



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 7CLV
BMRB ID : 36365
Title : Solution structure of mitochondrial Tim23 channel in complex with a signaling peptide
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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 : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

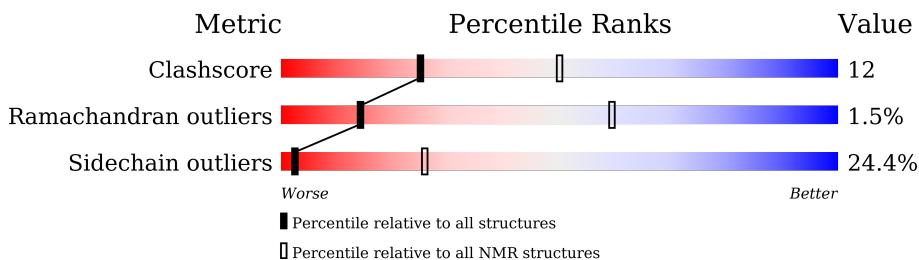
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 35%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	222	
1	B	222	
2	C	25	

2 Ensemble composition and analysis

This entry contains 15 models. Model 5 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:64-A:75, A:91-A:124, A:151-A:216, B:64-B:79, B:91-B:122, B:150-B:216 (227)	1.36	5

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 5, 6, 8, 9, 11, 12, 13, 14, 15
2	3, 4, 7, 10

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6985 atoms, of which 3514 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TIM23 isoform 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	222	3274	1026	1643	281	315	9	0
1	B	222	3274	1026	1643	281	315	9	0

- Molecule 2 is a protein called COX4 isoform 1.

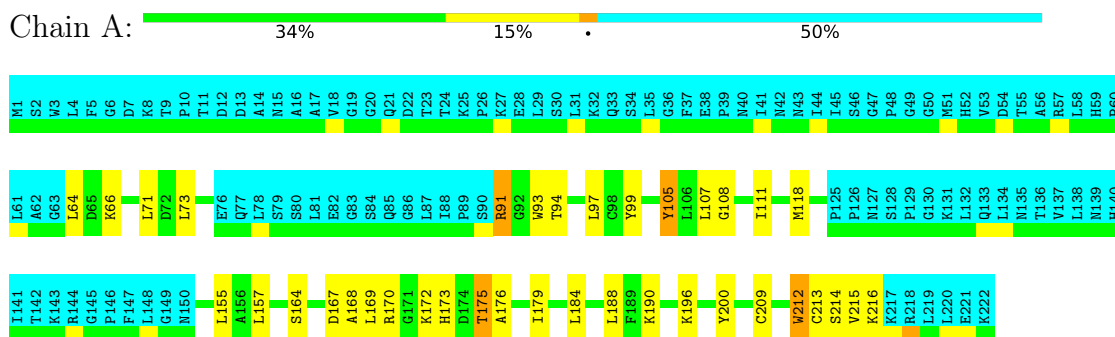
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	C	25	437	134	228	39	34	2	0

4 Residue-property plots [i](#)

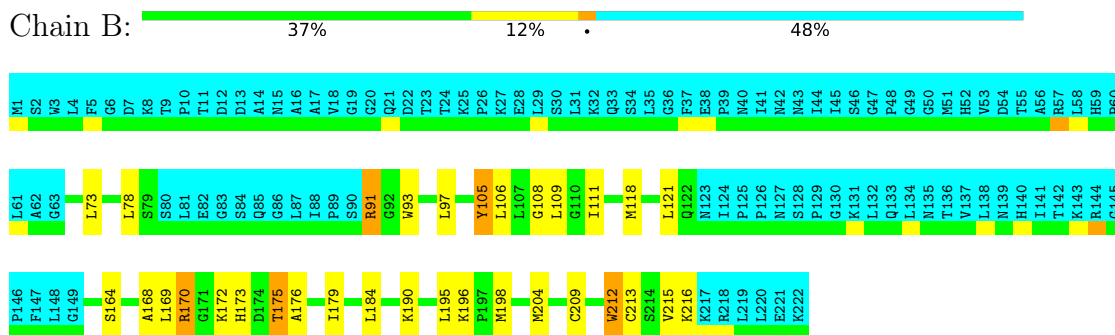
4.1 Average score per residue in the NMR ensemble

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.

