



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2KZU / pdb_00002kzu
BMRB ID : 17019
Title : DAXX helical bundle (DHB) domain / Rassf1C complex
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Deposited on : 2010-06-25

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We welcome your comments at validation@mail.wwpdb.org

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

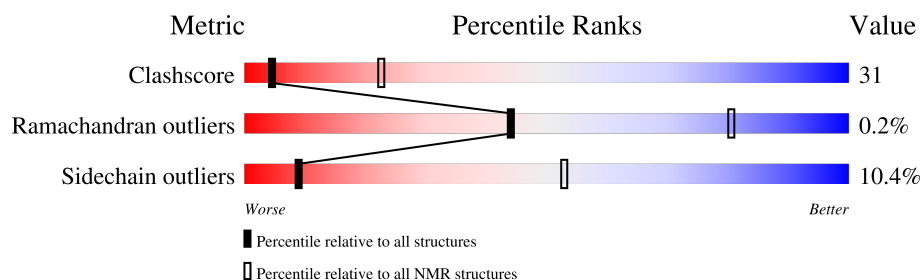
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	94	43% 37% 5% 15%
2	B	18	17% 50% 6% 28%

2 Ensemble composition and analysis

This entry contains 25 models. Model 15 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:59-A:138, B:27-B:39 (93)	0.35	15

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 5 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 9, 15, 18, 20, 24
2	1, 6, 8, 11, 14
3	4, 5, 7, 12, 22
4	13, 17, 23, 25
5	3, 10
Single-model clusters	16; 19; 21

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1836 atoms, of which 917 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Death-associated protein 6.

Mol	Chain	Residues	Atoms						Trace
1	A	94	Total	C	H	N	O	S	0
			1558	489	791	138	134	6	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	expression tag	UNP Q4VX54
A	52	SER	-	expression tag	UNP Q4VX54
A	53	HIS	-	expression tag	UNP Q4VX54
A	54	MET	-	expression tag	UNP Q4VX54

- Molecule 2 is a protein called Ras association (RalGDS/AF-6) domain family 1.

Mol	Chain	Residues	Atoms					Trace
2	B	18	Total	C	H	N	O	0
			278	92	126	24	36	

There are 2 discrepancies between the modelled and reference sequences:

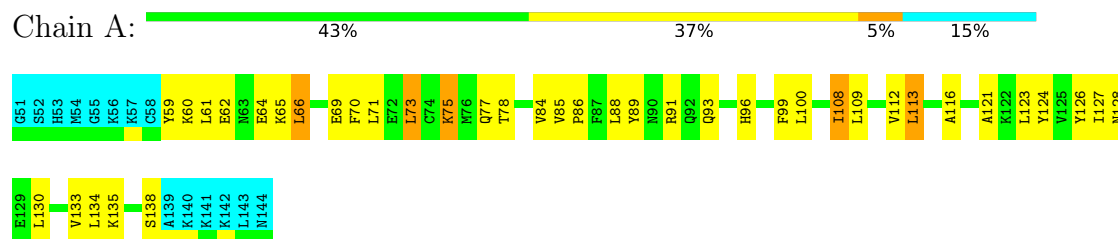
Chain	Residue	Modelled	Actual	Comment	Reference
B	22	GLY	-	expression tag	UNP Q5TZT2
B	39	TRP	-	expression tag	UNP Q5TZT2

4 Residue-property plots [i](#)

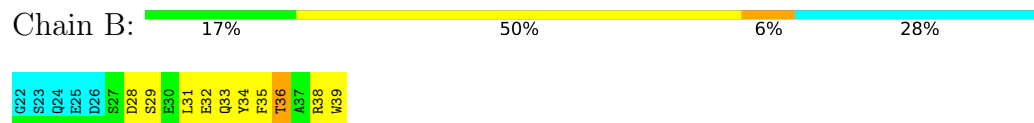
4.1 Average score per residue in the NMR ensemble

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: Death-associated protein 6



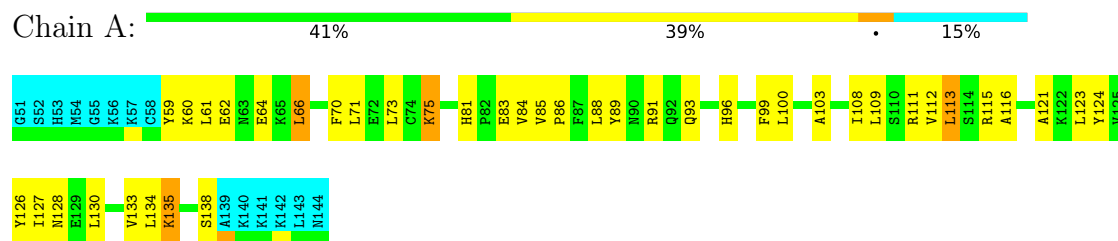
- Molecule 2: Ras association (RalGDS/AF-6) domain family 1



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

The representative model is number 15. Colouring as in section 4.1 above.

- Molecule 1: Death-associated protein 6



- Molecule 2: Ras association (RalGDS/AF-6) domain family 1



G22	S23	Q24	E25	D26	S27	D28	S29	E30	L31	E32	Q33	Y34	F35	T36	A37	R38	W39
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5 Refinement protocol and experimental data overview

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

Of the 120 calculated structures, 25 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
ARIA	structure solution	2.2
ARIA	refinement	2.2

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	1292
Number of shifts mapped to atoms	1292
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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	0.54±0.03	0±0/677 (0.0± 0.1%)	0.86±0.01	0±0/914 (0.0± 0.0%)
2	B	0.51±0.03	0±0/119 (0.0± 0.0%)	0.83±0.03	0±0/159 (0.0± 0.0%)
All	All	0.53	2/19900 (0.0%)	0.85	0/26825 (0.0%)

All 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	59	TYR	CE1-CZ	-5.81	1.24	1.38	5	1
1	A	59	TYR	CE2-CZ	5.61	1.51	1.38	5	1

There are no bond-angle outliers.

