.34
14	3	1	57	0	0	61	0.52	1.66	0.41	0.39
15	3	2	32	0	0	37	0.53	2.4	0.58	0.25
16	1	1	35	1	0	38	0.47	1.96	0.45	0.29
17	3	1	47	0	0	51	0.53	2.15	0.44	0.4
18	2	4	29	0	2	37	0.45	1.39	0.37	0.28
19	2	0	29	0	2	33	0.3	1.1	0.25	0.19
20	2	3	36	0	2	43	0.46	1.89	0.45	0.24

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 [\(i\)](#)



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

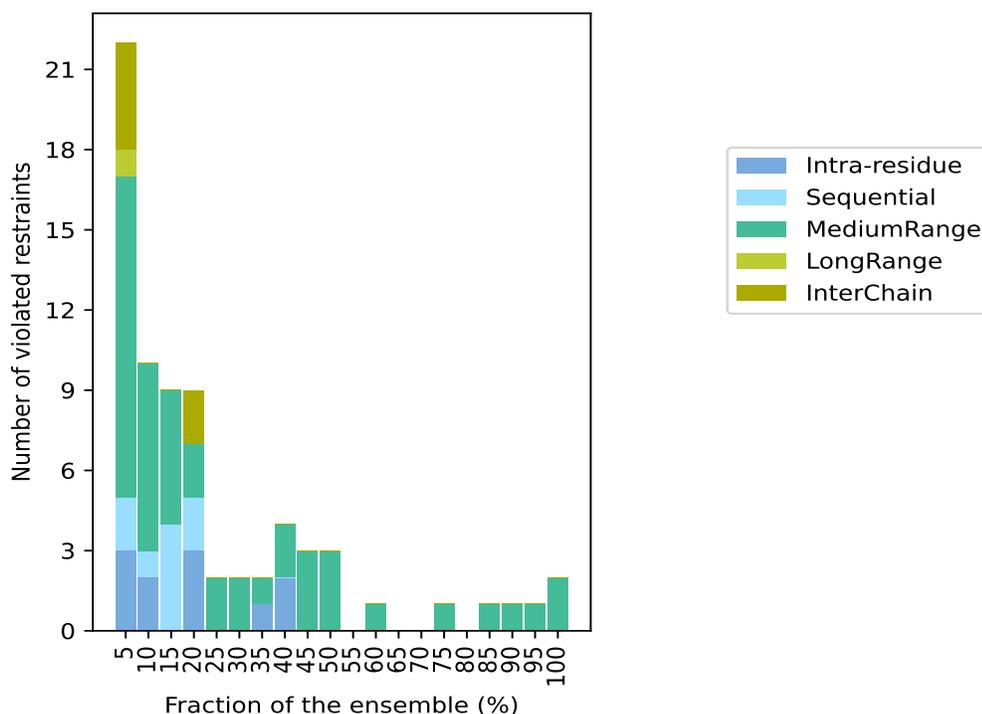
9.3 Distance violation statistics for the ensemble

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, 2910(IR:752, SQ:657, MR:976, LR:511, IC:14) 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	2	12	1	4	22	1	5.0
2	1	7	0	0	10	2	10.0
0	4	5	0	0	9	3	15.0
3	2	2	0	2	9	4	20.0
0	0	2	0	0	2	5	25.0
0	0	2	0	0	2	6	30.0
1	0	1	0	0	2	7	35.0
2	0	2	0	0	4	8	40.0
0	0	3	0	0	3	9	45.0
0	0	3	0	0	3	10	50.0
0	0	0	0	0	0	11	55.0
0	0	1	0	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	1	0	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	1	0	0	1	17	85.0
0	0	1	0	0	1	18	90.0
0	0	1	0	0	1	19	95.0
0	0	2	0	0	2	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

