



wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 36823
Title : ¹H, ¹³C, and ¹⁵N resonance assignments and solution structure of the first double strand RNA binding domain of DExH-Box Helicase30 (DHX30)
Authors : Abe, C.; Muto, Y.; He, F.; Takahashi, M.; Tsuda, K.; Nagata, T.; Tanaka, A.; Kobayashi, N.; Kigawa, T.; Guntert, P.; Shirouzu, M.; Yokoyama, S.; Kuwasako, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
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The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4-5-2 with Phenix2.2
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	:	v1.3.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

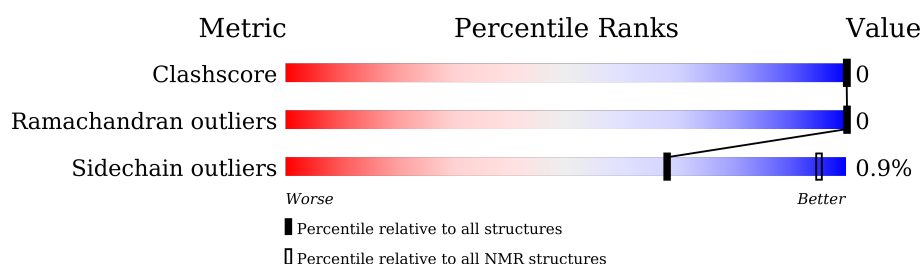
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	119	 76% . 23%

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:12-A:44, A:52-A:110 (92)	0.26	12

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 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1828 atoms, of which 926 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ATP-dependent RNA helicase DHX30.

Mol	Chain	Residues	Atoms						Trace
1	A	119	Total	C	H	N	O	S	0
			1828	571	926	166	164	1	

There are 12 discrepancies between the modelled and reference sequences:

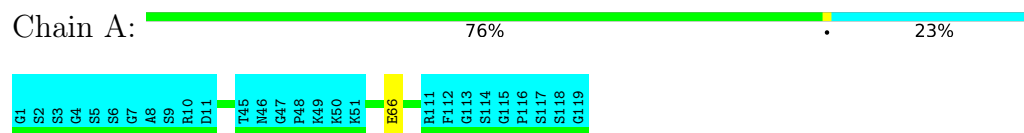
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q7L2E3
A	2	SER	-	expression tag	UNP Q7L2E3
A	3	SER	-	expression tag	UNP Q7L2E3
A	4	GLY	-	expression tag	UNP Q7L2E3
A	5	SER	-	expression tag	UNP Q7L2E3
A	6	SER	-	expression tag	UNP Q7L2E3
A	7	GLY	-	expression tag	UNP Q7L2E3
A	115	GLY	-	expression tag	UNP Q7L2E3
A	116	PRO	-	expression tag	UNP Q7L2E3
A	117	SER	-	expression tag	UNP Q7L2E3
A	118	SER	-	expression tag	UNP Q7L2E3
A	119	GLY	-	expression tag	UNP Q7L2E3

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.

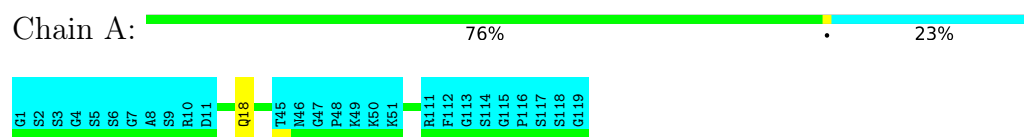
- Molecule 1: ATP-dependent RNA helicase DHX30



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

The representative model is number 12. Colouring as in section 4.1 above.

- Molecule 1: ATP-dependent RNA helicase DHX30



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with favorable non-bond energy*.

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

Software name	Classification	Version
CYANA	structure calculation	2.1
Amber	refinement	24
TALOS	geometry optimization	

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	1385
Number of shifts mapped to atoms	1385
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

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	0.83±0.01	0±0/740 (0.0± 0.0%)	1.44±0.02	2±1/999 (0.2± 0.1%)
All	All	0.83	0/14800 (0.0%)	1.44	39/19980 (0.2%)

There are no bond-length outliers.

5 of 9 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	66	GLU	CA-C-N	6.76	126.84	122.18	6	14
1	A	66	GLU	C-N-CA	6.76	126.84	122.18	6	14
1	A	95	PRO	CA-C-N	5.46	128.14	120.28	2	1
1	A	95	PRO	C-N-CA	5.46	128.14	120.28	2	1
1	A	18	GLN	CA-C-N	5.18	124.80	119.05	7	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	723	753	753	0±0
All	All	14460	15060	15060	-

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 -.

There are no clashes.

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	92/119 (77%)	91±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
All	All	1840/2380 (77%)	1823 (99%)	17 (1%)	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	74/93 (80%)	73±1 (99±1%)	1±1 (1±1%)	68	95
All	All	1480/1860 (80%)	1467 (99%)	13 (1%)	68	95

All 5 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	85	GLN	5
1	A	18	GLN	3
1	A	25	SER	2
1	A	61	LYS	2
1	A	14	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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 93% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *DSRM13*

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	1385
Number of shifts mapped to atoms	1385
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	112	-0.30 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	99	0.18 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}'$	102	-0.11 ± 0.07	None needed (< 0.5 ppm)
^{15}N	92	0.75 ± 0.30	Should be applied

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 93%, i.e. 1197 atoms were assigned a chemical shift out of a possible 1290. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	440/459 (96%)	183/187 (98%)	177/184 (96%)	80/88 (91%)
Sidechain	667/729 (91%)	456/476 (96%)	205/224 (92%)	6/29 (21%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	90/102 (88%)	45/51 (88%)	43/46 (93%)	2/5 (40%)
Overall	1197/1290 (93%)	684/714 (96%)	425/454 (94%)	88/122 (72%)