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	662	670	668	40±4
2	B	116	98	98	14±2
All	All	19450	19200	19150	1196

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 31.

5 of 185 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:GLU:HA	1:A:75:LYS:HD3	0.96	1.37	7	4
1:A:99:PHE:HB3	1:A:138:SER:HB3	0.93	1.38	24	10
1:A:71:LEU:HA	1:A:74:CYS:SG	0.92	2.03	16	1
1:A:122:LYS:HD3	2:B:39:TRP:HA	0.89	1.44	13	3
1:A:74:CYS:SG	1:A:85:VAL:HG22	0.82	2.14	16	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	80/94 (85%)	76±1 (95±1%)	4±1 (5±1%)	0±0 (0±0%)	100	100
2	B	12/18 (67%)	9±0 (77±4%)	3±1 (21±5%)	0±0 (2±3%)	9	53
All	All	2300/2800 (82%)	2138 (93%)	157 (7%)	5 (0%)	44	80

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	27	SER	4
2	B	36	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	73/84 (87%)	67±2 (92±2%)	6±2 (8±2%)	12	59
2	B	12/16 (75%)	9±1 (78±5%)	3±1 (22±5%)	2	30
All	All	2125/2500 (85%)	1904 (90%)	221 (10%)	9	53

5 of 25 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	66	LEU	25
1	A	73	LEU	25
1	A	113	LEU	25
2	B	34	TYR	25
2	B	36	THR	23

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 83% 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: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1292
Number of shifts mapped to atoms	1292
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	110	-0.68 ± 0.15	Should be checked
$^{13}\text{C}_\beta$	108	0.15 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	104	-0.40 ± 0.23	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 83%, i.e. 1112 atoms were assigned a chemical shift out of a possible 1346. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	366/459 (80%)	183/183 (100%)	93/186 (50%)	90/90 (100%)
Sidechain	644/747 (86%)	437/484 (90%)	199/229 (87%)	8/34 (24%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	102/140 (73%)	62/68 (91%)	39/66 (59%)	1/6 (17%)
Overall	1112/1346 (83%)	682/735 (93%)	331/481 (69%)	99/130 (76%)

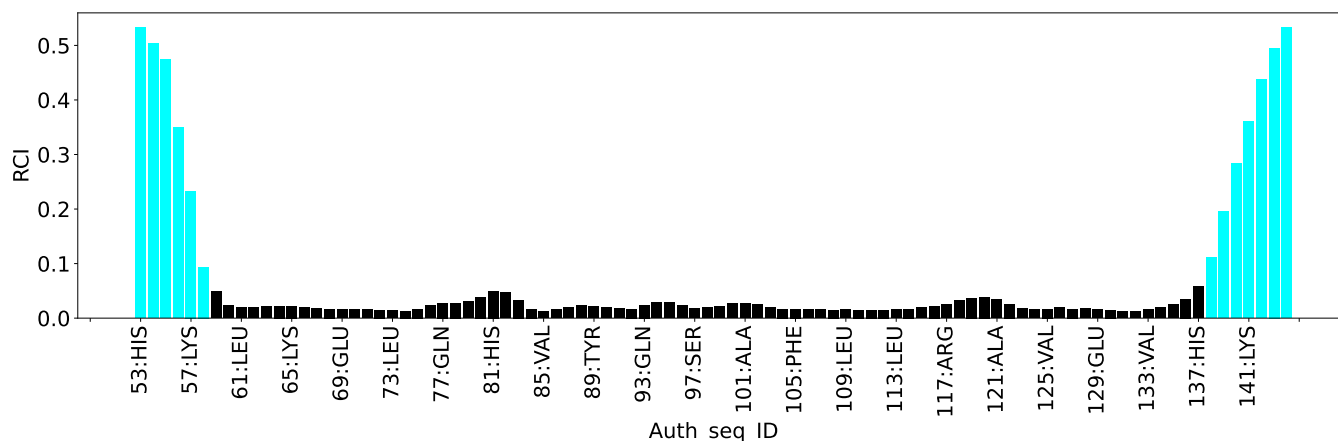
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

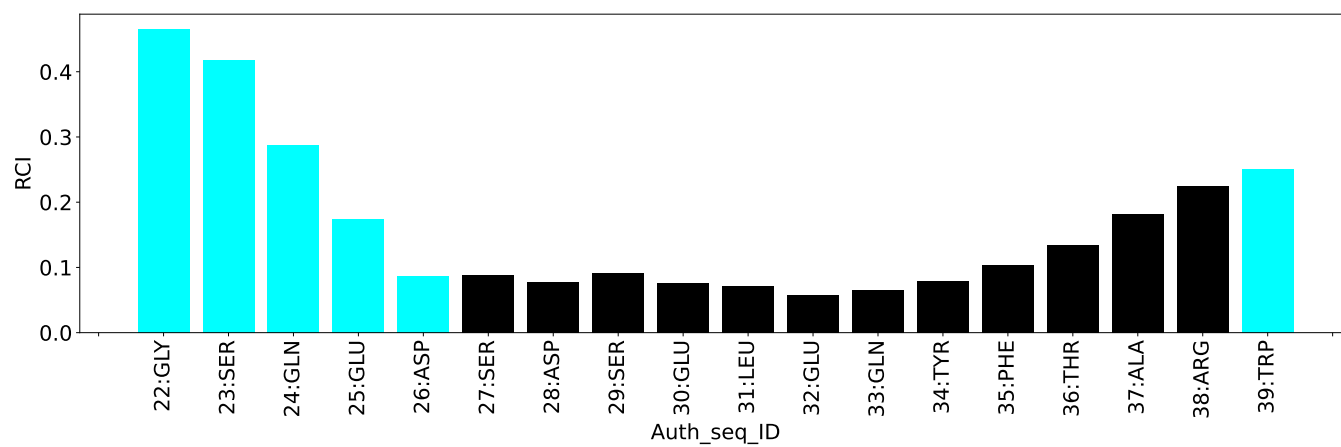
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



