



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 9DYU / pdb_00009dyu
BMRB ID : 52640
Title : Assembly and functional mechanisms of the Hsp70-Hsp40 chaperone machinery
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Deposited on : 2024-10-14

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

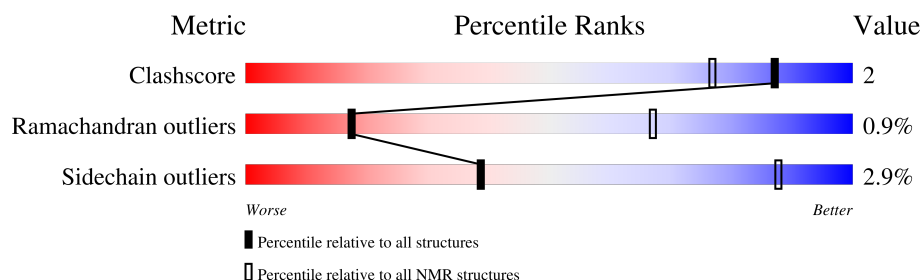
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	134	 84% .. 12% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:371-A:372, A:387-A:500 (116)	0.71	3

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1930 atoms, of which 967 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chaperone protein DnaK.

Mol	Chain	Residues	Atoms						Trace
1	A	132	Total	C	H	N	O	S	0
			1930	595	967	173	190	5	

There are 21 discrepancies between the modelled and reference sequences:

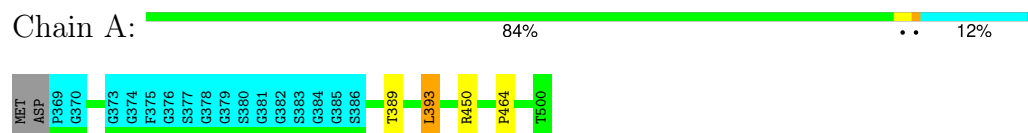
Chain	Residue	Modelled	Actual	Comment	Reference
A	367	MET	-	expression tag	UNP Q56235
A	368	ASP	-	expression tag	UNP Q56235
A	369	PRO	-	expression tag	UNP Q56235
A	370	GLY	-	expression tag	UNP Q56235
A	371	LEU	-	expression tag	UNP Q56235
A	372	PHE	-	expression tag	UNP Q56235
A	373	GLY	-	expression tag	UNP Q56235
A	374	GLY	-	expression tag	UNP Q56235
A	375	PHE	-	expression tag	UNP Q56235
A	376	GLY	-	expression tag	UNP Q56235
A	377	SER	-	expression tag	UNP Q56235
A	378	GLY	-	expression tag	UNP Q56235
A	379	GLY	-	expression tag	UNP Q56235
A	380	SER	-	expression tag	UNP Q56235
A	381	GLY	-	expression tag	UNP Q56235
A	382	GLY	-	expression tag	UNP Q56235
A	383	SER	-	expression tag	UNP Q56235
A	384	GLY	-	expression tag	UNP Q56235
A	385	GLY	-	expression tag	UNP Q56235
A	386	SER	-	expression tag	UNP Q56235
A	387	GLY	-	expression tag	UNP Q56235

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.

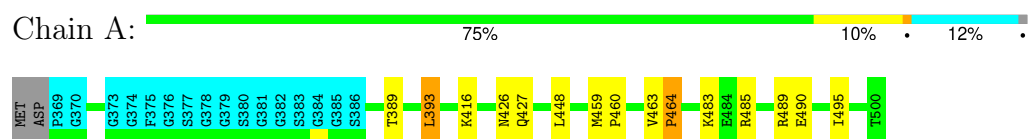
- Molecule 1: Chaperone protein DnaK



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

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

- Molecule 1: Chaperone protein DnaK



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	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1407
Number of shifts mapped to atoms	1380
Number of unparsed shifts	0
Number of shifts with mapping errors	27
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	1.23±0.04	1±1/895 (0.1± 0.1%)	0.87±0.01	0±0/1215 (0.0± 0.0%)
All	All	1.23	14/17900 (0.1%)	0.87	1/24300 (0.0%)

5 of 6 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	457	PRO	CA-C	8.31	1.56	1.51	14	1
1	A	412	ILE	CA-CB	5.87	1.60	1.55	12	3
1	A	406	ILE	CA-CB	5.81	1.58	1.54	15	3
1	A	466	ILE	CA-CB	5.69	1.60	1.53	13	3
1	A	456	ILE	C-N	5.44	1.38	1.33	14	2

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	497	ASN	CA-CB-CG	5.12	117.72	112.60	19	1

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	881	901	898	3±1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	17620	18020	17960	69

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

5 of 38 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:405:LEU:HD11	1:A:418:GLU:HB2	0.61	1.72	6	1
1:A:402:MET:SD	1:A:404:VAL:HG23	0.59	2.37	17	1
1:A:389:THR:HG21	1:A:393:LEU:HD21	0.57	1.75	18	14
1:A:421:THR:HB	1:A:465:GLN:HG3	0.57	1.76	5	2
1:A:448:LEU:HB3	1:A:495:ILE:HG21	0.56	1.77	19	8

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	115/134 (86%)	109±2 (95±2%)	5±2 (4±2%)	1±1 (1±0%)	17	67
All	All	2300/2680 (86%)	2187 (95%)	93 (4%)	20 (1%)	17	67

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	464	PRO	17
1	A	422	THR	1
1	A	423	ALA	1
1	A	428	THR	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	99/107 (93%)	96±2 (97±2%)	3±2 (3±2%)	39	88
All	All	1980/2140 (93%)	1923 (97%)	57 (3%)	39	88

5 of 19 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	393	LEU	15
1	A	450	ARG	10
1	A	371	LEU	6
1	A	416	LYS	5
1	A	412	ILE	2