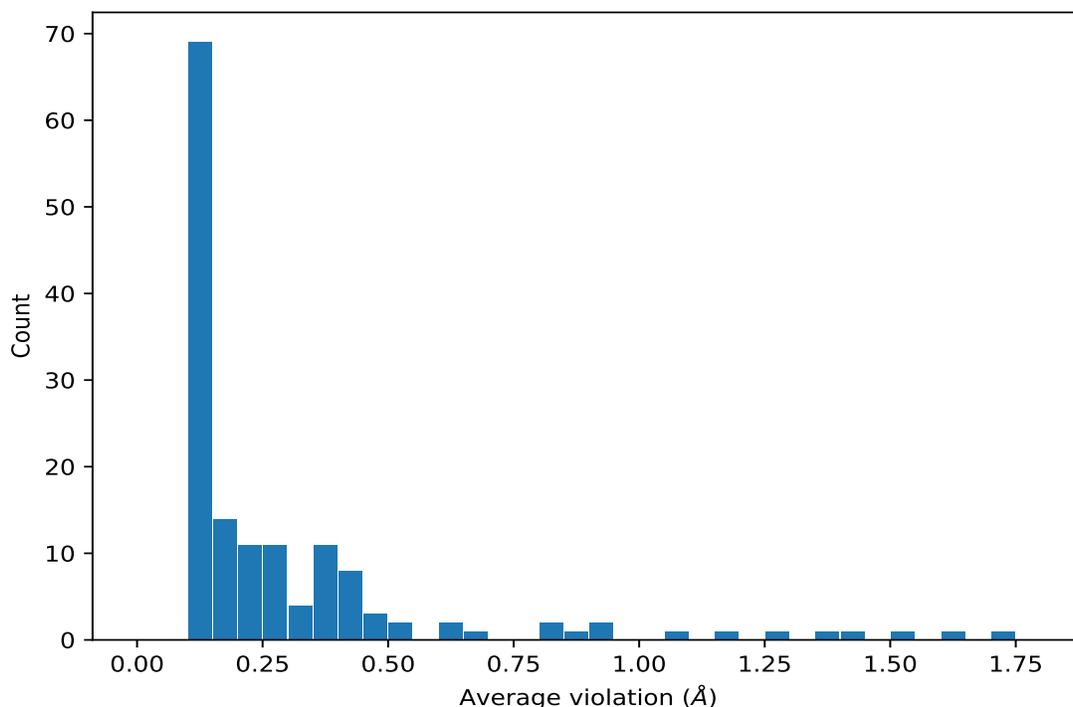
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