7.1.4 Statistically unusual chemical shifts [i](#)

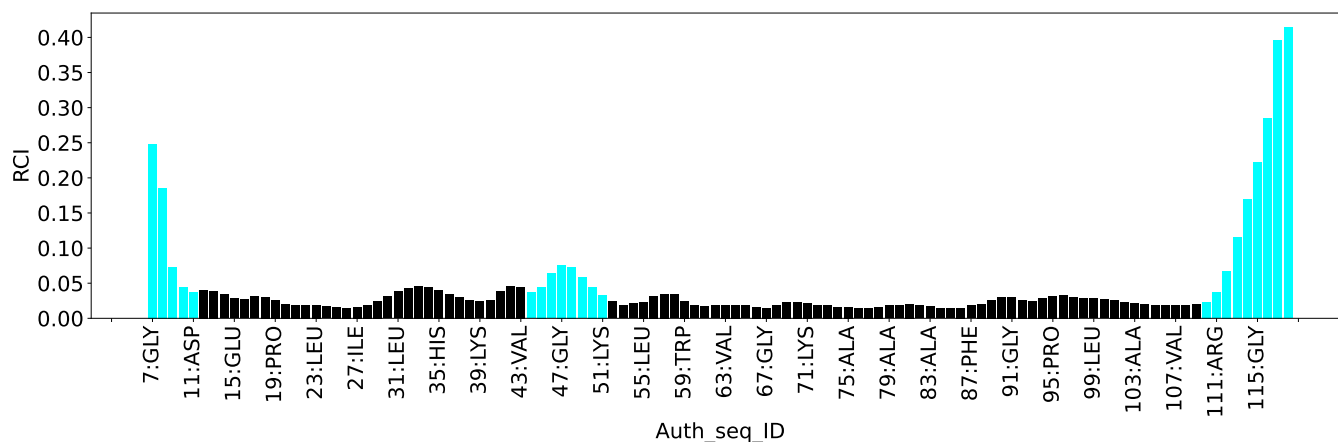
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	60	PRO	HB2	-0.34	0.37 – 3.78	-7.1
1	A	60	PRO	HG2	0.02	0.41 – 3.45	-6.3
1	A	60	PRO	HG3	0.09	0.33 – 3.48	-5.8
1	A	60	PRO	HA	2.67	2.78 – 6.00	-5.3

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

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	3123
Intra-residue ($ i-j =0$)	41
Sequential ($ i-j =1$)	845
Medium range ($ i-j >1$ and $ i-j <5$)	776
Long range ($ i-j \geq 5$)	1461
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	763
Number of unmapped restraints	0
Number of restraints per residue	32.7
Number of long range restraints per residue ¹	12.3

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)	16.1	0.2
0.2-0.5 (Medium)	139.1	0.5
>0.5 (Large)	1481.9	5.49

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)	9.6	9.66
10.0-20.0 (Medium)	4.7	19.69
>20.0 (Large)	160.3	134.11