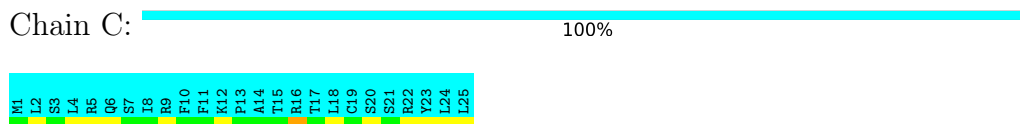
- Molecule 1: TIM23 isoform 1



- Molecule 1: TIM23 isoform 1



- Molecule 2: COX4 isoform 1



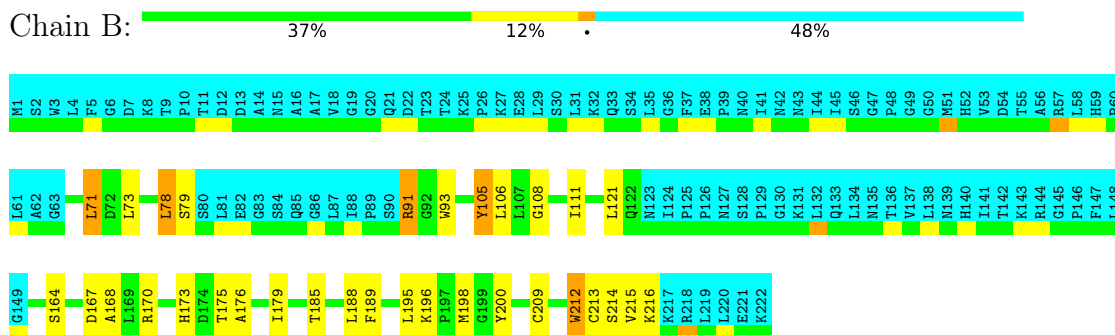
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

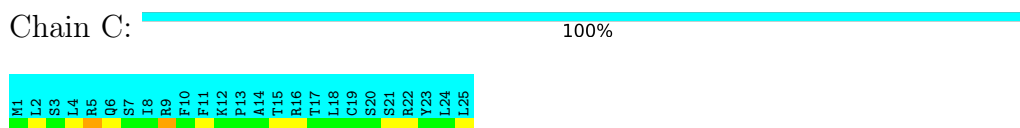
- Molecule 1: TIM23 isoform 1



- Molecule 1: TIM23 isoform 1



- Molecule 2: COX4 isoform 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 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
X-PLOR NIH	structure calculation	
X-PLOR NIH	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	1939
Number of shifts mapped to atoms	1939
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.9±0.2
1	B	0.0±0.0	2.0±0.0
All	All	0	59

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	170	ARG	Sidechain	15
1	B	91	ARG	Sidechain	15
1	B	170	ARG	Sidechain	15
1	A	91	ARG	Sidechain	14

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	807	809	809	22±5
1	B	831	828	828	21±5
2	C	0	0	0	0±0
All	All	24570	24555	24555	570

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 12.