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 85% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *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	1407
Number of shifts mapped to atoms	1380
Number of unparsed shifts	0
Number of shifts with mapping errors	27
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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 27) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	.	PRO	HA	4.455	0.00	.
1	A	.	PRO	HB2	2.324	0.01	.
1	A	.	PRO	HB3	2.025	0.00	.
1	A	.	PRO	HD2	3.619	0.01	.
1	A	.	PRO	HD3	3.542	0.01	.
1	A	.	PRO	HG2	2.082	0.00	.
1	A	.	PRO	HG3	1.887	0.01	.
1	A	.	PRO	C	176.899	0.00	.
1	A	.	PRO	CA	64.374	0.05	.
1	A	.	PRO	CB	32.364	0.07	.
1	A	.	PRO	CD	49.738	0.02	.
1	A	.	PRO	CG	27.098	0.01	.
1	A	367	MET	H	8.601	0.00	.
1	A	367	MET	HA	4.763	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	367	MET	HB2	2.38	0.01	.
1	A	367	MET	HB3	2.327	0.00	.
1	A	367	MET	C	175.614	0.00	.
1	A	367	MET	CA	54.293	0.08	.
1	A	367	MET	CB	33.183	0.07	.
1	A	367	MET	N	118.253	0.03	.
1	A	368	ASP	H	7.401	0.00	.
1	A	368	ASP	HA	4.773	0.01	.
1	A	368	ASP	HB2	2.529	0.01	2
1	A	368	ASP	HB3	2.529	0.01	2
1	A	368	ASP	CA	54.152	0.04	.
1	A	368	ASP	CB	39.967	0.06	.
1	A	368	ASP	N	121.809	0.05	.

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	122	-0.19 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	109	-0.13 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}'$	111	0.22 ± 0.12	None needed (< 0.5 ppm)
^{15}N	112	-0.34 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 1331 atoms were assigned a chemical shift out of a possible 1559. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	543/574 (95%)	223/234 (95%)	216/232 (93%)	104/108 (96%)
Sidechain	769/921 (83%)	524/602 (87%)	239/284 (84%)	6/35 (17%)
Aromatic	19/64 (30%)	19/32 (59%)	0/26 (0%)	0/6 (0%)
Overall	1331/1559 (85%)	766/868 (88%)	455/542 (84%)	110/149 (74%)

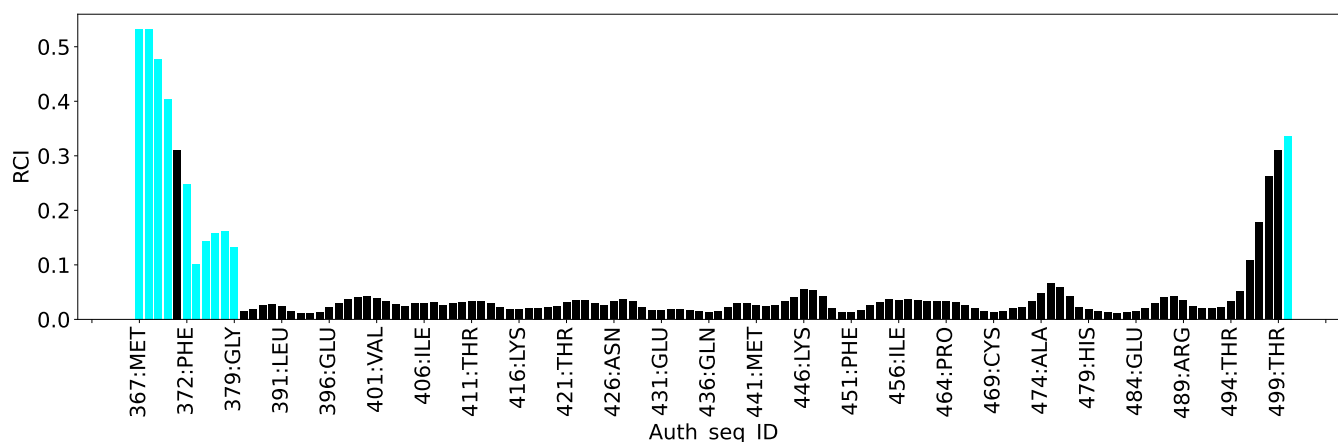
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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	1690
Intra-residue ($ i-j =0$)	327
Sequential ($ i-j =1$)	501
Medium range ($ i-j >1$ and $ i-j <5$)	124
Long range ($ i-j \geq 5$)	654
Inter-chain	0
Hydrogen bond restraints	84
Disulfide bond restraints	0
Total dihedral-angle restraints	182
Number of unmapped restraints	0
Number of restraints per residue	14.0
Number of long range restraints per residue ¹	5.5

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)	17.2	0.2
0.2-0.5 (Medium)	38.2	0.5
>0.5 (Large)	45.6	2.81

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)	41.3	9.78
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