9 Distance violation analysis ⓘ

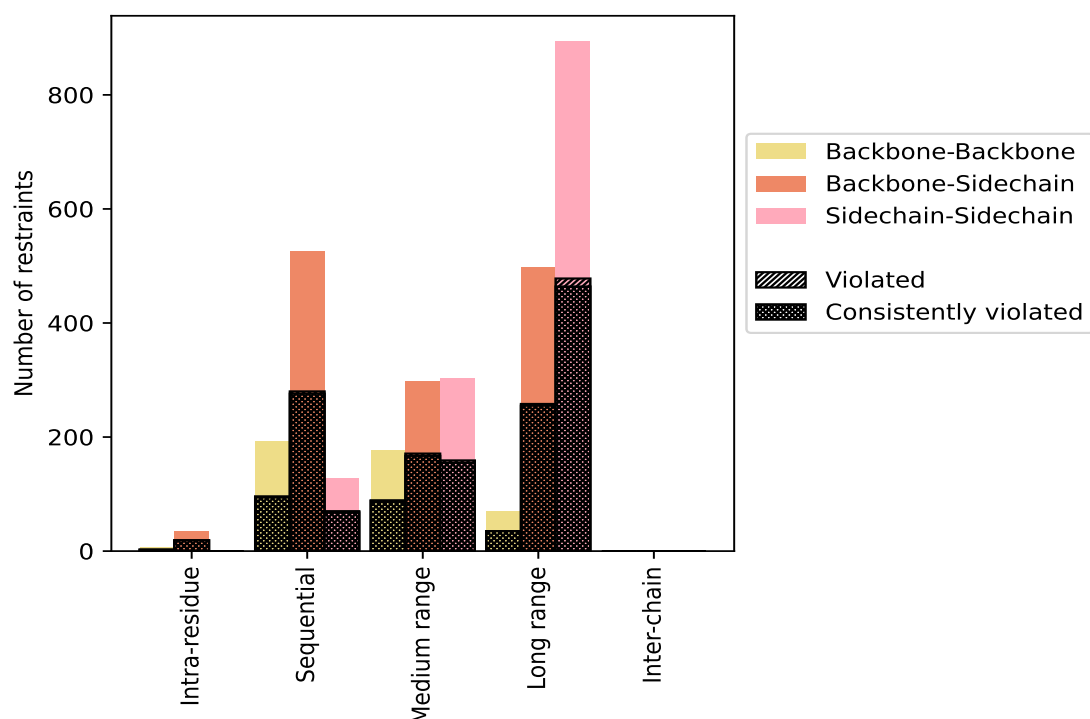
9.1 Summary of distance violations ⓘ

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)	41	1.3	22	53.7	0.7	21	51.2	0.7
Backbone-Backbone	6	0.2	3	50.0	0.1	2	33.3	0.1
Backbone-Sidechain	35	1.1	19	54.3	0.6	19	54.3	0.6
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	845	27.1	446	52.8	14.3	438	51.8	14.0
Backbone-Backbone	192	6.1	96	50.0	3.1	94	49.0	3.0
Backbone-Sidechain	526	16.8	280	53.2	9.0	276	52.5	8.8
Sidechain-Sidechain	127	4.1	70	55.1	2.2	68	53.5	2.2
Medium range (i-j >1 & i-j <5)	776	24.8	419	54.0	13.4	410	52.8	13.1
Backbone-Backbone	176	5.6	89	50.6	2.8	88	50.0	2.8
Backbone-Sidechain	298	9.5	171	57.4	5.5	167	56.0	5.3
Sidechain-Sidechain	302	9.7	159	52.6	5.1	155	51.3	5.0
Long range (i-j ≥5)	1461	46.8	771	52.8	24.7	754	51.6	24.1
Backbone-Backbone	70	2.2	35	50.0	1.1	35	50.0	1.1
Backbone-Sidechain	497	15.9	258	51.9	8.3	255	51.3	8.2
Sidechain-Sidechain	894	28.6	478	53.5	15.3	464	51.9	14.9
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3123	100.0	1658	53.1	53.1	1623	52.0	52.0
Backbone-Backbone	444	14.2	223	50.2	7.1	219	49.3	7.0
Backbone-Sidechain	1356	43.4	728	53.7	23.3	717	52.9	23.0
Sidechain-Sidechain	1323	42.4	707	53.4	22.6	687	51.9	22.0

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 disulfied bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	22	442	412	763	0	1639	1.73	5.4	0.94	1.73
2	22	443	412	763	0	1640	1.73	5.34	0.94	1.71
3	22	443	413	759	0	1637	1.73	5.42	0.94	1.72
4	21	440	413	763	0	1637	1.73	5.43	0.94	1.71
5	22	441	412	762	0	1637	1.74	5.45	0.94	1.71
6	22	444	413	764	0	1643	1.73	5.49	0.94	1.7
7	21	444	412	760	0	1637	1.72	5.47	0.94	1.69
8	22	441	414	760	0	1637	1.73	5.42	0.94	1.7
9	21	442	413	762	0	1638	1.74	5.45	0.94	1.72
10	21	439	413	765	0	1638	1.73	5.45	0.95	1.68

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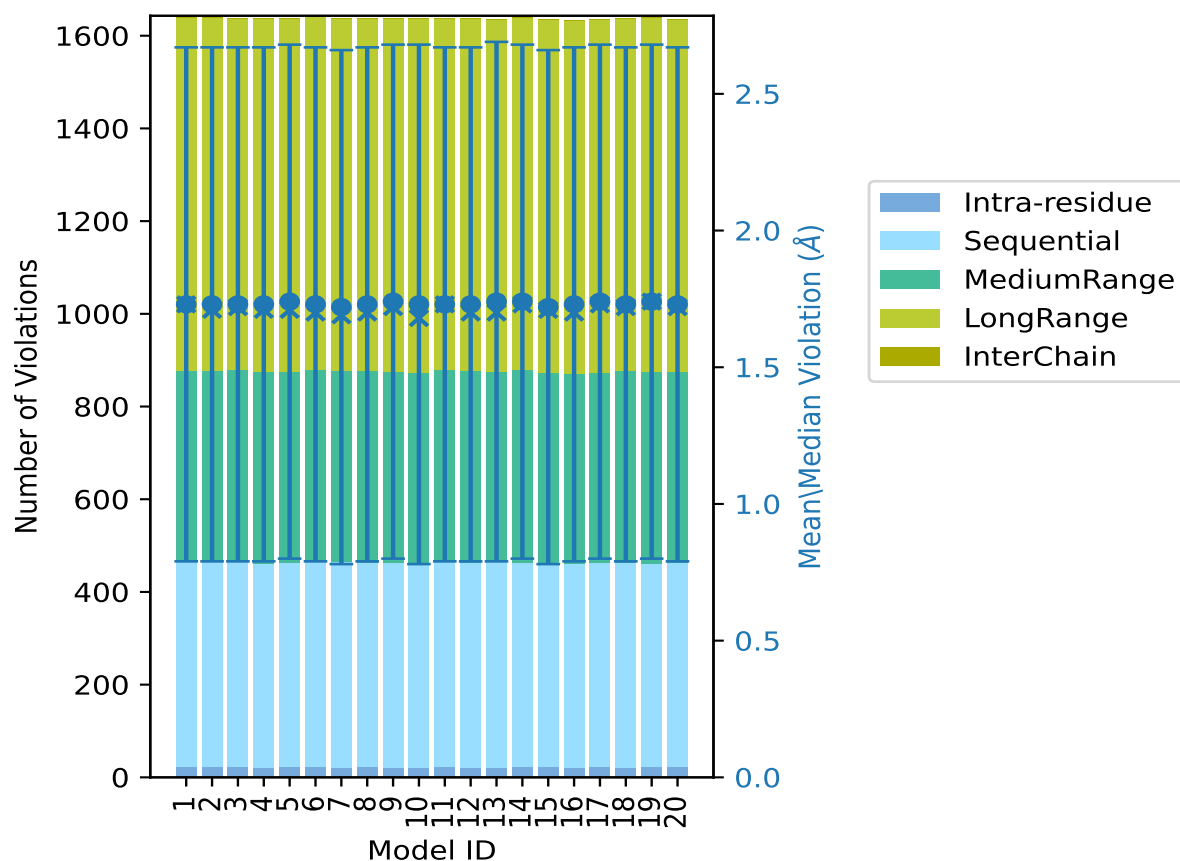
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	22	442	414	759	0	1637	1.73	5.45	0.94	1.73
12	21	443	413	761	0	1638	1.73	5.41	0.94	1.7
13	21	443	412	760	0	1636	1.74	5.44	0.95	1.7
14	22	442	415	760	0	1639	1.74	5.44	0.94	1.73
15	22	440	412	762	0	1636	1.72	5.42	0.94	1.71
16	21	439	411	762	0	1633	1.73	5.45	0.94	1.7
17	22	440	411	761	0	1634	1.74	5.44	0.94	1.73
18	21	442	413	761	0	1637	1.73	5.45	0.94	1.72
19	22	439	413	765	0	1639	1.74	5.36	0.94	1.74
20	22	440	413	760	0	1635	1.73	5.42	0.94	1.72