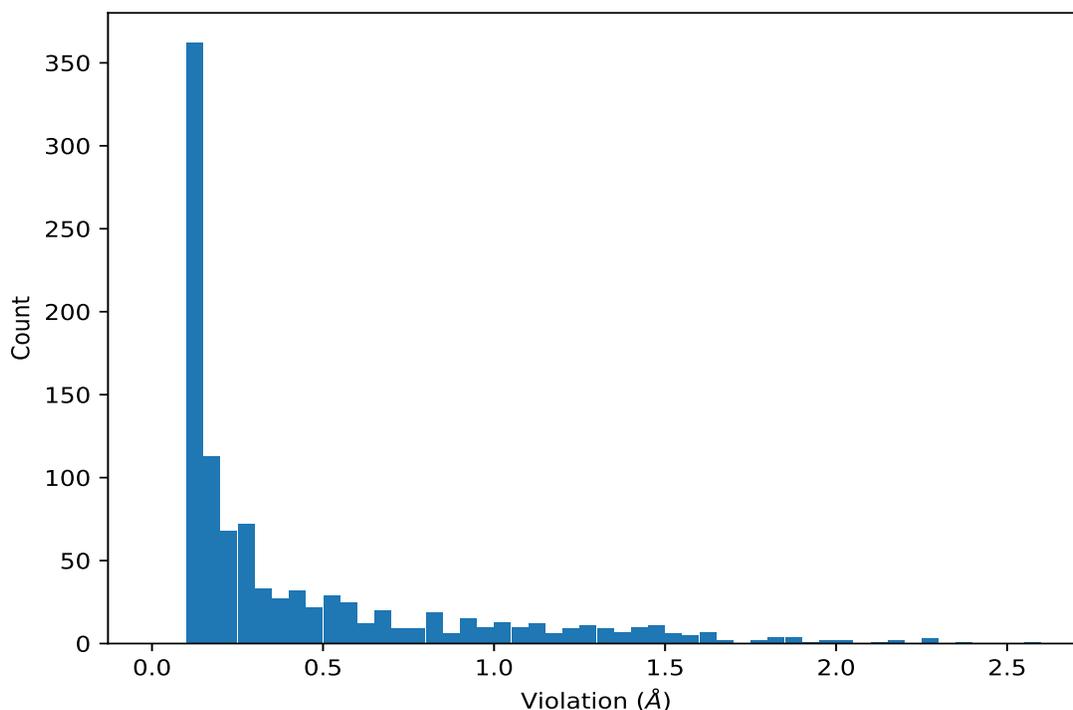
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	20	1.71	0.59	1.81
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	20	1.52	0.27	1.52
(10,61)	1:93:A:ASP:H	1:89:A:GLU:C	20	1.25	0.28	1.25
(9,62)	1:93:A:ASP:N	1:89:A:GLU:O	20	1.17	0.24	1.18
(10,62)	1:93:A:ASP:N	1:89:A:GLU:C	20	0.94	0.24	0.94
(9,59)	1:92:A:ARG:H	1:88:A:ASN:O	20	0.87	0.42	0.9
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	19	1.45	0.47	1.5
(3,11)	2:314:B:ALA:H	2:310:B:THR:C	19	0.84	0.28	0.86
(9,123)	1:151:A:PHE:H	1:147:A:GLY:O	19	0.23	0.06	0.21
(3,12)	2:314:B:ALA:N	2:310:B:THR:C	18	0.62	0.26	0.6

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)
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	10	2.6
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	15	2.4
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	2	2.29
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	12	2.27
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	10	2.25
(2,12)	2:314:B:ALA:N	2:310:B:THR:O	12	2.15
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	17	2.15
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	13	2.14
(2,11)	2:314:B:ALA:H	2:310:B:THR:O	3	2.05
(9,61)	1:93:A:ASP:H	1:89:A:GLU:O	9	2.03

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

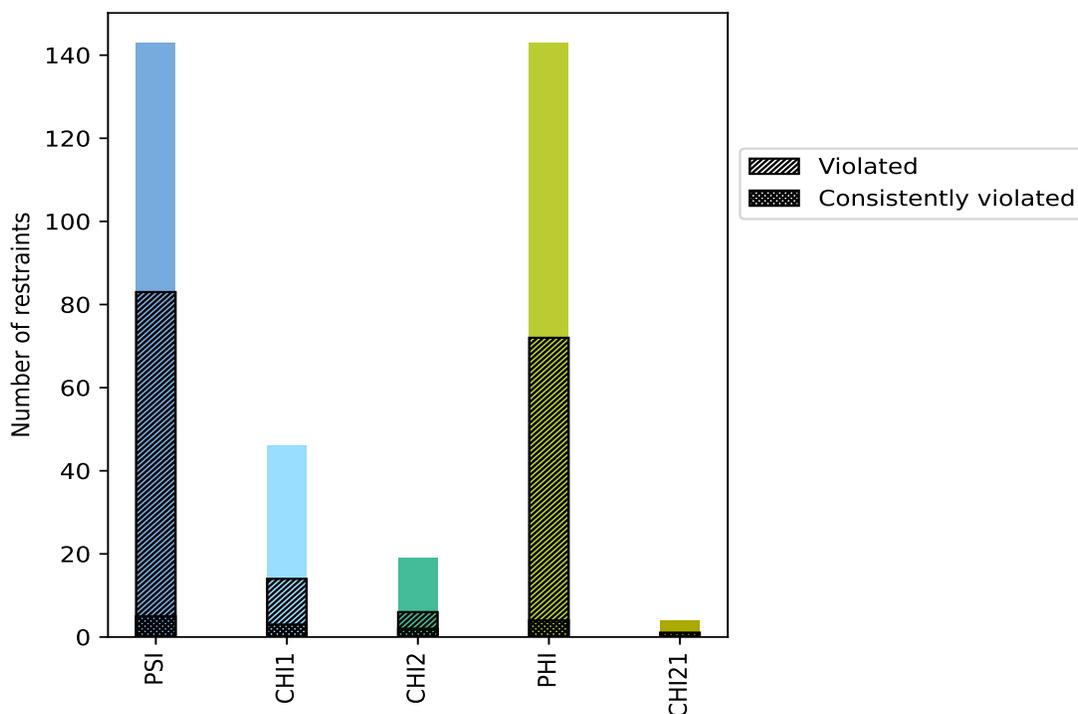
10.1 Summary of dihedral-angle violations [i](#)