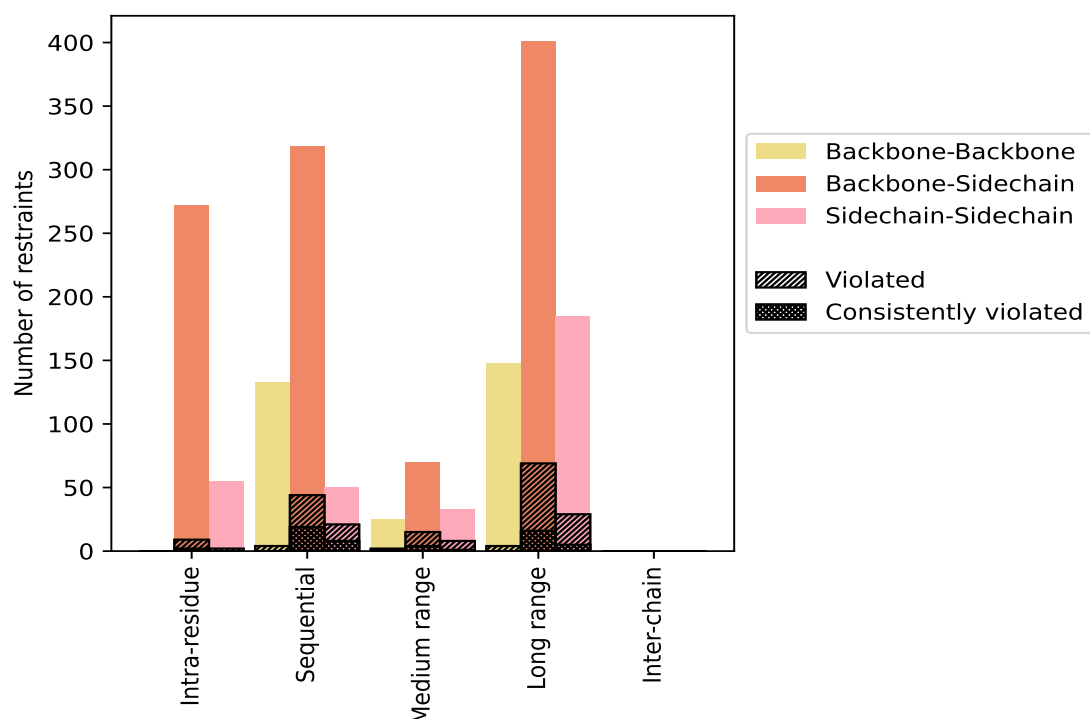
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	327	19.3	11	3.4	0.7	2	0.6	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	272	16.1	9	3.3	0.5	2	0.7	0.1
Sidechain-Sidechain	55	3.3	2	3.6	0.1	0	0.0	0.0
Sequential ($i-j =1$)	501	29.6	69	13.8	4.1	27	5.4	1.6
Backbone-Backbone	133	7.9	4	3.0	0.2	0	0.0	0.0
Backbone-Sidechain	318	18.8	44	13.8	2.6	19	6.0	1.1
Sidechain-Sidechain	50	3.0	21	42.0	1.2	8	16.0	0.5
Medium range ($i-j >1$ & $i-j <5$)	124	7.3	25	20.2	1.5	6	4.8	0.4
Backbone-Backbone	25	1.5	2	8.0	0.1	1	4.0	0.1
Backbone-Sidechain	66	3.9	15	22.7	0.9	4	6.1	0.2
Sidechain-Sidechain	33	2.0	8	24.2	0.5	1	3.0	0.1
Long range ($i-j \geq 5$)	654	38.7	99	15.1	5.9	21	3.2	1.2
Backbone-Backbone	148	8.8	4	2.7	0.2	0	0.0	0.0
Backbone-Sidechain	321	19.0	66	20.6	3.9	16	5.0	0.9
Sidechain-Sidechain	185	10.9	29	15.7	1.7	5	2.7	0.3
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	84	5.0	3	3.6	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1690	100.0	207	12.2	12.2	56	3.3	3.3
Backbone-Backbone	306	18.1	10	3.3	0.6	1	0.3	0.1
Backbone-Sidechain	1061	62.8	137	12.9	8.1	41	3.9	2.4
Sidechain-Sidechain	323	19.1	60	18.6	3.6	14	4.3	0.8

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	6	38	13	41	0	98	0.56	1.65	0.38	0.45
2	6	39	13	43	0	101	0.57	1.59	0.37	0.49
3	6	40	11	44	0	101	0.53	1.79	0.38	0.46
4	5	42	14	41	0	102	0.58	1.57	0.36	0.49
5	5	44	14	47	0	110	0.53	1.94	0.36	0.46
6	6	44	12	44	0	106	0.56	2.09	0.4	0.46
7	5	40	14	45	0	104	0.57	1.5	0.35	0.5
8	5	43	14	45	0	107	0.52	1.56	0.35	0.42
9	6	42	13	44	0	105	0.56	1.65	0.37	0.44
10	4	44	12	43	0	103	0.51	1.52	0.35	0.42

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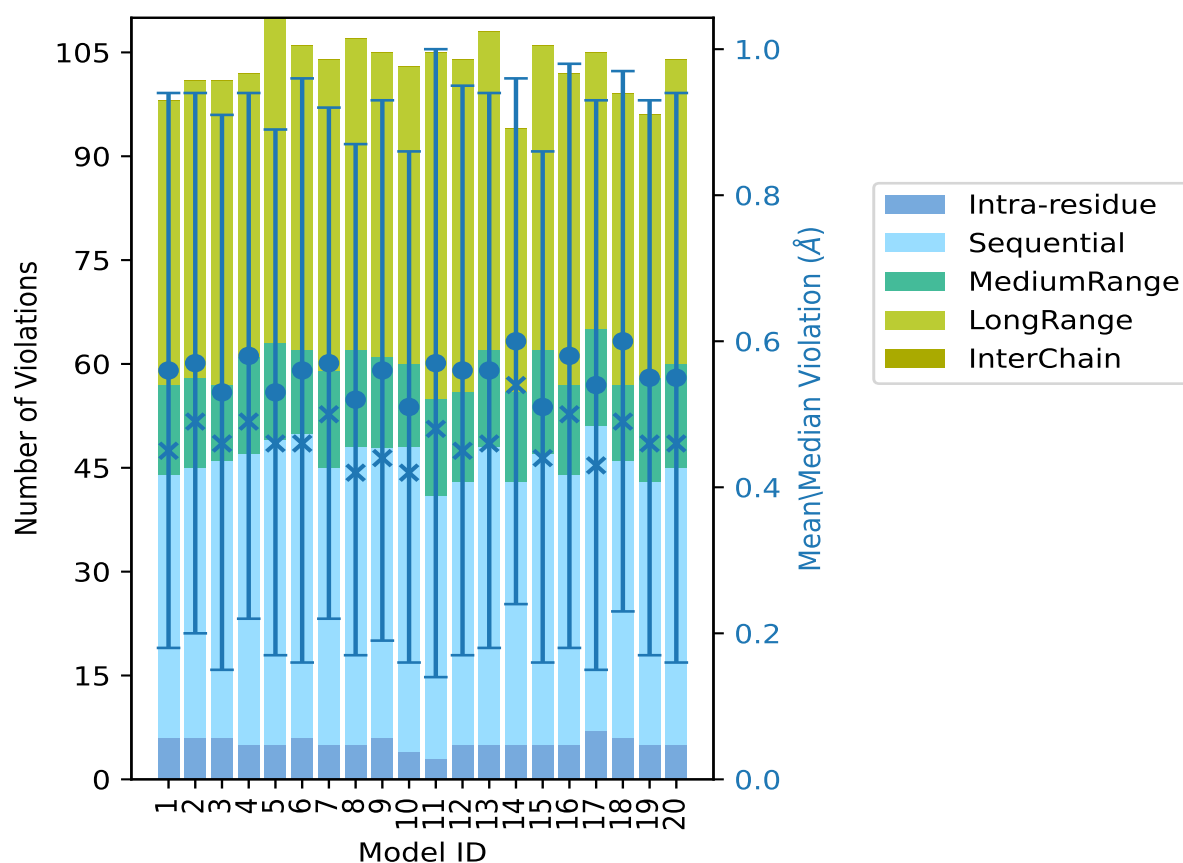
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	38	14	50	0	105	0.57	2.81	0.43	0.48
12	5	38	13	48	0	104	0.56	1.61	0.39	0.45
13	5	43	14	46	0	108	0.56	1.88	0.38	0.46
14	5	38	13	38	0	94	0.6	2.06	0.36	0.54
15	5	42	15	44	0	106	0.51	1.61	0.35	0.44
16	5	39	13	45	0	102	0.58	2.14	0.4	0.5
17	7	44	14	40	0	105	0.54	1.81	0.39	0.43
18	6	40	11	42	0	99	0.6	1.6	0.37	0.49
19	5	38	15	38	0	96	0.55	1.83	0.38	0.46
20	5	40	15	44	0	104	0.55	1.81	0.39	0.46