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

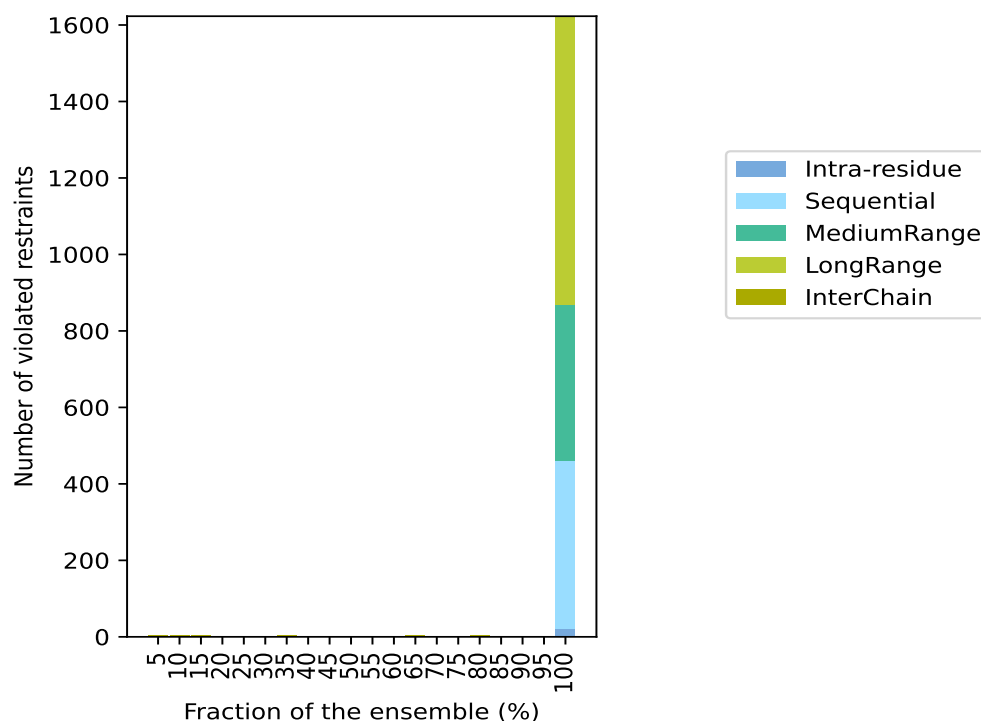
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1465(IR:19, SQ:399, MR:357, LR:690, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	3	1	0	4	1	5.0
0	1	0	3	0	4	2	10.0
0	1	2	1	0	4	3	15.0
0	0	0	0	0	0	4	20.0
0	1	0	1	0	2	5	25.0
0	0	0	1	0	1	6	30.0
0	1	1	2	0	4	7	35.0
0	0	0	0	0	0	8	40.0
0	1	1	0	0	2	9	45.0
0	0	0	1	0	1	10	50.0
0	1	0	0	0	1	11	55.0
1	0	0	0	0	1	12	60.0
0	0	1	2	0	3	13	65.0
0	0	0	2	0	2	14	70.0
0	0	0	0	0	0	15	75.0
0	2	1	0	0	3	16	80.0
0	0	0	2	0	2	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	1	0	1	19	95.0
21	438	410	754	0	1623	20	100.0

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

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

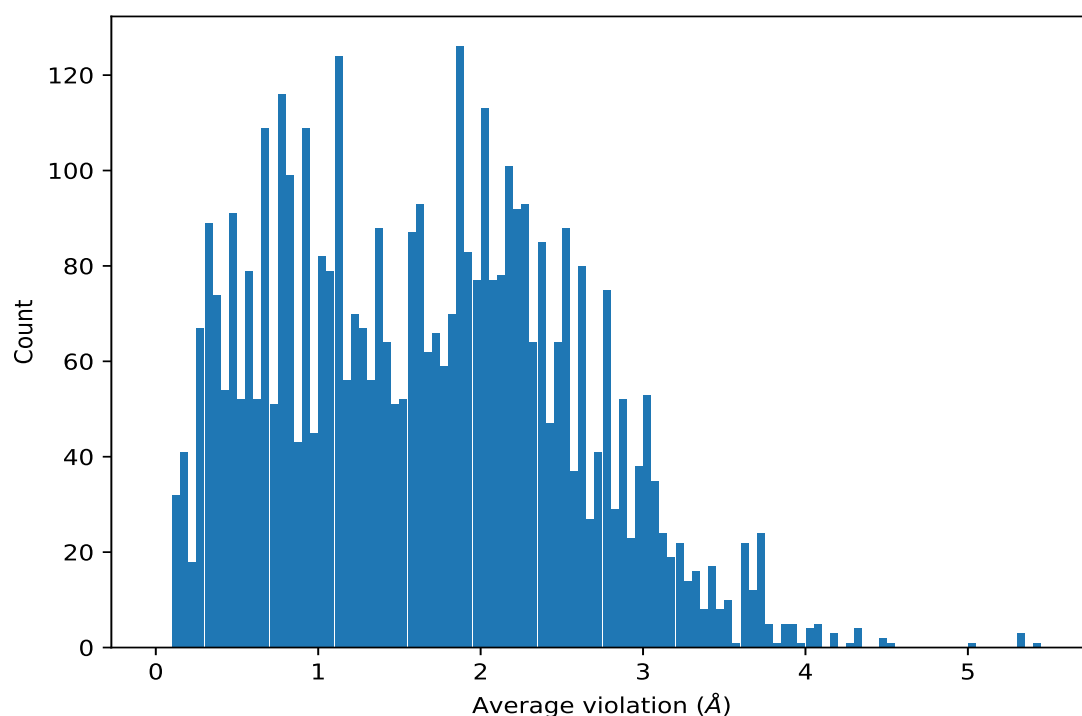
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