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	2287
Intra-residue ($ i-j =0$)	949
Sequential ($ i-j =1$)	480
Medium range ($ i-j >1$ and $ i-j <5$)	409
Long range ($ i-j \geq 5$)	340
Inter-chain	109
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	162
Number of unmapped restraints	0
Number of restraints per residue	21.9
Number of long range restraints per residue ¹	3.0

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)	108.6	0.2
0.2-0.5 (Medium)	242.8	0.5
>0.5 (Large)	218.0	4.35

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)	12.9	7.01
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

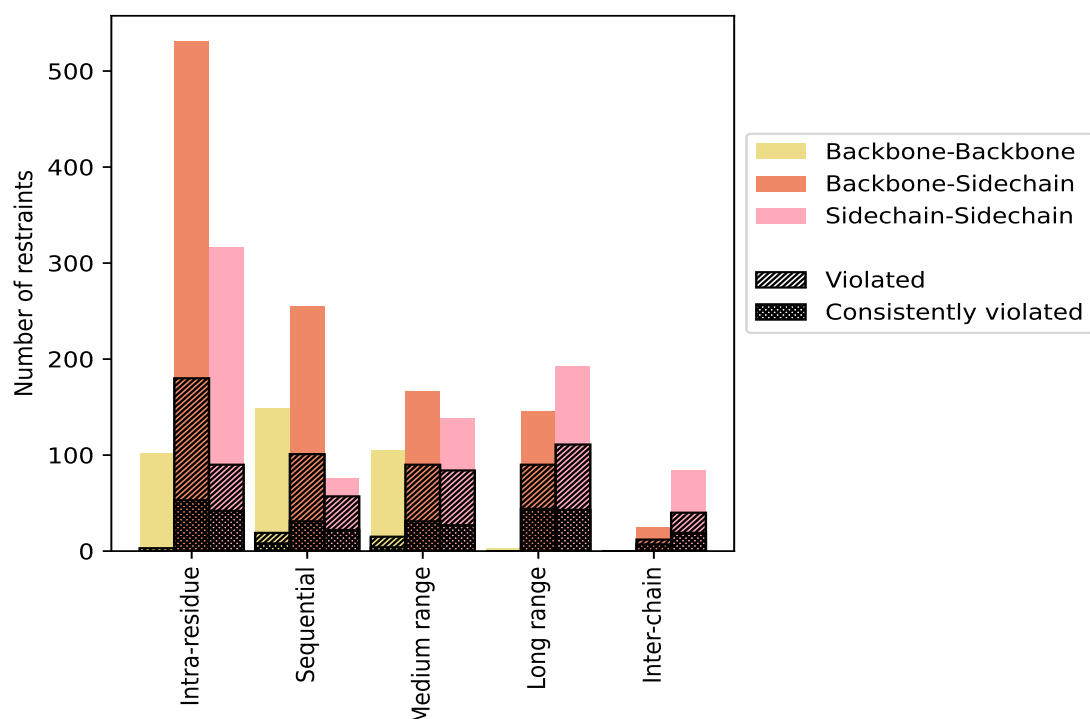
9.1 Summary of distance violations ⓘ

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)	949	41.5	273	28.8	11.9	95	10.0	4.2
Backbone-Backbone	102	4.5	3	2.9	0.1	0	0.0	0.0
Backbone-Sidechain	531	23.2	180	33.9	7.9	53	10.0	2.3
Sidechain-Sidechain	316	13.8	90	28.5	3.9	42	13.3	1.8
Sequential (i-j =1)	480	21.0	177	36.9	7.7	61	12.7	2.7
Backbone-Backbone	149	6.5	19	12.8	0.8	8	5.4	0.3
Backbone-Sidechain	255	11.1	101	39.6	4.4	31	12.2	1.4
Sidechain-Sidechain	76	3.3	57	75.0	2.5	22	28.9	1.0
Medium range (i-j >1 & i-j <5)	409	17.9	189	46.2	8.3	62	15.2	2.7
Backbone-Backbone	105	4.6	15	14.3	0.7	4	3.8	0.2
Backbone-Sidechain	166	7.3	90	54.2	3.9	31	18.7	1.4
Sidechain-Sidechain	138	6.0	84	60.9	3.7	27	19.6	1.2
Long range (i-j ≥5)	340	14.9	201	59.1	8.8	87	25.6	3.8
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	145	6.3	90	62.1	3.9	44	30.3	1.9
Sidechain-Sidechain	192	8.4	111	57.8	4.9	43	22.4	1.9
Inter-chain	109	4.8	52	47.7	2.3	26	23.9	1.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	25	1.1	12	48.0	0.5	7	28.0	0.3
Sidechain-Sidechain	84	3.7	40	47.6	1.7	19	22.6	0.8
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	2287	100.0	892	39.0	39.0	331	14.5	14.5
Backbone-Backbone	359	15.7	37	10.3	1.6	12	3.3	0.5
Backbone-Sidechain	1122	49.1	473	42.2	20.7	166	14.8	7.3
Sidechain-Sidechain	806	35.2	382	47.4	16.7	153	19.0	6.7

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	159	116	134	132	33	574	0.6	3.59	0.58	0.4
2	165	121	132	122	37	577	0.58	3.73	0.58	0.4
3	163	118	132	126	35	574	0.56	3.64	0.54	0.39
4	156	119	132	126	35	568	0.57	3.69	0.56	0.39
5	168	118	134	129	37	586	0.57	3.66	0.56	0.4
6	163	122	125	124	33	567	0.62	4.35	0.61	0.42
7	163	117	132	132	32	576	0.57	3.57	0.56	0.4
8	156	117	127	129	32	561	0.6	3.69	0.58	0.4
9	154	122	139	126	35	576	0.59	3.76	0.6	0.39
10	158	129	131	133	32	583	0.59	3.57	0.57	0.42