5 of 249 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:THR:HG21	1:A:212:TRP:CD1	0.86	2.05	14	2
1:A:175:THR:HG23	1:B:105:TYR:CZ	0.85	2.07	2	9
1:A:105:TYR:CZ	1:B:175:THR:HG23	0.81	2.10	13	9
1:A:173:HIS:O	1:A:215:VAL:HG22	0.81	1.74	7	1
1:A:176:ALA:HB1	1:A:179:ILE:CG1	0.79	2.08	1	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	112/222 (50%)	101±3 (90±2%)	10±3 (9±2%)	2±1 (1±1%)	15	61
1	B	115/222 (52%)	103±2 (89±2%)	11±2 (9±2%)	2±1 (2±1%)	14	59
2	C	0	-	-	-	-	-
All	All	3405/7035 (48%)	3049 (90%)	306 (9%)	50 (1%)	14	59

5 of 12 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	175	THR	12
1	B	175	THR	12
1	A	214	SER	8
1	B	214	SER	5
1	B	216	LYS	3

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	81/173 (47%)	62±4 (76±5%)	19±4 (24±5%)	2	26
1	B	84/173 (49%)	63±4 (75±5%)	21±4 (25±5%)	2	25
2	C	0	-	-	-	-
All	All	2475/5550 (45%)	1871 (76%)	604 (24%)	2	26

5 of 122 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	212	TRP	15
1	B	212	TRP	15
1	A	105	TYR	13
1	B	172	LYS	12
1	A	172	LYS	11

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 35% for the well-defined parts and 31% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping i

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

Total number of shifts	1939
Number of shifts mapped to atoms	1939
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

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	29	LEU	HD11	0.788	.	2
1	A	29	LEU	HD12	0.788	.	2
1	A	29	LEU	HD13	0.788	.	2
1	A	73	LEU	HD11	0.846	.	2
1	A	73	LEU	HD12	0.846	.	2
1	A	73	LEU	HD13	0.846	.	2
1	A	78	LEU	HD11	0.822	.	2
1	A	78	LEU	HD12	0.822	.	2
1	A	78	LEU	HD13	0.822	.	2
1	A	148	LEU	HD11	0.864	.	2
1	A	148	LEU	HD12	0.864	.	2
1	A	148	LEU	HD13	0.864	.	2
1	A	71	LEU	HD11	0.828	.	2
1	A	71	LEU	HD12	0.828	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	LEU	HD13	0.828	.	2
1	A	35	LEU	HD11	0.725	.	2
1	A	35	LEU	HD12	0.725	.	2
1	A	35	LEU	HD13	0.725	.	2
1	A	81	LEU	HD11	0.797	.	2
1	A	81	LEU	HD12	0.797	.	2
1	A	81	LEU	HD13	0.797	.	2
1	A	109	LEU	HD11	0.757	0.002	2
1	A	109	LEU	HD12	0.757	0.002	2
1	A	109	LEU	HD13	0.757	0.002	2
1	A	121	LEU	HD11	0.796	0.008	2
1	A	121	LEU	HD12	0.796	0.008	2
1	A	121	LEU	HD13	0.796	0.008	2
1	A	132	LEU	HD11	0.787	0.004	2
1	A	132	LEU	HD12	0.787	0.004	2
1	A	132	LEU	HD13	0.787	0.004	2
1	A	169	LEU	HD11	0.783	0.003	2
1	A	169	LEU	HD12	0.783	0.003	2
1	A	169	LEU	HD13	0.783	0.003	2
1	A	188	LEU	HD11	0.737	0.019	2
1	A	188	LEU	HD12	0.737	0.019	2
1	A	188	LEU	HD13	0.737	0.019	2
1	A	87	LEU	HD11	0.784	.	2
1	A	87	LEU	HD12	0.784	.	2
1	A	87	LEU	HD13	0.784	.	2
1	A	106	LEU	HD11	0.788	.	2
1	A	106	LEU	HD12	0.788	.	2
1	A	106	LEU	HD13	0.788	.	2
1	A	134	LEU	HD11	0.779	.	2
1	A	134	LEU	HD12	0.779	.	2
1	A	134	LEU	HD13	0.779	.	2
1	A	184	LEU	HD11	0.802	.	2
1	A	184	LEU	HD12	0.802	.	2
1	A	184	LEU	HD13	0.802	.	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	211	0.40 \pm 0.14	None needed (< 0.5 ppm)