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	143	40.3	83	58.0	23.4	5	3.5	1.4
CHI1	46	13.0	14	30.4	3.9	3	6.5	0.8
CHI2	19	5.4	6	31.6	1.7	2	10.5	0.6
PHI	143	40.3	72	50.3	20.3	4	2.8	1.1
CHI21	4	1.1	1	25.0	0.3	1	25.0	0.3
Total	355	100.0	176	49.6	49.6	15	4.2	4.2

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](#)



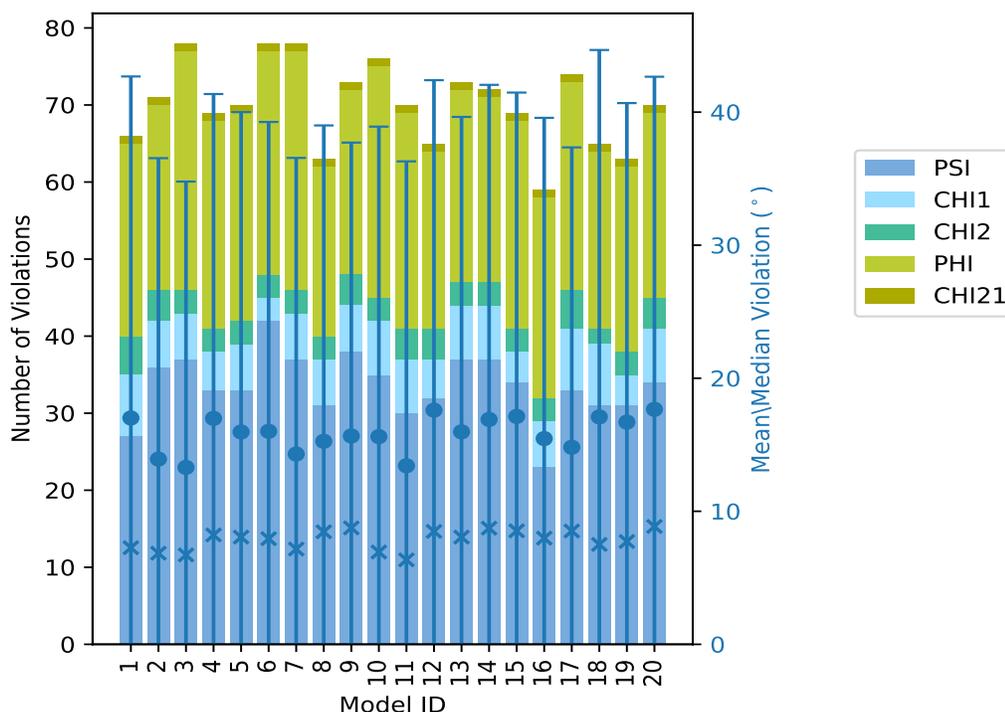
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [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	CHI1	CHI2	PHI	CHI21	Total				
1	27	8	5	25	1	66	17.01	130.26	25.67	7.26
2	36	6	4	24	1	71	13.92	128.17	22.62	6.85
3	37	6	3	31	1	78	13.3	133.61	21.48	6.72
4	33	5	3	27	1	69	16.98	132.83	24.38	8.22
5	33	6	3	27	1	70	15.96	129.29	24.04	8.06
6	42	3	3	29	1	78	16.01	131.63	23.25	7.94
7	37	6	3	31	1	78	14.3	131.61	22.26	7.16
8	31	6	3	22	1	63	15.26	132.37	23.74	8.46
9	38	6	4	24	1	73	15.66	130.82	22.05	8.75
10	35	7	3	30	1	76	15.61	135.02	23.3	6.94
11	30	7	4	28	1	70	13.42	131.51	22.88	6.35
12	32	5	4	23	1	65	17.6	135.21	24.8	8.49
13	37	7	3	25	1	73	15.97	129.58	23.67	8.06
14	37	7	3	24	1	72	16.9	133.52	25.15	8.73
15	34	4	3	27	1	69	17.13	131.47	24.34	8.53
16	23	6	3	26	1	59	15.46	129.75	24.11	7.98
17	33	8	5	27	1	74	14.81	131.06	22.54	8.52
18	31	8	2	23	1	65	17.09	129.51	27.58	7.51
19	31	4	3	24	1	63	16.7	131.13	23.98	7.73
20	34	7	4	24	1	70	17.66	127.23	25.0	8.86