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

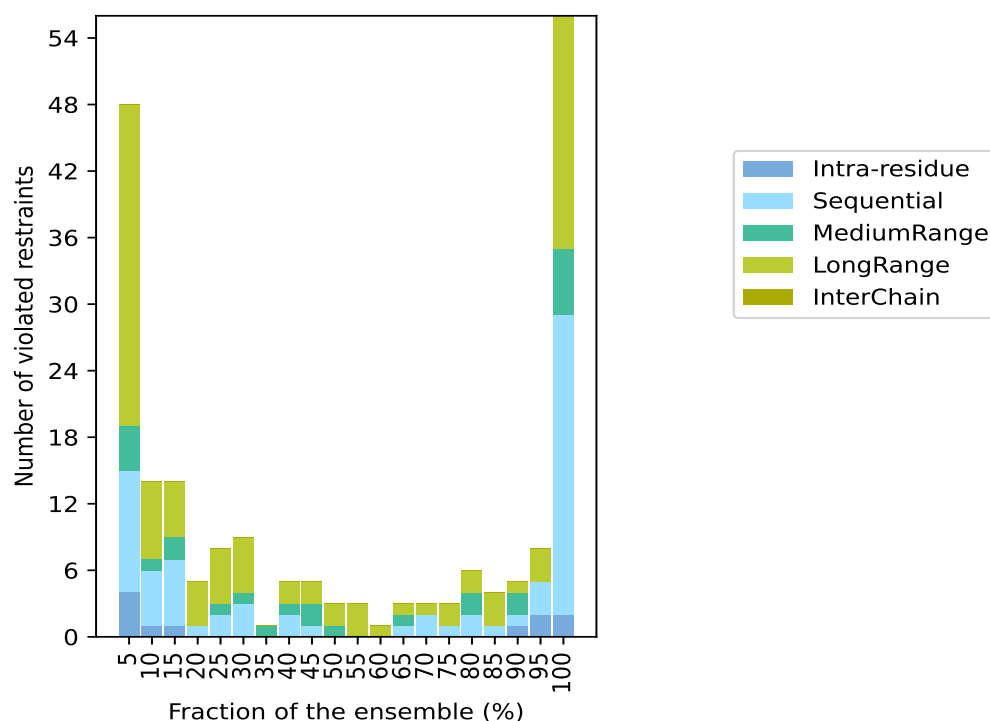
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1402(IR:316, SQ:432, MR:99, LR:555, IC:0) restraints are 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	%
4	11	4	29	0	48	1	5.0
1	5	1	7	0	14	2	10.0
1	6	2	5	0	14	3	15.0
0	1	0	4	0	5	4	20.0
0	2	1	5	0	8	5	25.0
0	3	1	5	0	9	6	30.0
0	0	1	0	0	1	7	35.0
0	2	1	2	0	5	8	40.0
0	1	2	2	0	5	9	45.0
0	0	1	2	0	3	10	50.0
0	0	0	3	0	3	11	55.0
0	0	0	1	0	1	12	60.0
0	1	1	1	0	3	13	65.0
0	2	0	1	0	3	14	70.0
0	1	0	2	0	3	15	75.0
0	2	2	2	0	6	16	80.0
0	1	0	3	0	4	17	85.0
1	1	2	1	0	5	18	90.0
2	3	0	3	0	8	19	95.0
2	27	6	21	0	56	20	100.0