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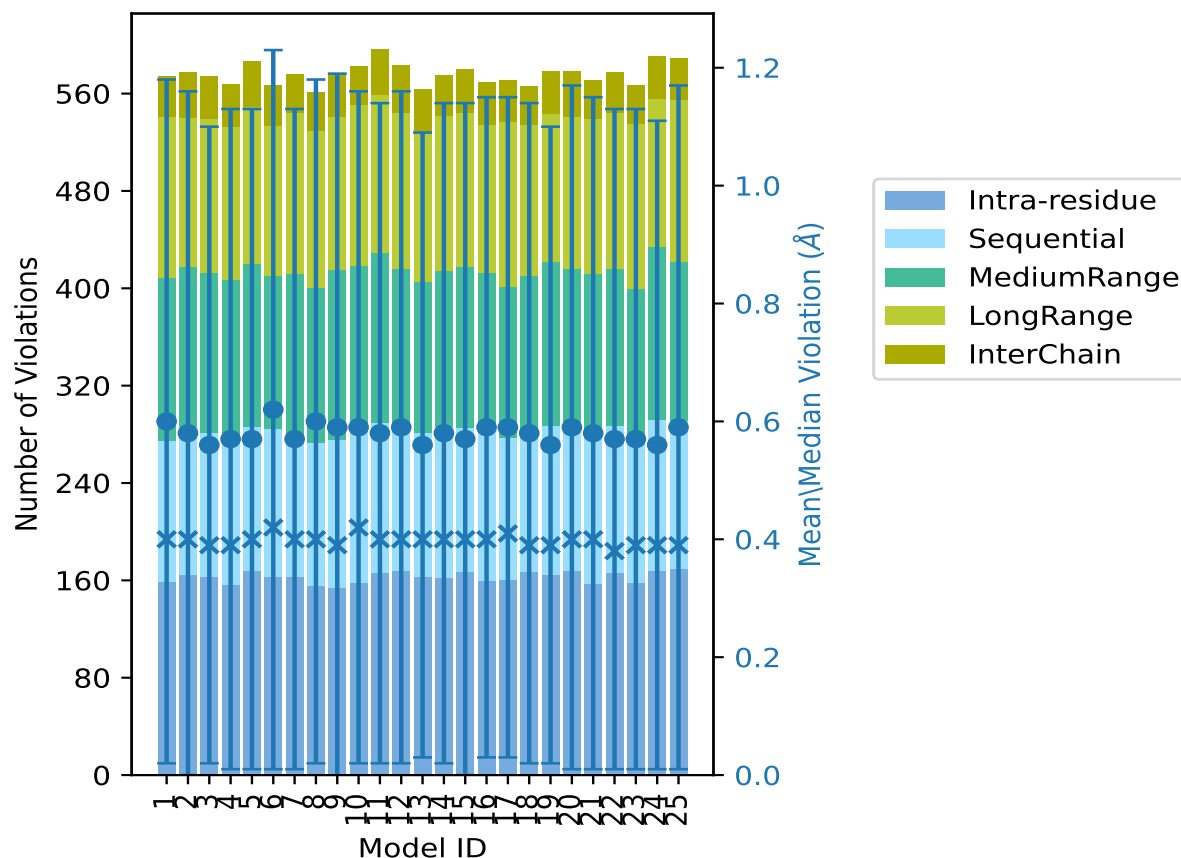
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	166	124	139	130	37	596	0.58	3.62	0.56	0.4
12	168	115	133	128	39	583	0.59	3.74	0.57	0.4
13	163	118	124	123	36	564	0.56	3.9	0.53	0.4
14	162	124	128	128	33	575	0.58	3.66	0.56	0.4
15	167	118	133	126	36	580	0.57	3.64	0.57	0.4
16	160	123	130	121	35	569	0.59	3.58	0.56	0.4
17	161	116	124	136	34	571	0.59	3.61	0.56	0.41
18	167	116	127	124	32	566	0.58	3.66	0.56	0.39
19	165	122	135	121	35	578	0.56	3.55	0.54	0.39
20	168	122	126	125	37	578	0.59	3.75	0.58	0.4
21	157	126	129	127	32	571	0.58	3.69	0.57	0.4
22	166	121	129	128	33	577	0.57	3.69	0.56	0.38
23	158	121	121	135	32	567	0.57	3.69	0.56	0.39
24	168	124	142	122	35	591	0.56	3.54	0.55	0.39
25	170	121	131	133	34	589	0.59	3.61	0.58	0.39

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 [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1395(IR:676, SQ:303, MR:220, LR:139, IC:57) 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	%
27	8	15	12	6	68	1	4.0
14	7	7	6	3	37	2	8.0
14	10	11	9	1	45	3	12.0
11	11	4	5	1	32	4	16.0
10	10	2	4	1	27	5	20.0
9	10	4	3	0	26	6	24.0