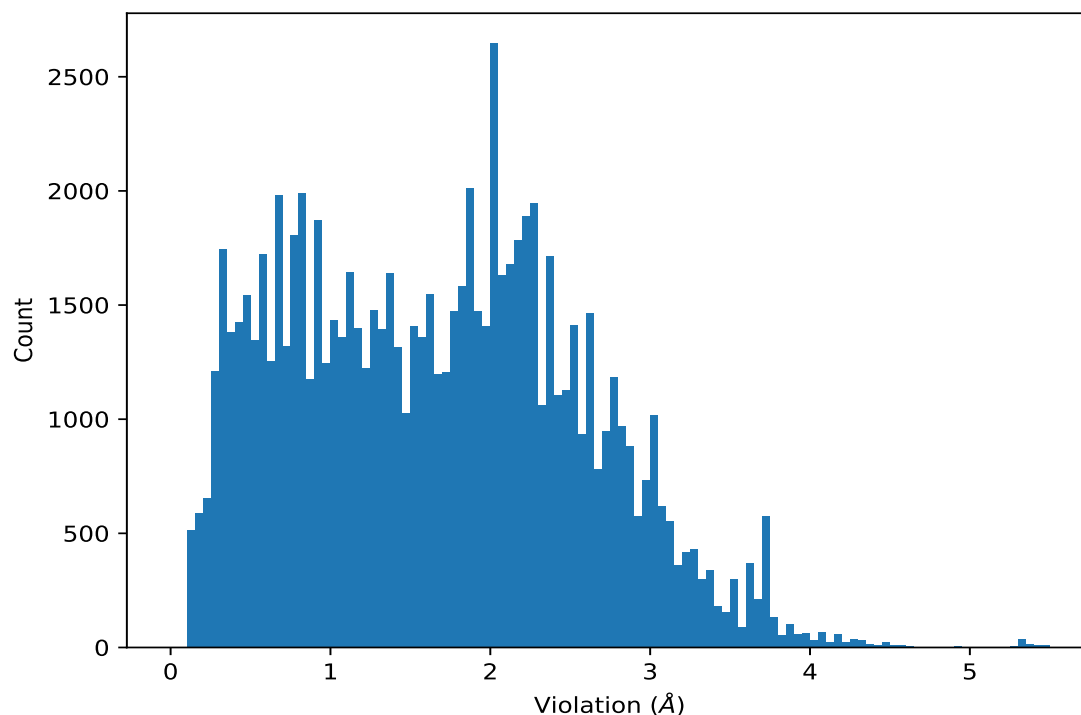
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,112)	1:100:A:PHE:H	1:104:A:LYS:HD2	20	5.43	0.04	5.44
(3,852)	1:87:A:PHE:HB2	1:105:A:TYR:HE1	20	5.35	0.01	5.35
(3,852)	1:87:A:PHE:HB2	1:105:A:TYR:HE2	20	5.35	0.01	5.35
(3,630)	1:27:A:ILE:HG13	1:60:A:PRO:HD2	20	5.33	0.07	5.32
(3,442)	1:45:A:THR:HA	1:52:A:LYS:HB2	20	5.03	0.25	5.12
(3,180)	1:75:A:ALA:H	1:76:A:GLU:HB3	20	4.54	0.04	4.54
(3,334)	1:23:A:LEU:HB3	1:84:A:CYS:HA	20	4.48	0.02	4.48
(3,406)	1:71:A:LYS:HB3	1:74:A:ASP:HA	20	4.46	0.12	4.42
(3,970)	1:55:A:LEU:HB2	1:65:A:VAL:HB	20	4.35	0.02	4.34
(3,1155)	1:22:A:LEU:HB2	1:23:A:LEU:HD11	20	4.31	0.07	4.28
(3,1155)	1:22:A:LEU:HB2	1:23:A:LEU:HD12	20	4.31	0.07	4.28
(3,1155)	1:22:A:LEU:HB2	1:23:A:LEU:HD13	20	4.31	0.07	4.28
(3,1228)	1:39:A:LYS:H	1:58:A:LYS:HG2	20	4.29	0.55	4.01

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)
(3,112)	1:100:A:PHE:H	1:104:A:LYS:HD2	6	5.49
(3,630)	1:27:A:ILE:HG13	1:60:A:PRO:HD2	7	5.47
(3,112)	1:100:A:PHE:H	1:104:A:LYS:HD2	5	5.45
(3,112)	1:100:A:PHE:H	1:104:A:LYS:HD2	7	5.45
(3,112)	1:100:A:PHE:H	1:104:A:LYS:HD2	9	5.45
(3,112)	1:100:A:PHE:H	1:104:A:LYS:HD2	10	5.45
(3,112)	1:100:A:PHE:H	1:104:A:LYS:HD2	11	5.45
(3,112)	1:100:A:PHE:H	1:104:A:LYS:HD2	16	5.45
(3,112)	1:100:A:PHE:H	1:104:A:LYS:HD2	18	5.45
(3,630)	1:27:A:ILE:HG13	1:60:A:PRO:HD2	17	5.44

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

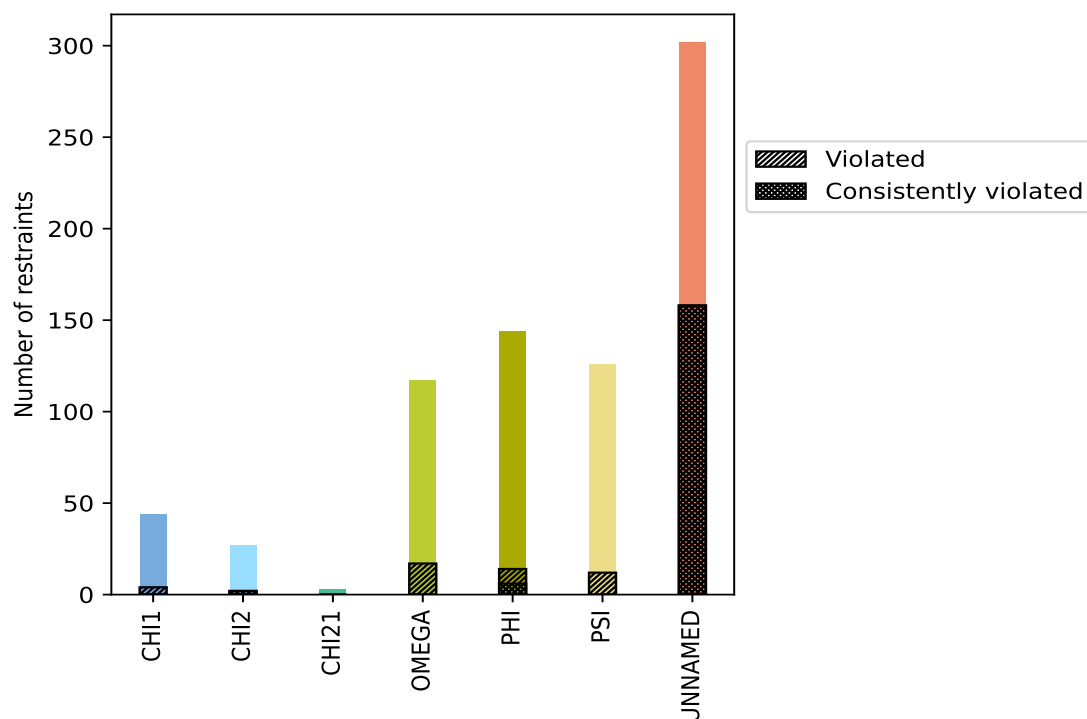
10.1 Summary of dihedral-angle violations [i](#)