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Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\beta$	178	0.71 ± 0.04	Should be checked
$^{13}\text{C}'$	197	0.11 ± 0.12	None needed (< 0.5 ppm)
^{15}N	198	0.71 ± 0.27	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 35%, i.e. 1005 atoms were assigned a chemical shift out of a possible 2833. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	519/1167 (44%)	207/488 (42%)	209/454 (46%)	103/225 (46%)
Sidechain	463/1474 (31%)	328/978 (34%)	135/459 (29%)	0/37 (0%)
Aromatic	23/192 (12%)	21/92 (23%)	0/94 (0%)	2/6 (33%)
Overall	1005/2833 (35%)	556/1558 (36%)	344/1007 (34%)	105/268 (39%)

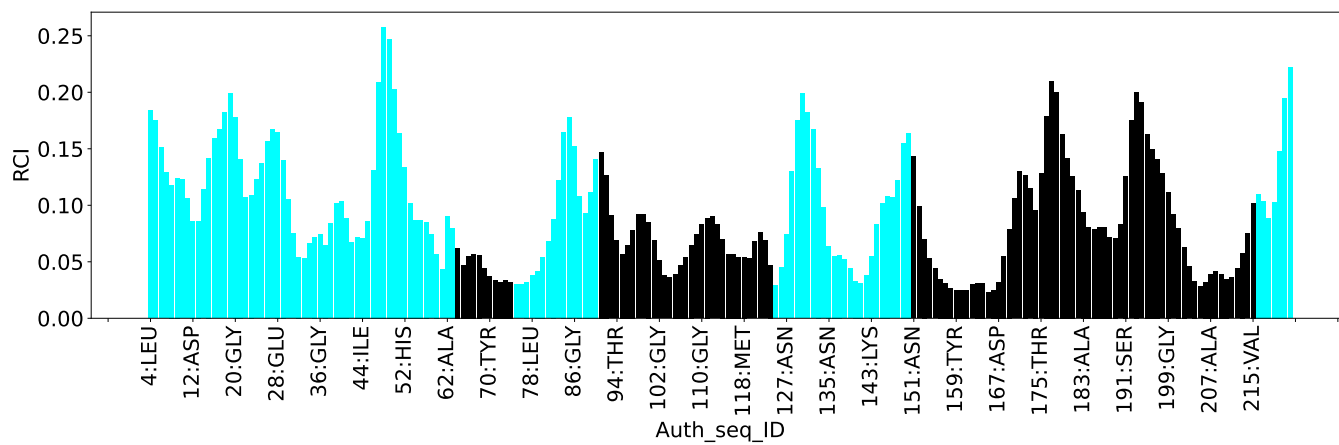
7.1.4 Statistically unusual chemical shifts [i](#)

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:



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	3104
Intra-residue ($ i-j =0$)	954
Sequential ($ i-j =1$)	960
Medium range ($ i-j >1$ and $ i-j <5$)	368
Long range ($ i-j \geq 5$)	228
Inter-chain	594
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	752
Number of unmapped restraints	2
Number of restraints per residue	8.2
Number of long range restraints per residue ¹	0.5

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)	216.5	0.2
0.2-0.5 (Medium)	209.1	0.5
>0.5 (Large)	486.2	20.64

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)	25.1	10.0
10.0-20.0 (Medium)	9.8	19.8
>20.0 (Large)	66.1	157.2