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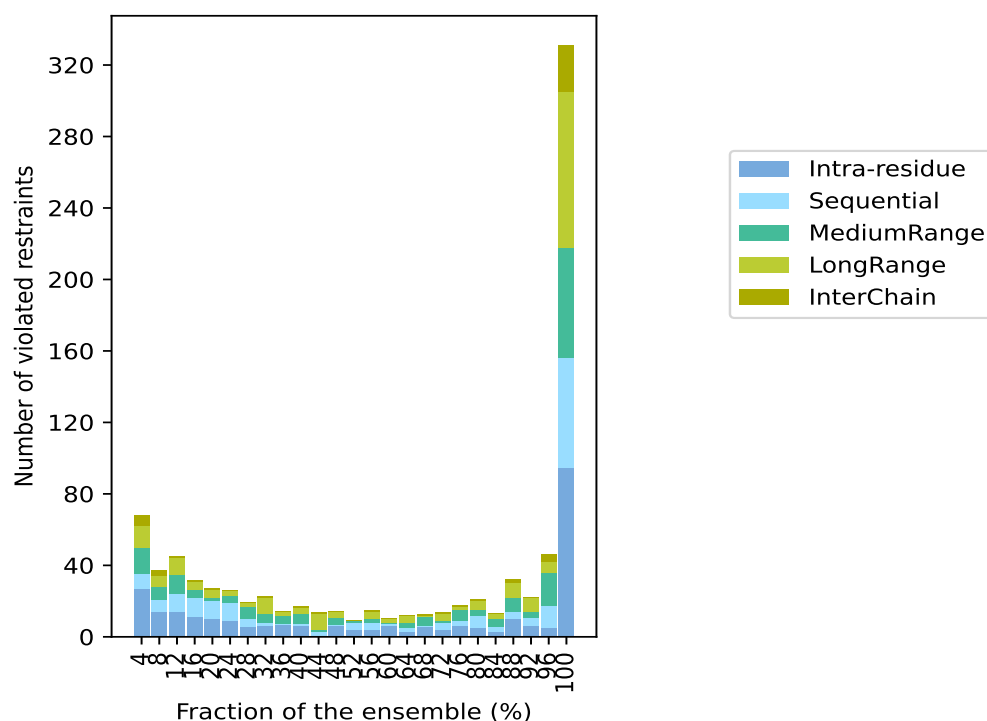
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
6	4	7	2	0	19	7	28.0
6	2	5	9	1	23	8	32.0
7	0	5	2	0	14	9	36.0
6	1	6	3	1	17	10	40.0
0	3	1	9	1	14	11	44.0
6	1	4	3	0	14	12	48.0
4	4	1	0	0	9	13	52.0
4	4	2	4	1	15	14	56.0
6	1	1	2	0	10	15	60.0
3	2	3	4	0	12	16	64.0
6	0	5	1	1	13	17	68.0
4	4	1	4	1	14	18	72.0
6	3	6	2	1	18	19	76.0
5	7	3	5	1	21	20	80.0
3	3	4	3	0	13	21	84.0
10	4	8	8	2	32	22	88.0
6	5	3	8	0	22	23	92.0
5	12	19	6	4	46	24	96.0
95	61	62	87	26	331	25	100.0

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

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

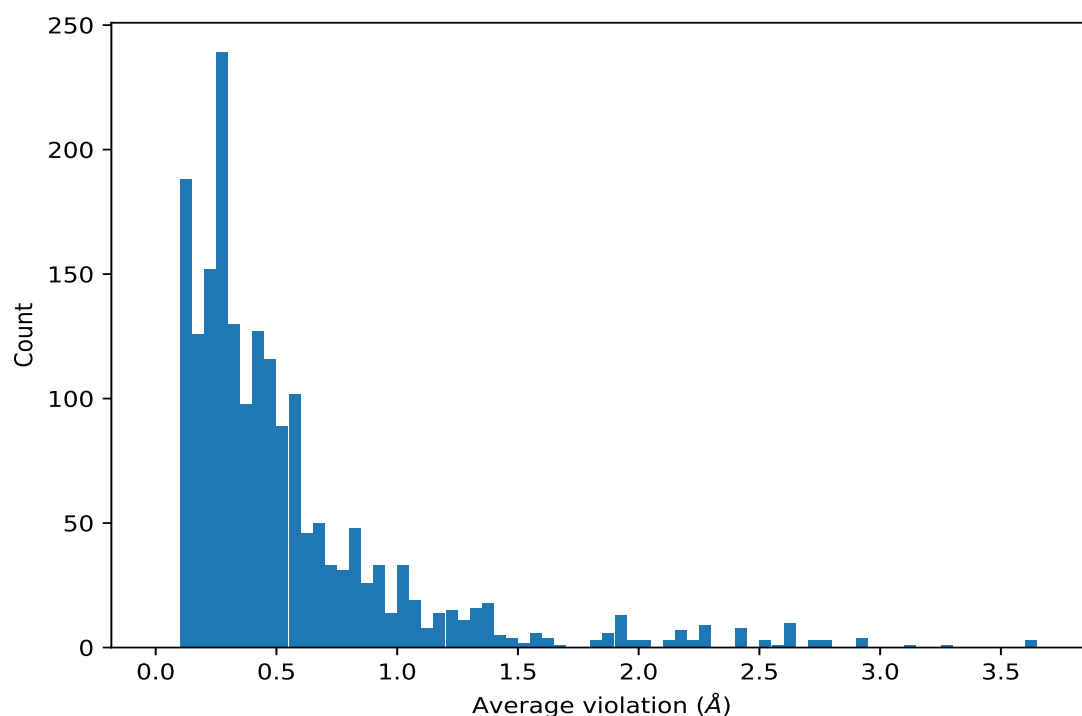
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	25	3.65	0.09	3.64
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	25	3.65	0.09	3.64
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	25	3.65	0.09	3.64
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	25	3.27	0.1	3.27
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	25	3.13	0.18	3.13
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	25	2.94	0.11	2.94
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	25	2.92	0.23	2.87
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	25	2.92	0.23	2.87
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG12	25	2.92	0.23	2.87
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	25	2.77	0.15	2.77
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	25	2.77	0.15	2.77
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG12	25	2.77	0.15	2.77
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD22	25	2.7	0.17	2.69
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	25	2.7	0.17	2.69
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD23	25	2.7	0.17	2.69
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	25	2.64	0.11	2.64