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	CHI1	CHI2	PHI	CHI21	Total	Count ¹	%
11	2	1	13	0	27	1	5.0
10	3	0	12	0	25	2	10.0
7	1	1	2	0	11	3	15.0
9	1	0	7	0	17	4	20.0
8	1	0	1	0	10	5	25.0
2	0	0	4	0	6	6	30.0
0	0	1	6	0	7	7	35.0
2	0	0	2	0	4	8	40.0
2	0	0	2	0	4	9	45.0
3	0	0	1	0	4	10	50.0
1	0	0	2	0	3	11	55.0

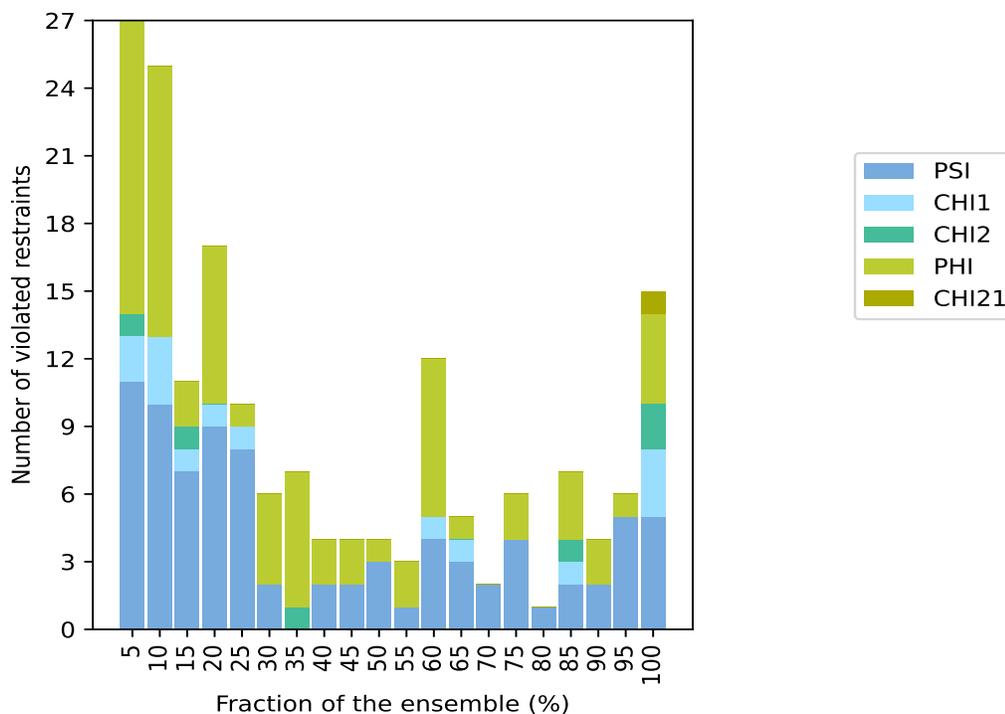
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PSI	Number of violated restraints					Fraction of the ensemble	
	CHI1	CHI2	PHI	CHI21	Total	Count ¹	%
4	1	0	7	0	12	12	60.0
3	1	0	1	0	5	13	65.0
2	0	0	0	0	2	14	70.0
4	0	0	2	0	6	15	75.0
1	0	0	0	0	1	16	80.0
2	1	1	3	0	7	17	85.0
2	0	0	2	0	4	18	90.0
5	0	0	1	0	6	19	95.0
5	3	2	4	1	15	20	100.0