9 Distance violation analysis i

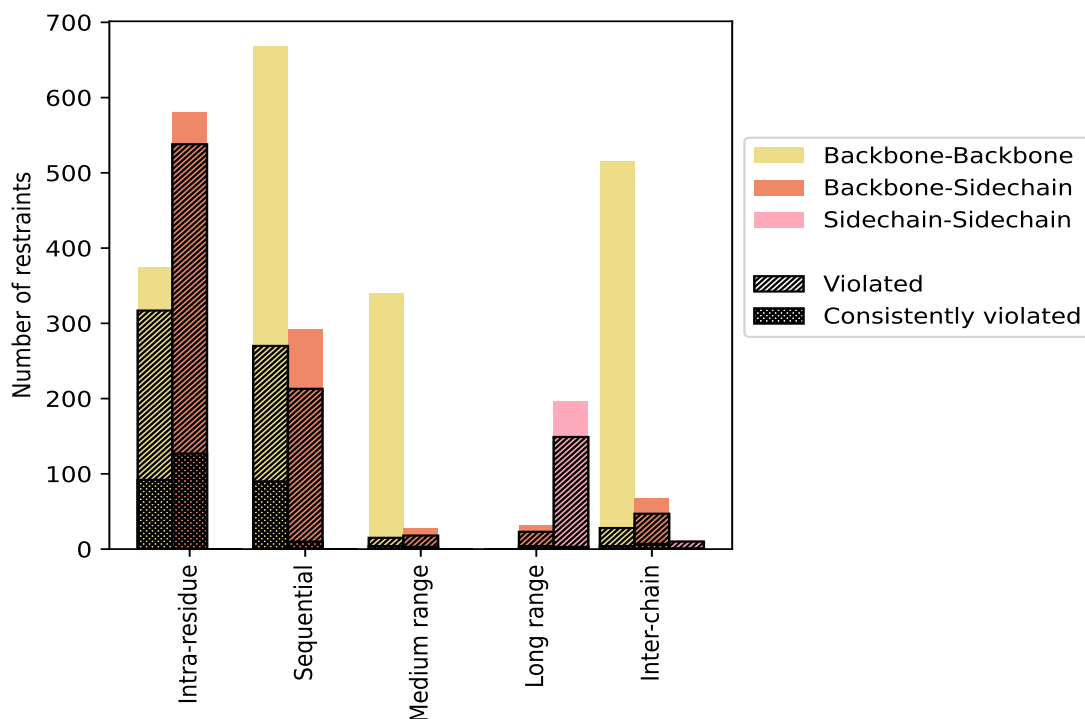
9.1 Summary of distance violations i

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	954	30.7	855	89.6	27.5	219	23.0	7.1
Backbone-Backbone	374	12.0	317	84.8	10.2	92	24.6	3.0
Backbone-Sidechain	580	18.7	538	92.8	17.3	127	21.9	4.1
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	960	30.9	483	50.3	15.6	100	10.4	3.2
Backbone-Backbone	668	21.5	270	40.4	8.7	90	13.5	2.9
Backbone-Sidechain	292	9.4	213	72.9	6.9	10	3.4	0.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	368	11.9	33	9.0	1.1	7	1.9	0.2
Backbone-Backbone	340	11.0	15	4.4	0.5	4	1.2	0.1
Backbone-Sidechain	28	0.9	18	64.3	0.6	3	10.7	0.1
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	228	7.3	172	75.4	5.5	7	3.1	0.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	32	1.0	23	71.9	0.7	4	12.5	0.1
Sidechain-Sidechain	196	6.3	149	76.0	4.8	3	1.5	0.1
Inter-chain	594	19.1	85	14.3	2.7	12	2.0	0.4
Backbone-Backbone	515	16.6	28	5.4	0.9	4	0.8	0.1
Backbone-Sidechain	67	2.2	47	70.1	1.5	7	10.4	0.2
Sidechain-Sidechain	12	0.4	10	83.3	0.3	1	8.3	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	3104	100.0	1628	52.4	52.4	345	11.1	11.1
Backbone-Backbone	1897	61.1	630	33.2	20.3	190	10.0	6.1
Backbone-Sidechain	999	32.2	839	84.0	27.0	151	15.1	4.9
Sidechain-Sidechain	208	6.7	159	76.4	5.1	4	1.9	0.1