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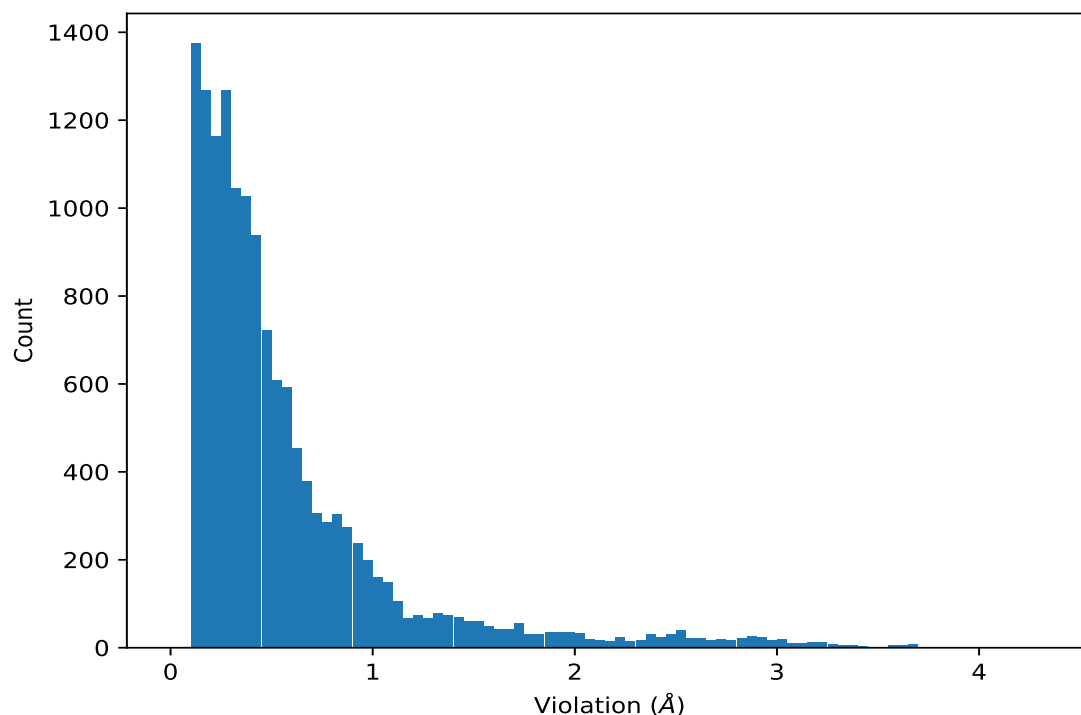
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1026)	1:109:A:LEU:HD13	1:67:A:PHE:HE1	25	2.63	0.89	2.95
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	25	2.63	0.89	2.95
(1,1026)	1:109:A:LEU:HD12	1:67:A:PHE:HE1	25	2.63	0.89	2.95
(1,1105)	1:134:A:LEU:HD22	1:99:A:PHE:HE1	25	2.61	0.66	2.73

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

The following table provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	6	4.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	13	3.9
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	9	3.76
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	20	3.75
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	12	3.74
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	2	3.73
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	21	3.69
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	4	3.69
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	8	3.69
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	23	3.69

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

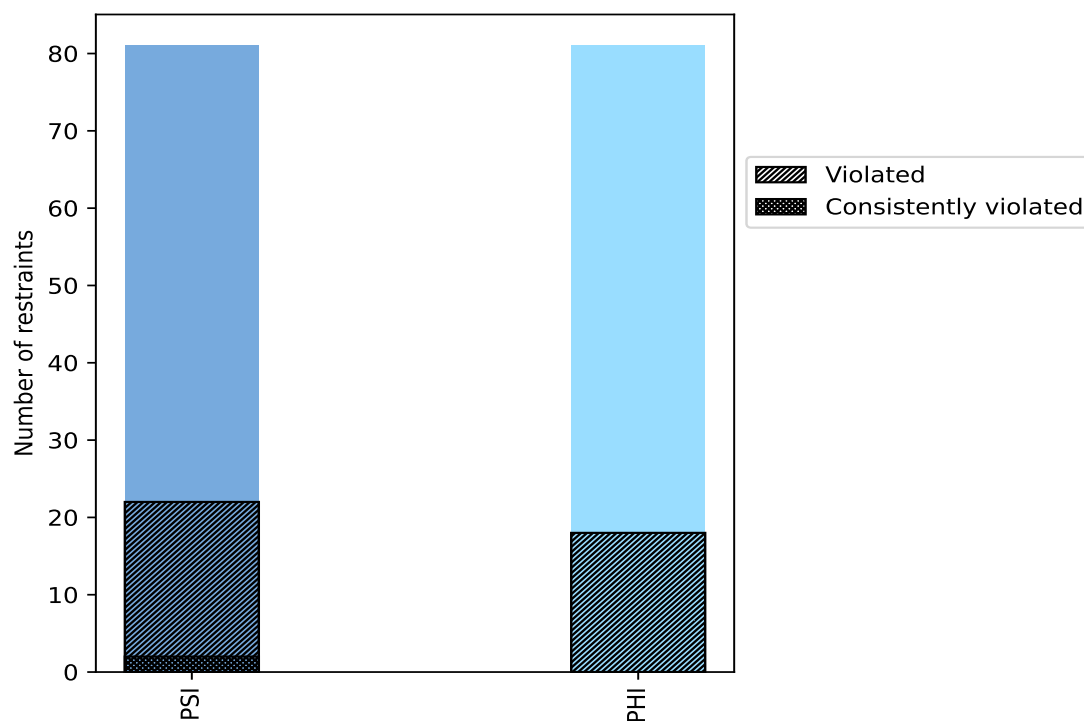
10.1 Summary of dihedral-angle violations [i](#)

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	81	50.0	22	27.2	13.6	2	2.5	1.2
PHI	81	50.0	18	22.2	11.1	0	0.0	0.0
Total	162	100.0	40	24.7	24.7	2	1.2	1.2

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](#)