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

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

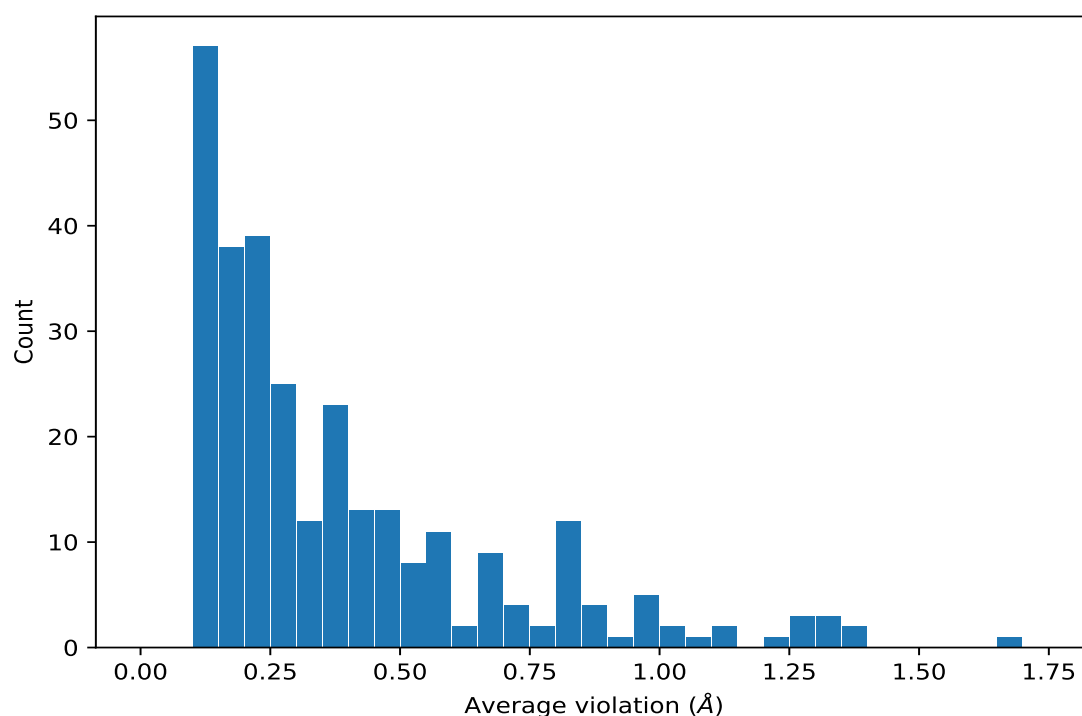
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

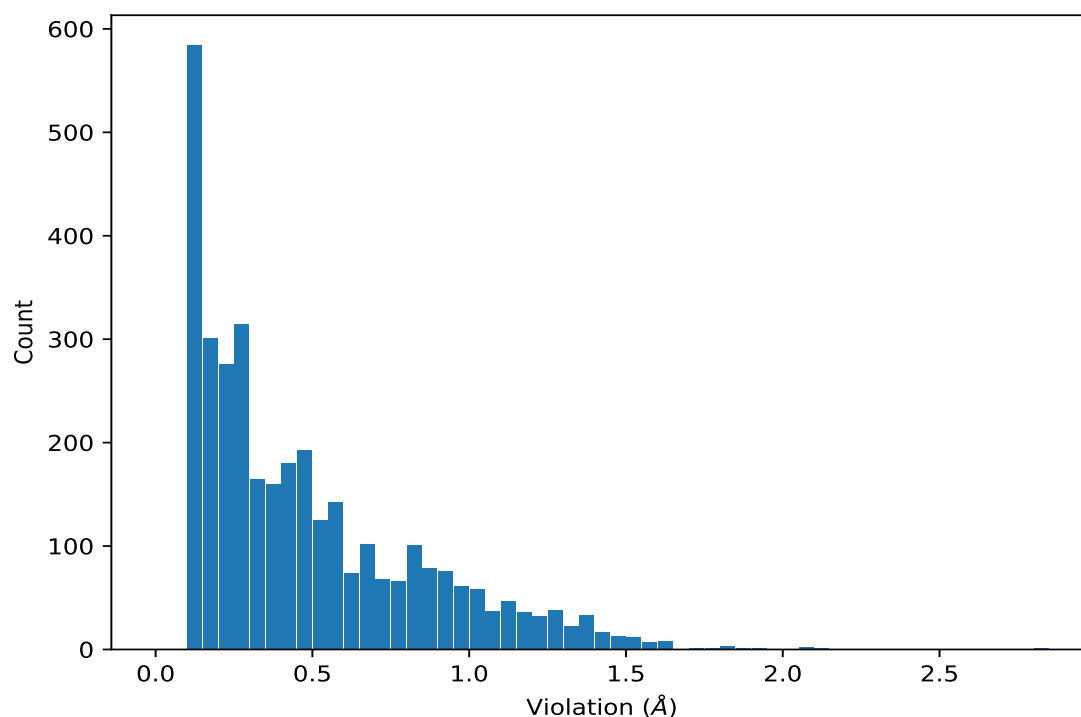
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,480)	1:467:A:GLU:HB2	1:483:A:LYS:HB2	20	1.69	0.42	1.65
(2,1316)	1:488:A:GLY:H	1:489:A:ARG:HB3	20	1.4	0.33	1.48
(2,408)	1:408:A:ARG:HG2	1:409:A:ASN:HB3	20	1.36	0.16	1.36
(2,397)	1:407:A:PRO:HB3	1:409:A:ASN:H	20	1.32	0.06	1.34
(2,1537)	1:471:A:ASP:H	1:472:A:ILE:HG13	20	1.3	0.11	1.28
(2,23)	1:438:A:GLU:HG2	1:439:A:ARG:HD2	20	1.3	0.24	1.23
(2,64)	1:390:A:PRO:HB3	1:391:A:LEU:HD11	20	1.27	0.1	1.25
(2,64)	1:390:A:PRO:HB3	1:391:A:LEU:HD12	20	1.27	0.1	1.25
(2,64)	1:390:A:PRO:HB3	1:391:A:LEU:HD13	20	1.27	0.1	1.25
(2,407)	1:408:A:ARG:HD3	1:409:A:ASN:HA	20	1.23	0.1	1.25
(2,424)	1:411:A:THR:HA	1:412:A:ILE:HG12	20	1.14	0.09	1.12
(2,405)	1:390:A:PRO:HA	1:408:A:ARG:HG2	20	1.05	0.15	1.05