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	551	245	18	69	42	925	0.72	20.28	1.42	0.54
2	536	239	21	70	48	914	0.74	20.34	1.44	0.56
3	541	241	16	57	36	891	0.7	20.42	1.42	0.54
4	549	242	18	66	47	922	0.71	20.31	1.41	0.54
5	550	244	19	74	37	924	0.7	20.12	1.39	0.55
6	539	243	25	53	44	904	0.74	20.17	1.43	0.55
7	521	240	18	59	38	876	0.72	20.64	1.45	0.55
8	544	245	21	75	36	921	0.71	20.3	1.41	0.54
9	560	253	19	65	38	935	0.69	20.13	1.38	0.52
10	530	251	19	63	41	904	0.7	20.16	1.41	0.54
11	541	240	19	84	41	925	0.7	20.13	1.39	0.54

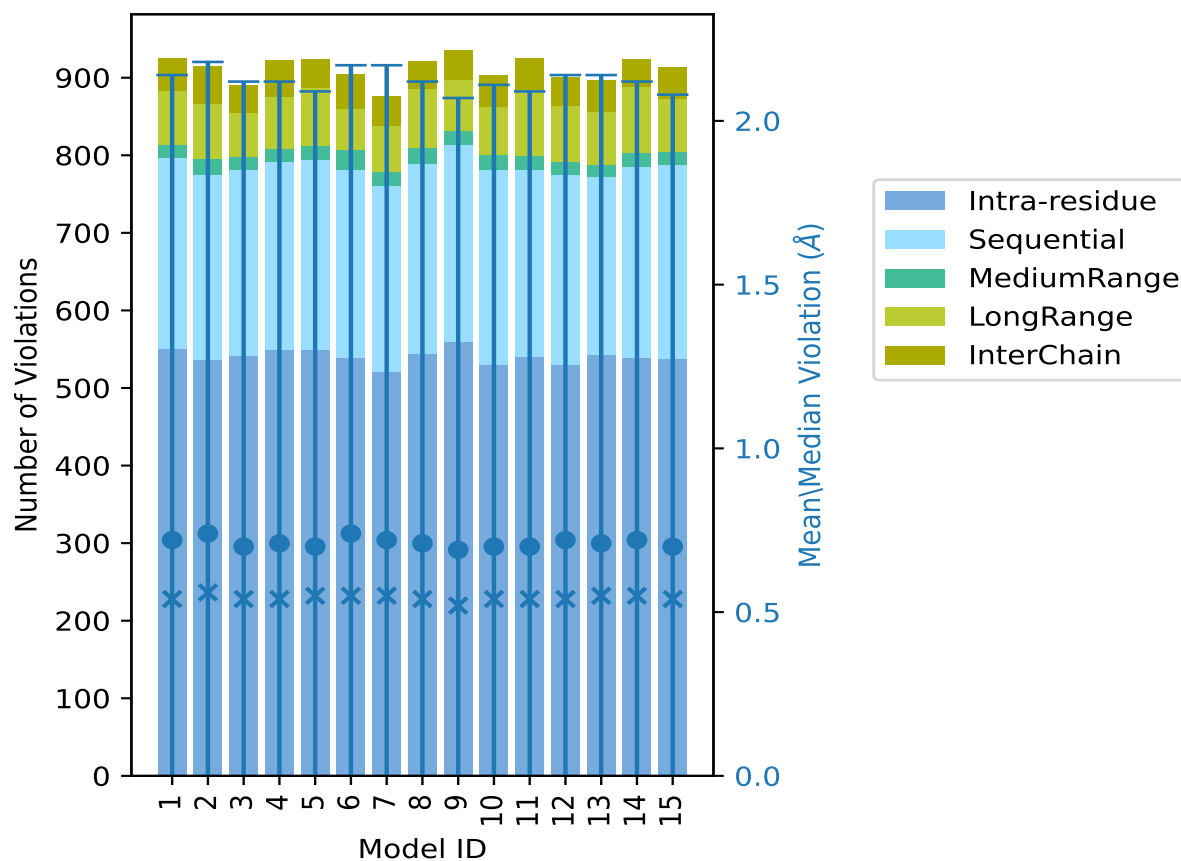
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	530	245	17	72	37	901	0.72	20.14	1.42	0.54
13	543	229	16	68	40	896	0.71	20.54	1.43	0.55
14	539	246	19	84	36	924	0.72	20.3	1.4	0.55
15	538	249	18	68	41	914	0.7	19.81	1.38	0.54