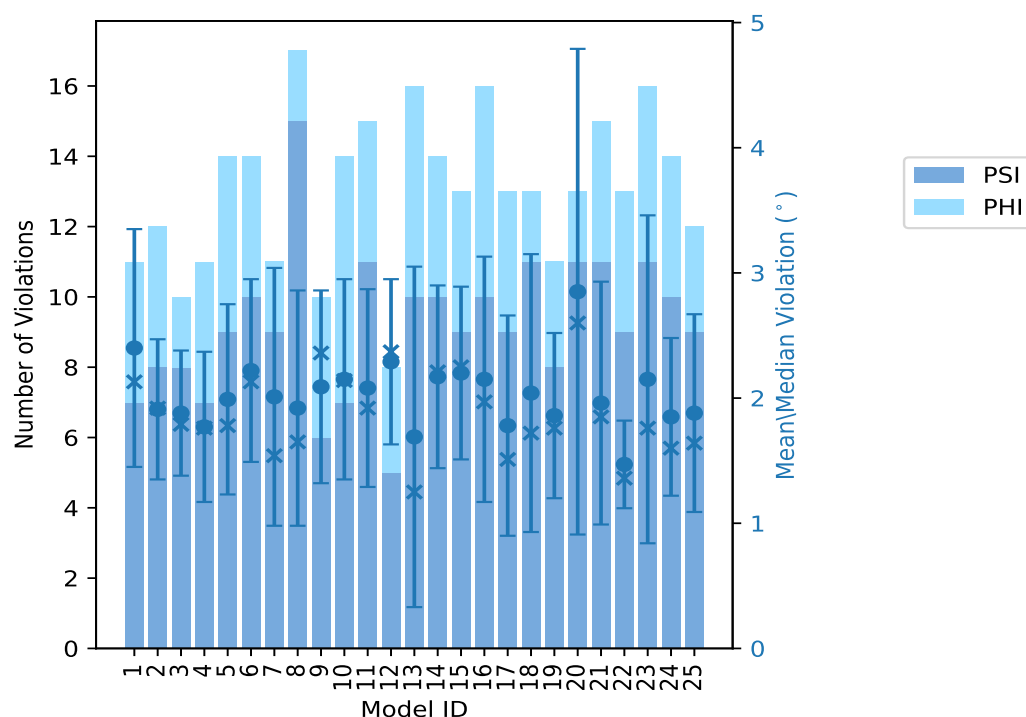
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	7	4	11	2.4	4.04	0.95	2.13
2	8	4	12	1.91	2.85	0.56	1.92
3	8	2	10	1.88	2.99	0.5	1.79
4	7	4	11	1.77	2.72	0.6	1.76
5	9	5	14	1.99	4.13	0.76	1.78
6	10	4	14	2.22	3.63	0.73	2.13
7	9	2	11	2.01	4.78	1.03	1.54
8	15	2	17	1.92	4.69	0.94	1.65
9	6	4	10	2.09	3.15	0.77	2.36
10	7	7	14	2.15	3.63	0.8	2.14
11	11	4	15	2.08	4.22	0.79	1.92
12	5	3	8	2.29	3.33	0.66	2.37
13	10	6	16	1.69	6.8	1.36	1.25
14	10	4	14	2.17	3.19	0.73	2.21
15	9	4	13	2.2	3.02	0.69	2.25
16	10	6	16	2.15	4.84	0.98	1.97
17	9	4	13	1.78	4.66	0.88	1.51
18	11	2	13	2.04	5.01	1.11	1.72
19	8	3	11	1.86	3.13	0.66	1.76
20	11	2	13	2.85	7.01	1.94	2.6
21	11	4	15	1.96	4.74	0.97	1.85
22	9	4	13	1.47	2.11	0.35	1.36
23	11	5	16	2.15	6.68	1.31	1.76
24	10	4	14	1.85	2.99	0.63	1.6
25	9	3	12	1.88	3.89	0.79	1.64

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
4	4	8	1	4.0
1	4	5	2	8.0
0	1	1	3	12.0
1	4	5	4	16.0
1	0	1	5	20.0
2	1	3	6	24.0
0	1	1	7	28.0
1	0	1	8	32.0
3	0	3	9	36.0
1	0	1	10	40.0
0	0	0	11	44.0

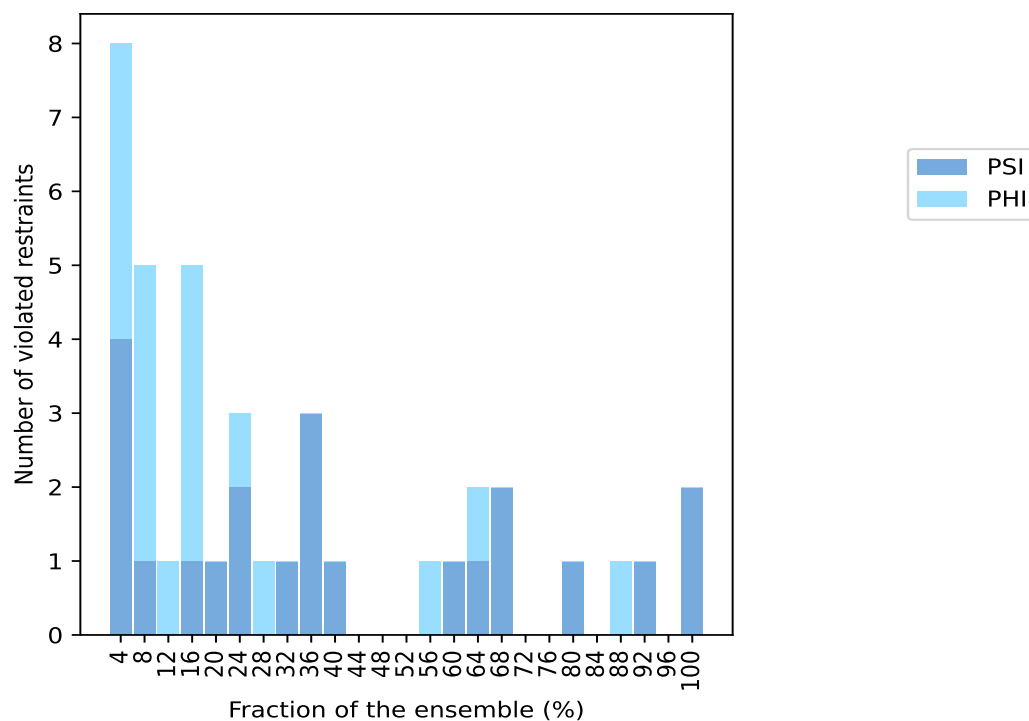
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	48.0
0	0	0	13	52.0
0	1	1	14	56.0
1	0	1	15	60.0
1	1	2	16	64.0
2	0	2	17	68.0
0	0	0	18	72.0
0	0	0	19	76.0
1	0	1	20	80.0
0	0	0	21	84.0
0	1	1	22	88.0
1	0	1	23	92.0
0	0	0	24	96.0
2	0	2	25	100.0