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)
(2,480)	1:467:A:GLU:HB2	1:483:A:LYS:HB2	11	2.81
(2,480)	1:467:A:GLU:HB2	1:483:A:LYS:HB2	16	2.14
(2,480)	1:467:A:GLU:HB2	1:483:A:LYS:HB2	6	2.09
(2,480)	1:467:A:GLU:HB2	1:483:A:LYS:HB2	14	2.06
(2,480)	1:467:A:GLU:HB2	1:483:A:LYS:HB2	5	1.94
(2,480)	1:467:A:GLU:HB2	1:483:A:LYS:HB2	13	1.88
(2,298)	1:372:A:PHE:HB3	1:422:A:THR:HB	19	1.83
(2,480)	1:467:A:GLU:HB2	1:483:A:LYS:HB2	17	1.81
(2,480)	1:467:A:GLU:HB2	1:483:A:LYS:HB2	20	1.81
(2,480)	1:467:A:GLU:HB2	1:483:A:LYS:HB2	3	1.79

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

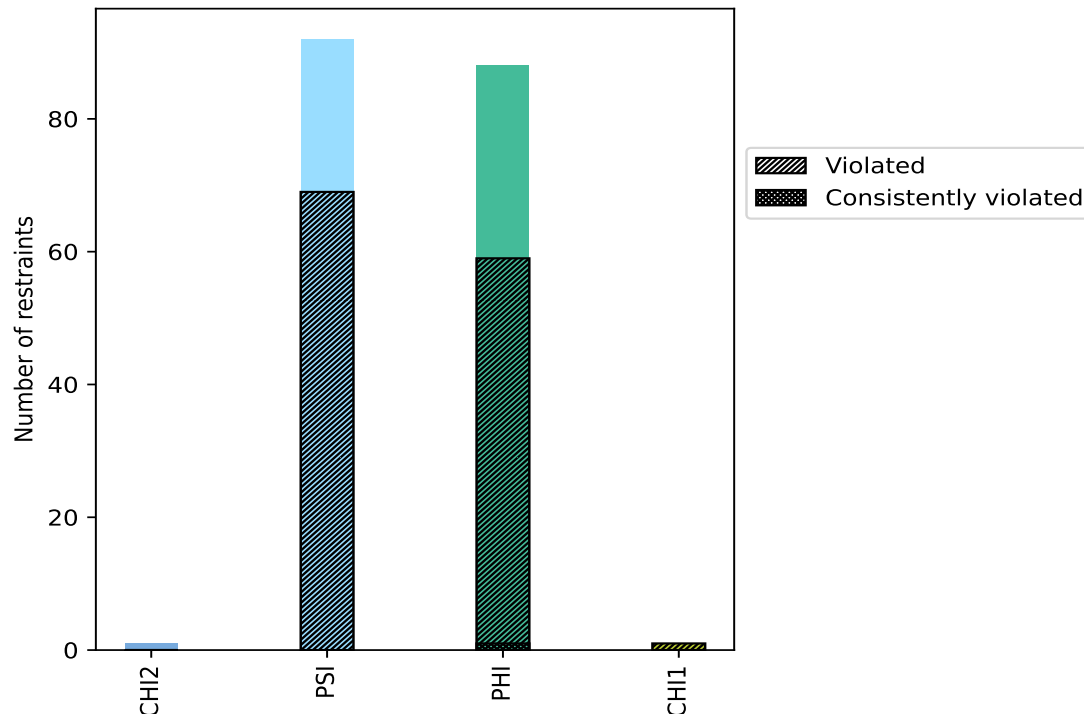
10.1 Summary of dihedral-angle violations [i](#)

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
CHI2	1	0.5	0	0.0	0.0	0	0.0	0.0
PSI	92	50.5	69	75.0	37.9	0	0.0	0.0
PHI	88	48.4	59	67.0	32.4	1	1.1	0.5
CHI1	1	0.5	1	100.0	0.5	0	0.0	0.0
Total	182	100.0	129	70.9	70.9	1	0.5	0.5

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](#)



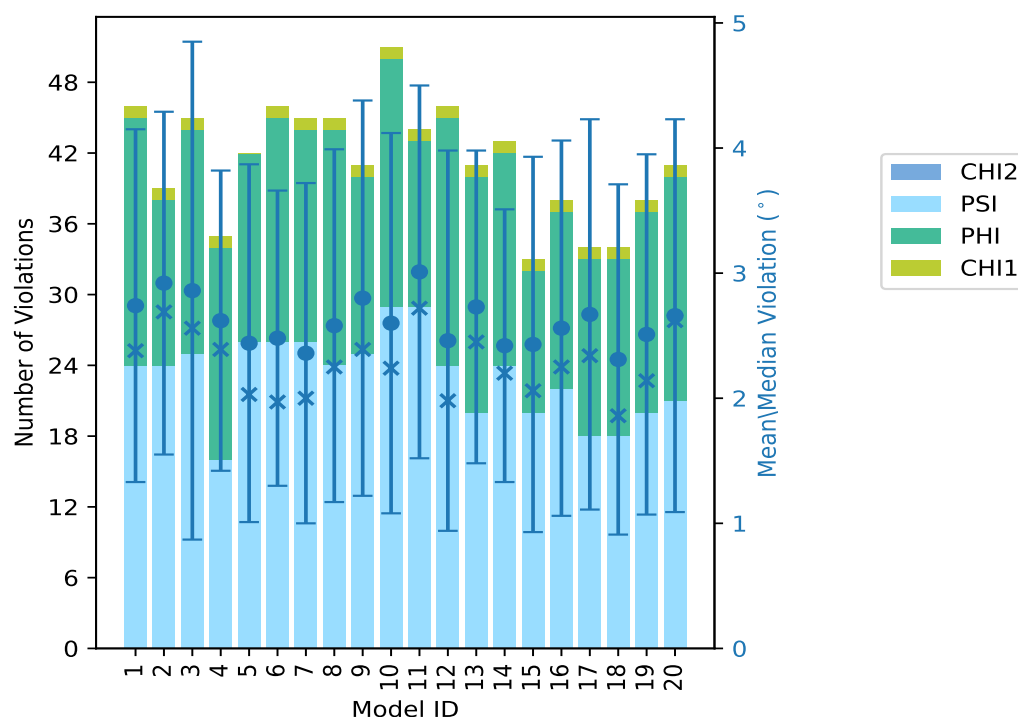
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	CHI2	PSI	PHI	CHI1	Total				
1	0	24	21	1	46	2.74	8.23	1.41	2.38
2	0	24	14	1	39	2.92	7.74	1.37	2.69
3	0	25	19	1	45	2.86	9.06	1.99	2.56
4	0	16	18	1	35	2.62	7.01	1.2	2.39
5	0	26	16	0	42	2.44	9.26	1.43	2.03
6	0	26	19	1	46	2.48	6.08	1.18	1.97
7	0	26	18	1	45	2.36	9.27	1.36	2.0
8	0	24	20	1	45	2.58	8.54	1.41	2.25
9	0	25	15	1	41	2.8	9.18	1.58	2.39
10	0	29	21	1	51	2.6	9.78	1.52	2.24
11	0	29	14	1	44	3.01	7.62	1.49	2.72
12	0	24	21	1	46	2.46	9.33	1.52	1.98
13	0	20	20	1	41	2.73	8.26	1.25	2.45
14	0	24	18	1	43	2.42	6.14	1.09	2.2
15	0	20	12	1	33	2.43	9.17	1.5	2.06
16	0	22	15	1	38	2.56	8.31	1.5	2.25
17	0	18	15	1	34	2.67	8.74	1.56	2.34
18	0	18	15	1	34	2.31	8.03	1.4	1.86
19	0	20	17	1	38	2.51	8.11	1.44	2.14
20	0	21	19	1	41	2.66	9.06	1.57	2.62