¹ Number of models with violations

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

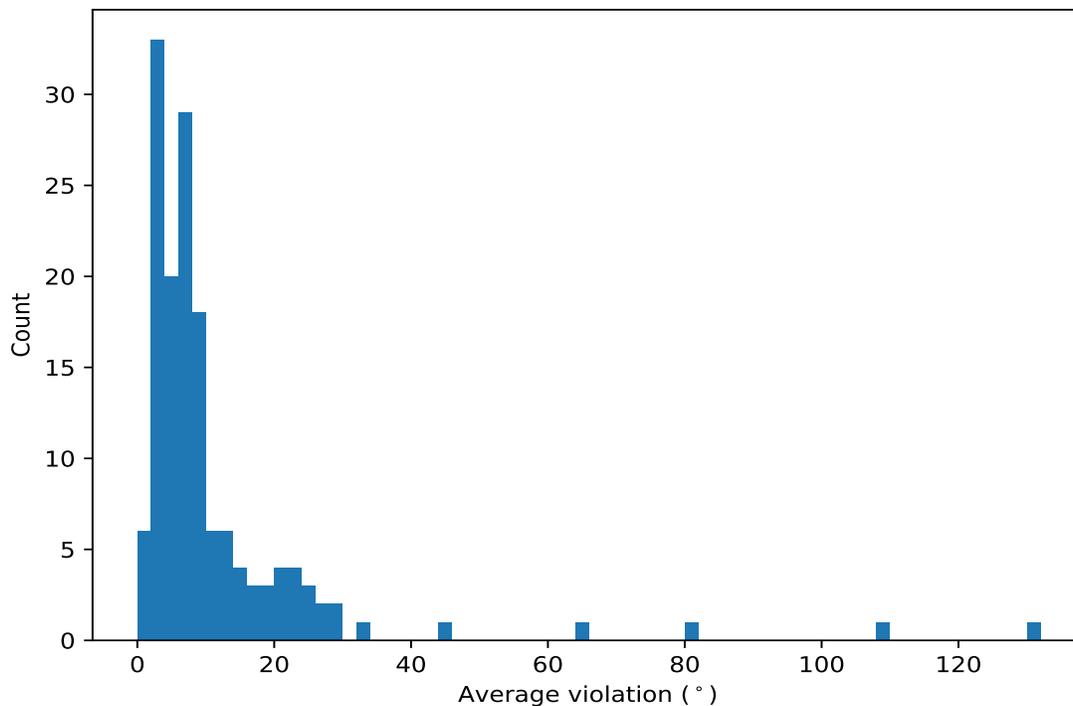


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

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

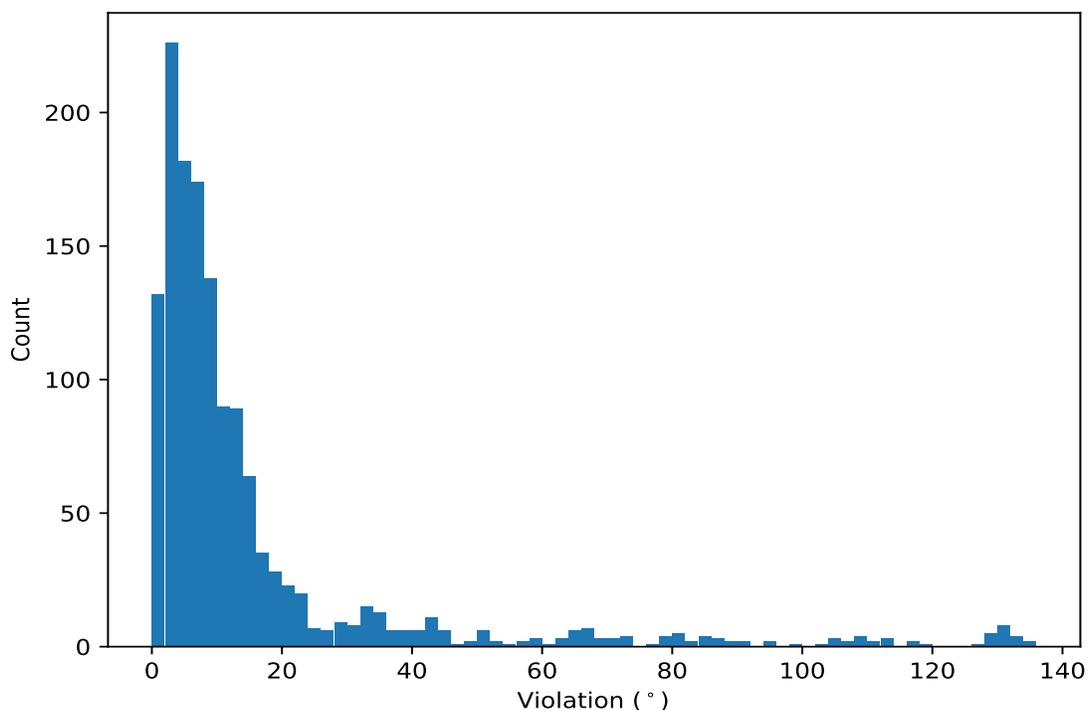
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	20	131.28	2.04	131.3
(2,15)	1:8:A:LEU:N	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	20	108.9	5.65	108.9
(2,16)	1:8:A:LEU:CA	1:8:A:LEU:CB	1:8:A:LEU:CG	1:8:A:LEU:CD1	20	64.1	4.32	65.15
(1,151)	1:95:A:VAL:C	1:96:A:ASN:N	1:96:A:ASN:CA	1:96:A:ASN:C	20	45.39	3.36	44.92
(2,40)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:CB	1:123:A:VAL:CG1	20	33.1	36.67	10.69
(1,274)	2:314:B:ALA:N	2:314:B:ALA:CA	2:314:B:ALA:C	2:315:B:TYR:N	20	22.44	9.77	20.1
(2,8)	1:90:A:LEU:CA	1:90:A:LEU:CB	1:90:A:LEU:CG	1:90:A:LEU:CD1	20	18.76	23.74	8.96
(1,150)	1:95:A:VAL:N	1:95:A:VAL:CA	1:95:A:VAL:C	1:96:A:ASN:N	20	14.94	5.24	15.34
(1,128)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:GLU:N	20	14.25	2.15	14.36
(1,35)	1:19:A:GLN:C	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	20	12.22	3.53	13.44

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	12	135.21
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	10	135.02
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	3	133.61
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	14	133.52
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	4	132.83
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	8	132.37
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	6	131.63
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	7	131.61
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	11	131.51
(1,126)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:PHE:N	15	131.47