¹ Number of models with violations

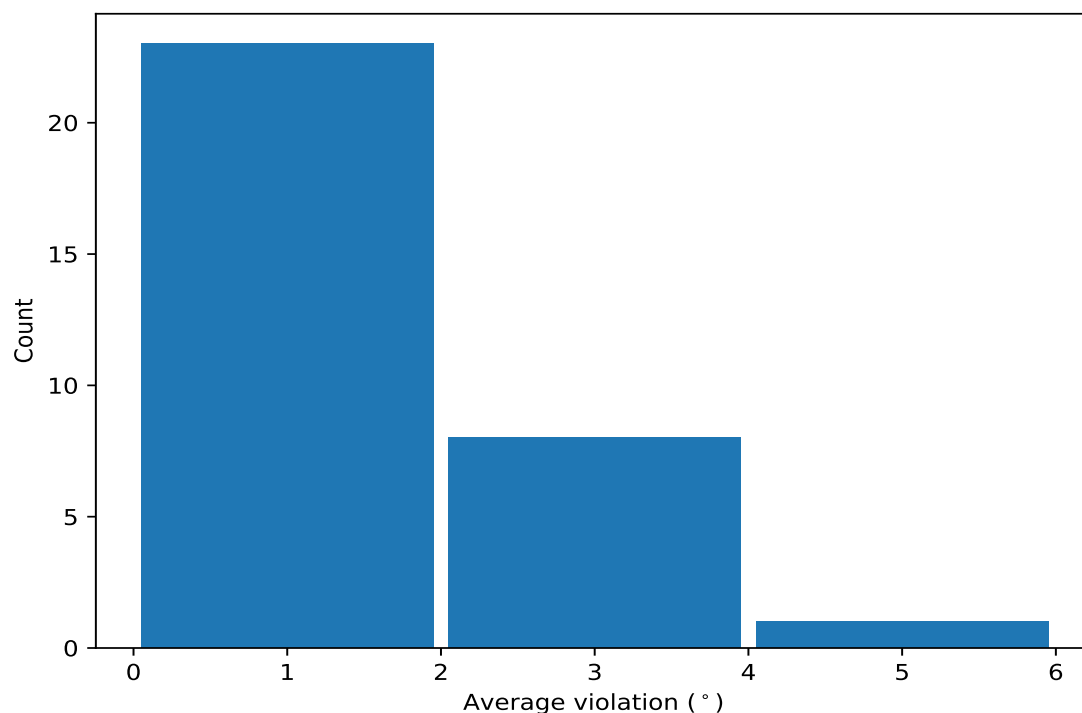
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

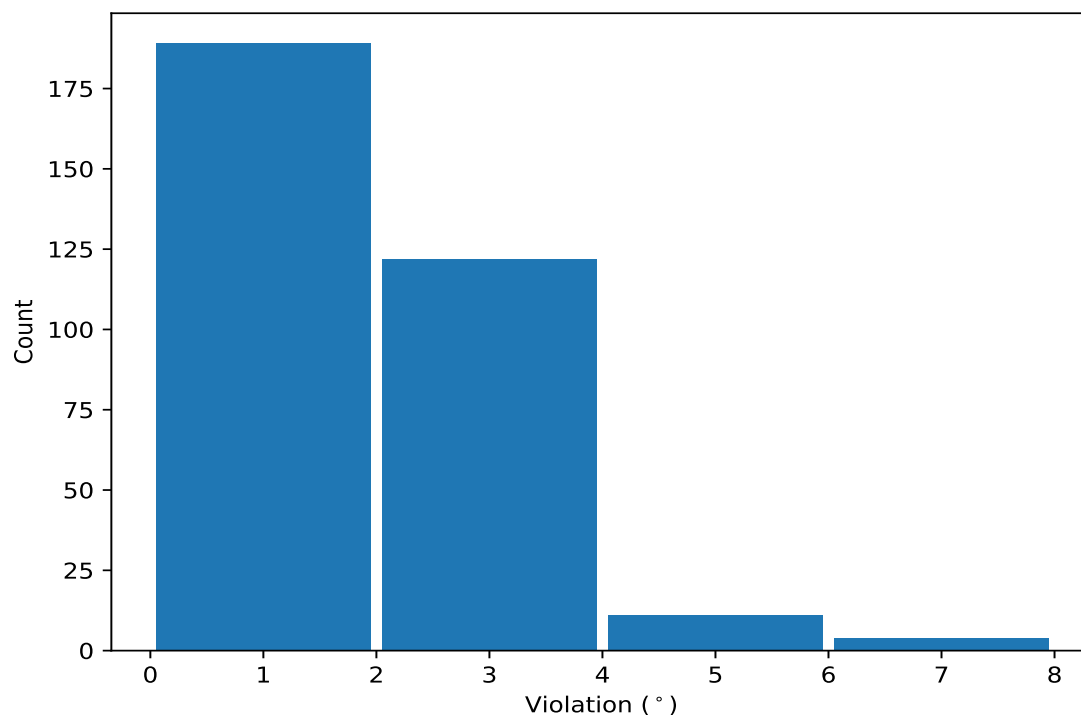
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	25	2.86	0.86	2.63
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	25	2.12	0.49	2.16
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	23	2.49	0.49	2.61
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	22	1.92	0.63	1.9
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	20	1.67	0.68	1.5
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	17	2.43	0.77	2.33
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	17	1.85	0.44	1.92
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	16	1.99	0.92	1.75
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	16	1.44	0.41	1.32
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	15	1.81	0.73	1.46

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 (°)
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	20	7.01
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	13	6.8
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	20	6.72
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	23	6.68
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	18	5.01
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	16	4.84
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	7	4.78
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	21	4.74
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	8	4.69
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	17	4.66