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	
CHI2	PSI	PHI	CHI1	Total	Count ¹	%
0	11	12	0	23	1	5.0
0	9	2	0	11	2	10.0
0	6	9	0	15	3	15.0
0	4	7	0	11	4	20.0
0	5	4	0	9	5	25.0
0	5	5	0	10	6	30.0
0	3	3	0	6	7	35.0
0	5	1	0	6	8	40.0
0	1	5	0	6	9	45.0
0	3	2	0	5	10	50.0
0	1	1	0	2	11	55.0

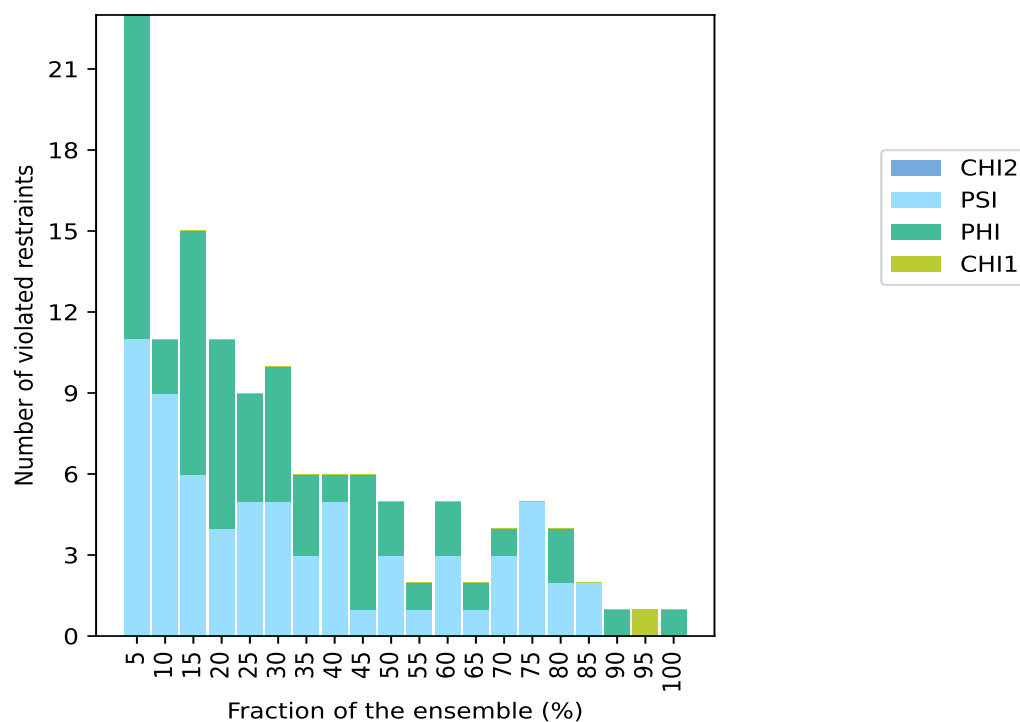
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Number of violated restraints					Fraction of the ensemble	
CHI2	PSI	PHI	CHI1	Total	Count ¹	%
0	3	2	0	5	12	60.0
0	1	1	0	2	13	65.0
0	3	1	0	4	14	70.0
0	5	0	0	5	15	75.0
0	2	2	0	4	16	80.0
0	2	0	0	2	17	85.0
0	0	1	0	1	18	90.0
0	0	0	1	1	19	95.0
0	0	1	0	1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