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
CHI1	44	5.8	4	9.1	0.5	0	0.0	0.0
CHI2	27	3.5	2	7.4	0.3	2	7.4	0.3
CHI21	3	0.4	0	0.0	0.0	0	0.0	0.0
OMEGA	117	15.3	17	14.5	2.2	0	0.0	0.0
PHI	144	18.9	14	9.7	1.8	6	4.2	0.8
PSI	126	16.5	12	9.5	1.6	0	0.0	0.0
UNNAMED	302	39.6	158	52.3	20.7	158	52.3	20.7
Total	763	100.0	207	27.1	27.1	166	21.8	21.8

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](#)



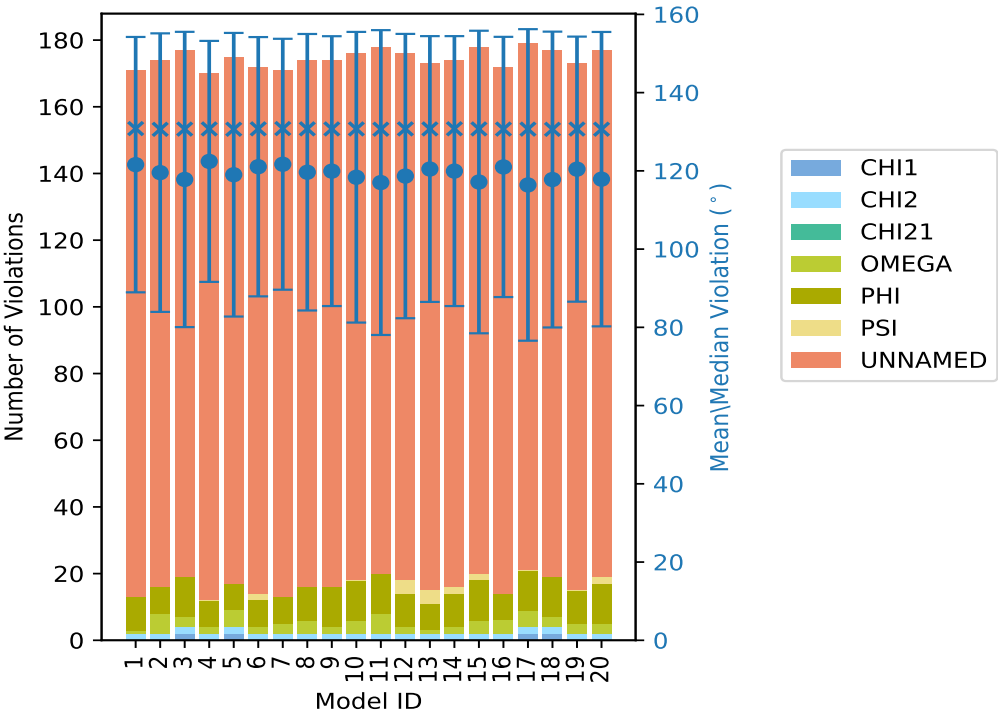
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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							Total	Mean (°)	Max (°)	SD (°)	Median (°)
	CHI1	CHI2	CHI21	OMEGA	PHI	PSI	UNNAMED					
1	0	2	0	1	10	0	158	171	121.59	133.55	32.64	130.81
2	0	2	0	6	8	0	158	174	119.55	133.65	35.6	130.62
3	2	2	0	3	12	0	158	177	117.8	133.57	37.74	130.68
4	0	2	0	2	8	0	158	170	122.42	134.11	30.8	130.72
5	2	2	0	5	8	0	158	175	119.01	133.89	36.25	130.64
6	0	2	0	2	8	2	158	172	121.06	133.55	33.14	130.74
7	0	2	0	3	8	0	158	171	121.69	134.01	32.07	130.81
8	0	2	0	4	10	0	158	174	119.65	133.66	35.34	130.74
9	0	2	0	2	12	0	158	174	119.93	133.56	34.49	130.72
10	0	2	0	4	12	0	158	176	118.37	133.63	37.15	130.72
11	0	2	0	6	12	0	158	178	117.01	133.88	38.96	130.65
12	0	2	0	2	10	4	158	176	118.67	134.01	36.34	130.73
13	0	2	0	1	8	4	158	173	120.47	133.53	33.97	130.72
14	0	2	0	2	10	2	158	174	119.94	133.64	34.5	130.76
15	0	2	0	4	12	2	158	178	117.15	133.84	38.67	130.72
16	0	2	0	4	8	0	158	172	121.0	133.9	33.26	130.68
17	2	2	0	5	12	0	158	179	116.4	133.79	39.82	130.67
18	2	2	0	3	12	0	158	177	117.78	133.8	37.81	130.62
19	0	2	0	3	10	0	158	173	120.44	133.97	33.88	130.69
20	0	2	0	3	12	2	158	177	117.88	133.77	37.63	130.65