¹ Number of models with violations

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

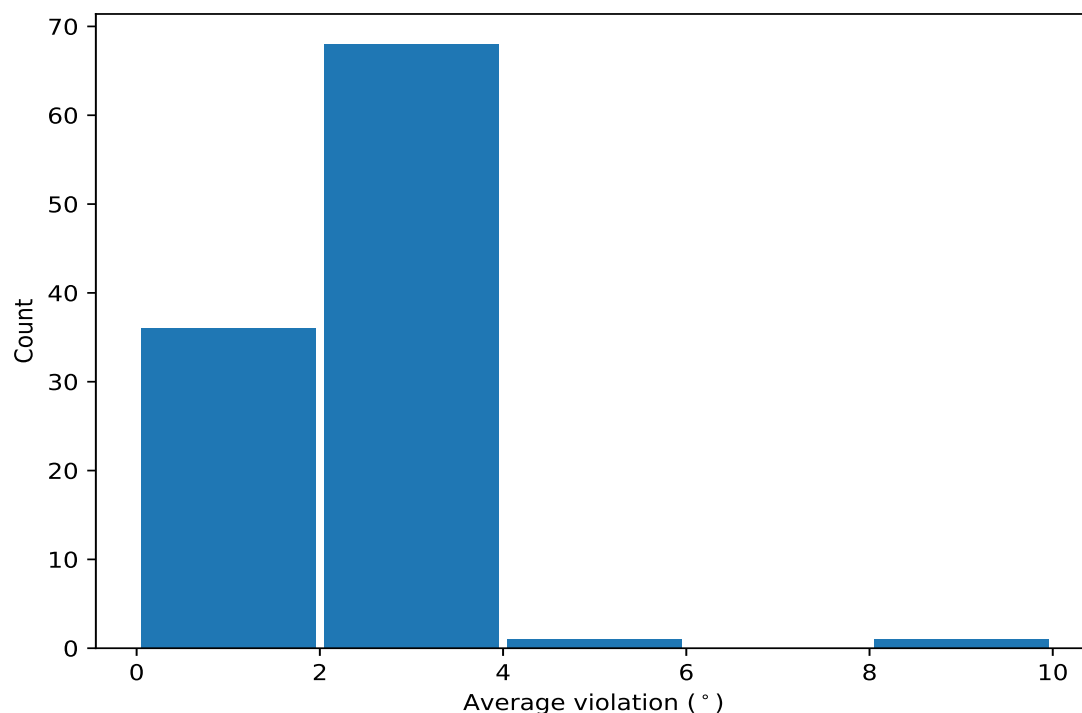


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

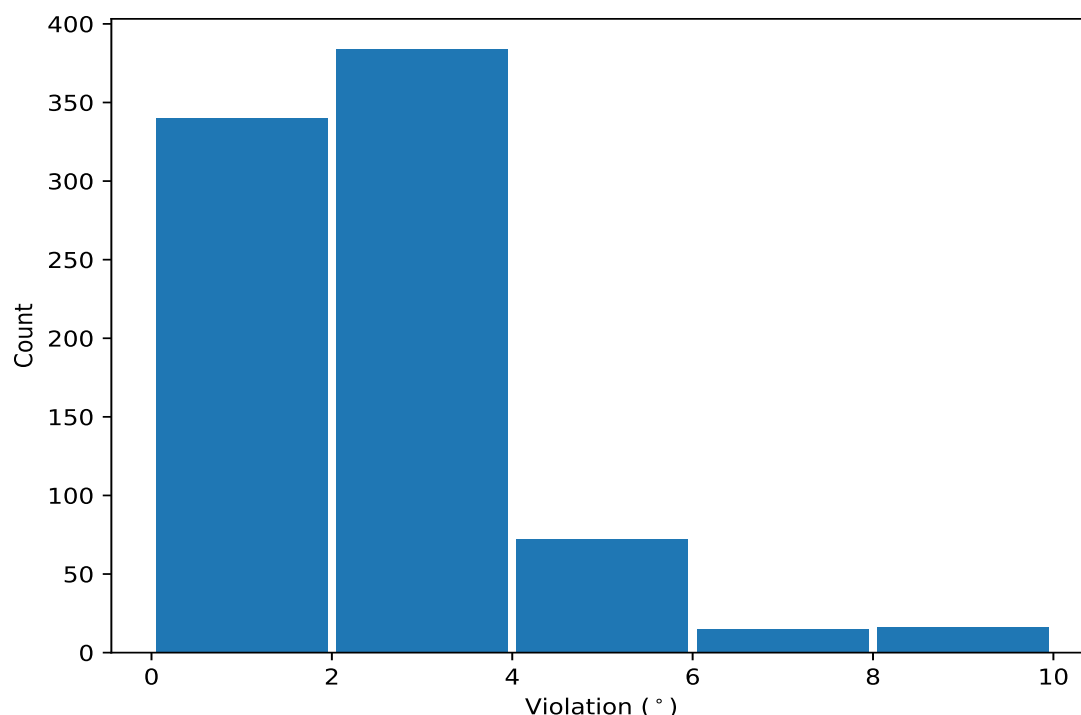
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	20	8.35	1.0	8.43
(1,181)	1:372:A:PHE:N	1:372:A:PHE:CA	1:372:A:PHE:CB	1:372:A:PHE:CG	19	2.97	1.35	2.68
(1,15)	1:394:A:GLY:C	1:395:A:VAL:N	1:395:A:VAL:CA	1:395:A:VAL:C	18	3.49	1.16	3.53
(1,71)	1:430:A:VAL:N	1:430:A:VAL:CA	1:430:A:VAL:C	1:431:A:GLU:N	17	3.93	1.82	3.16
(1,148)	1:479:A:HIS:N	1:479:A:HIS:CA	1:479:A:HIS:C	1:480:A:VAL:N	17	2.65	0.94	2.47
(1,40)	1:410:A:THR:N	1:410:A:THR:CA	1:410:A:THR:C	1:411:A:THR:N	16	2.92	0.94	3.17
(1,95)	1:445:A:ASN:C	1:446:A:LYS:N	1:446:A:LYS:CA	1:446:A:LYS:C	16	2.67	1.04	2.53
(1,30)	1:403:A:THR:N	1:403:A:THR:CA	1:403:A:THR:C	1:404:A:VAL:N	16	2.48	0.93	2.78
(1,68)	1:428:A:THR:C	1:429:A:ALA:N	1:429:A:ALA:CA	1:429:A:ALA:C	16	1.9	0.64	1.82
(1,178)	1:494:A:THR:N	1:494:A:THR:CA	1:494:A:THR:C	1:495:A:ILE:N	15	3.1	1.14	3.22

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 (°)
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	10	9.78
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	12	9.33
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	7	9.27
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	5	9.26
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	9	9.18
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	15	9.17
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	3	9.06
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	20	9.06
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	17	8.74
(1,11)	1:392:A:SER:C	1:393:A:LEU:N	1:393:A:LEU:CA	1:393:A:LEU:C	8	8.54