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

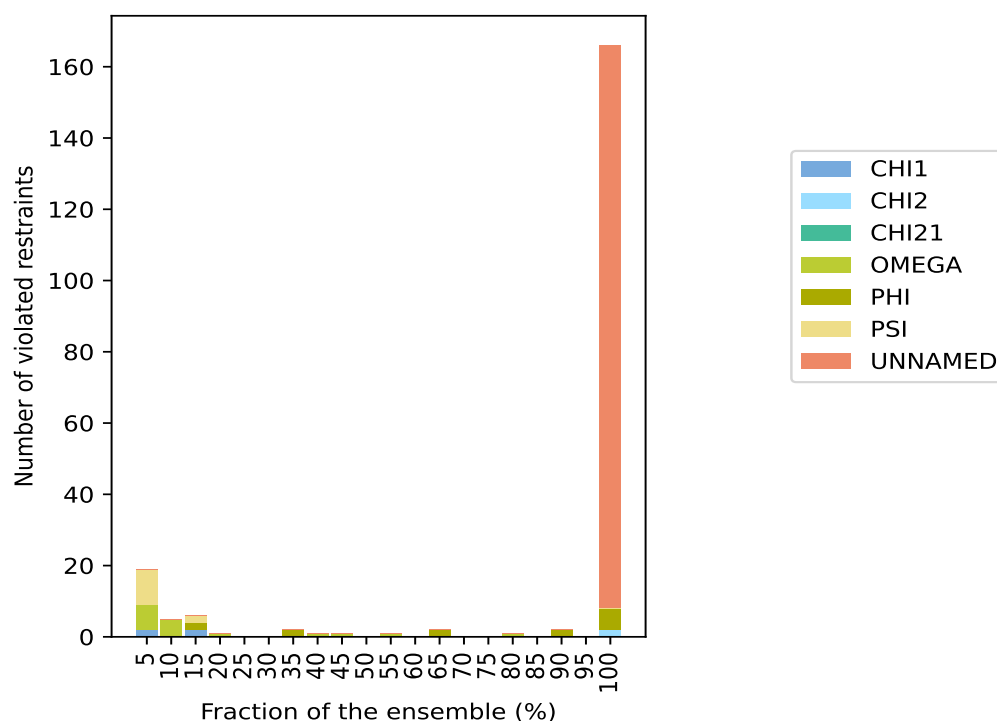
10.3 Dihedral-angle violation statistics for the ensemble

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	
CHI1	CHI2	CHI21	OMEGA	PHI	PSI	UNNAMED	Total	Count ¹	%
2	0	0	7	0	10	0	19	1	5.0
0	0	0	5	0	0	0	5	2	10.0
2	0	0	0	2	2	0	6	3	15.0
0	0	0	1	0	0	0	1	4	20.0
0	0	0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	0	0	6	30.0
0	0	0	0	2	0	0	2	7	35.0
0	0	0	1	0	0	0	1	8	40.0
0	0	0	1	0	0	0	1	9	45.0
0	0	0	0	0	0	0	0	10	50.0
0	0	0	1	0	0	0	1	11	55.0
0	0	0	0	0	0	0	0	12	60.0
0	0	0	0	2	0	0	2	13	65.0
0	0	0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	0	0	15	75.0
0	0	0	1	0	0	0	1	16	80.0
0	0	0	0	0	0	0	0	17	85.0
0	0	0	0	2	0	0	2	18	90.0
0	0	0	0	0	0	0	0	19	95.0
0	2	0	0	6	0	158	166	20	100.0

¹ Number of models with violations

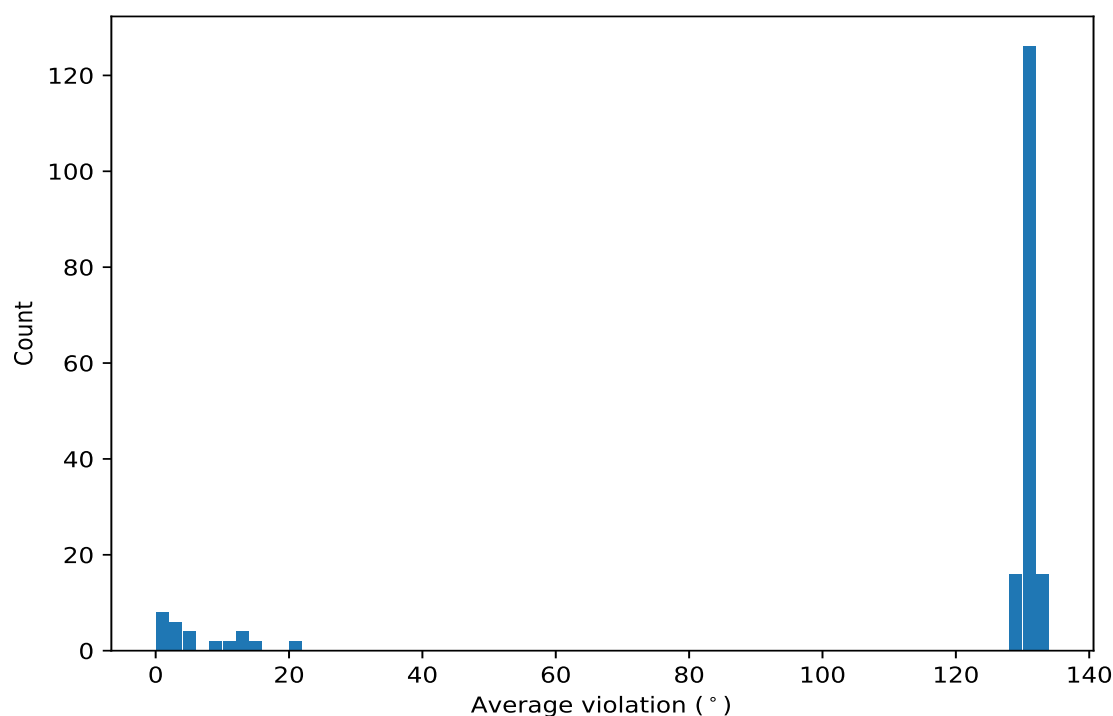
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

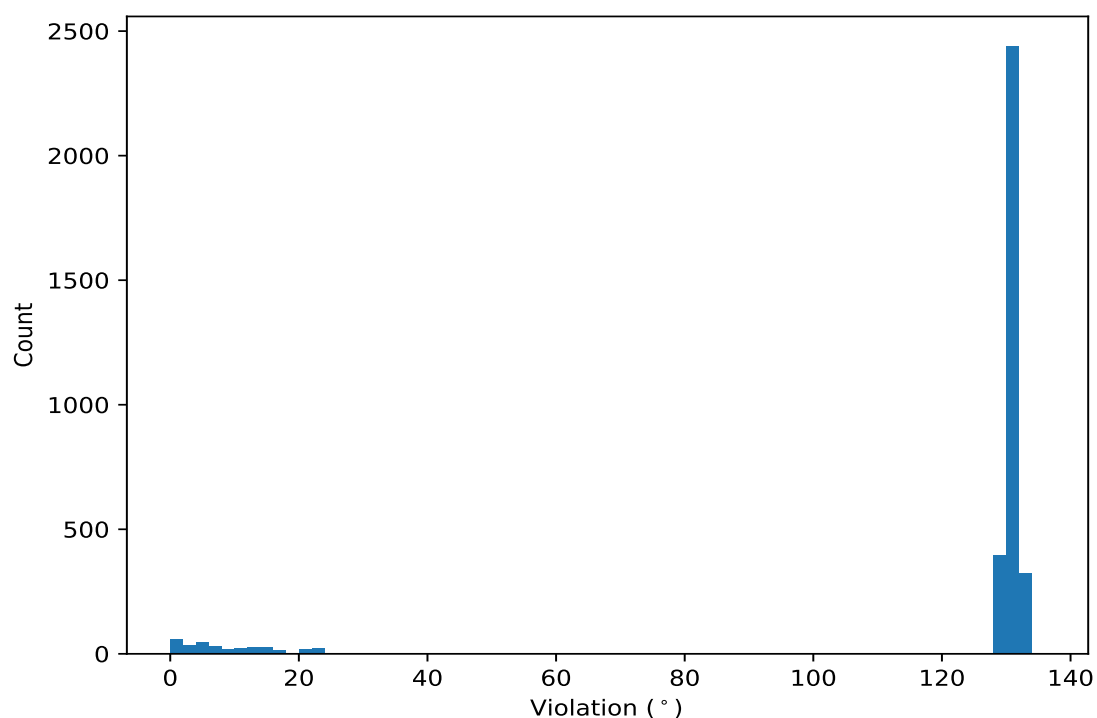
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Med
(1,37)	1:17:A:PRO:CA	1:17:A:PRO:CG	1:17:A:PRO:HB3	1:17:A:PRO:HB2	20	133.64	0.09	133.
(1,243)	1:95:A:PRO:CA	1:95:A:PRO:CG	1:95:A:PRO:HB3	1:95:A:PRO:HB2	20	133.42	0.05	133.
(1,116)	1:48:A:PRO:CA	1:48:A:PRO:CG	1:48:A:PRO:HB3	1:48:A:PRO:HB2	20	133.19	0.54	133.
(1,294)	1:116:A:PRO:CA	1:116:A:PRO:CG	1:116:A:PRO:HB3	1:116:A:PRO:HB2	20	133.16	0.58	133.
(1,46)	1:19:A:PRO:CG	1:19:A:PRO:N	1:19:A:PRO:HD3	1:19:A:PRO:HD2	20	133.05	0.28	133.
(1,44)	1:19:A:PRO:CA	1:19:A:PRO:CG	1:19:A:PRO:HB3	1:19:A:PRO:HB2	20	132.77	0.07	132.
(1,160)	1:60:A:PRO:CB	1:60:A:PRO:CD	1:60:A:PRO:HG3	1:60:A:PRO:HG2	20	132.72	0.09	132.
(1,63)	1:25:A:SER:CA	1:25:A:SER:OG	1:25:A:SER:HB3	1:25:A:SER:HB2	20	132.63	0.23	132.
(1,161)	1:60:A:PRO:CG	1:60:A:PRO:N	1:60:A:PRO:HD3	1:60:A:PRO:HD2	20	132.61	0.03	132.
(1,117)	1:48:A:PRO:CB	1:48:A:PRO:CD	1:48:A:PRO:HG3	1:48:A:PRO:HG2	20	132.53	0.51	132.

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 (°)
(1,116)	1:48:A:PRO:CA	1:48:A:PRO:CG	1:48:A:PRO:HB3	1:48:A:PRO:HB2	4	134.11
(1,294)	1:116:A:PRO:CA	1:116:A:PRO:CG	1:116:A:PRO:HB3	1:116:A:PRO:HB2	12	134.01
(1,116)	1:48:A:PRO:CA	1:48:A:PRO:CG	1:48:A:PRO:HB3	1:48:A:PRO:HB2	7	134.01
(1,294)	1:116:A:PRO:CA	1:116:A:PRO:CG	1:116:A:PRO:HB3	1:116:A:PRO:HB2	19	133.97
(1,116)	1:48:A:PRO:CA	1:48:A:PRO:CG	1:48:A:PRO:HB3	1:48:A:PRO:HB2	16	133.9
(1,116)	1:48:A:PRO:CA	1:48:A:PRO:CG	1:48:A:PRO:HB3	1:48:A:PRO:HB2	5	133.89
(1,294)	1:116:A:PRO:CA	1:116:A:PRO:CG	1:116:A:PRO:HB3	1:116:A:PRO:HB2	11	133.88
(1,37)	1:17:A:PRO:CA	1:17:A:PRO:CG	1:17:A:PRO:HB3	1:17:A:PRO:HB2	15	133.84
(1,46)	1:19:A:PRO:CG	1:19:A:PRO:N	1:19:A:PRO:HD3	1:19:A:PRO:HD2	18	133.8
(1,37)	1:17:A:PRO:CA	1:17:A:PRO:CG	1:17:A:PRO:HB3	1:17:A:PRO:HB2	17	133.79