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](#)

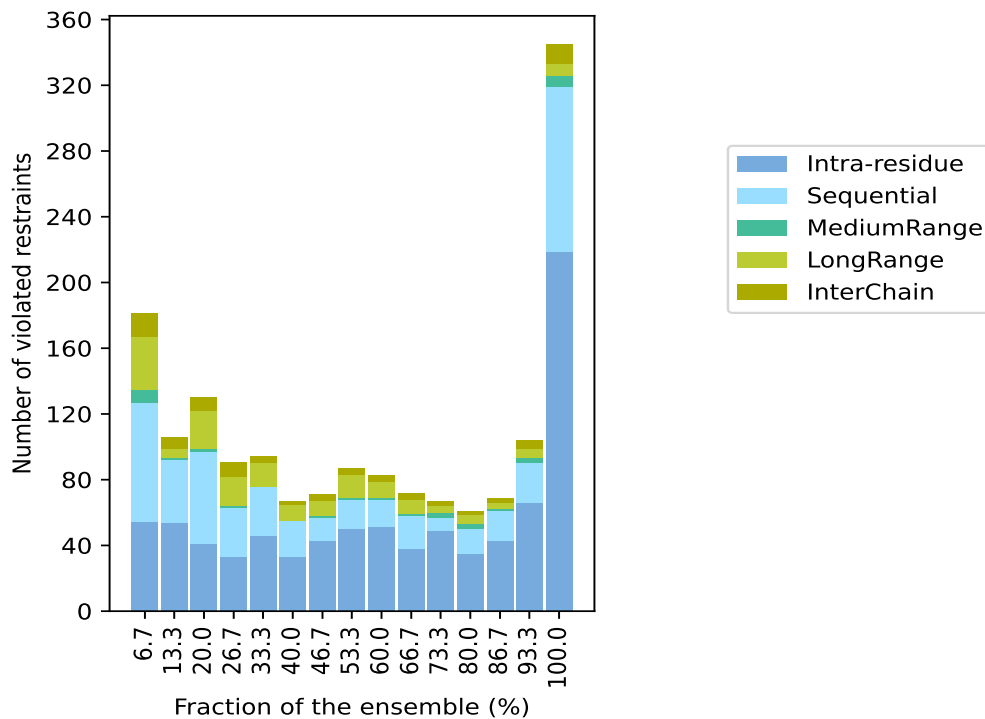
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for

a given fraction of the ensemble. In total, 1476(IR:99, SQ:477, MR:335, LR:56, IC:509) 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	%
54	73	8	32	14	181	1	6.7
54	38	1	6	7	106	2	13.3
41	56	2	23	8	130	3	20.0
33	30	1	18	9	91	4	26.7
46	30	0	14	4	94	5	33.3
33	22	0	10	2	67	6	40.0
43	14	1	9	4	71	7	46.7
50	18	1	14	4	87	8	53.3
51	17	1	10	4	83	9	60.0
38	20	1	9	4	72	10	66.7
49	8	3	4	3	67	11	73.3
35	15	3	6	2	61	12	80.0
43	18	1	4	3	69	13	86.7
66	24	3	6	5	104	14	93.3
219	100	7	7	12	345	15	100.0

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

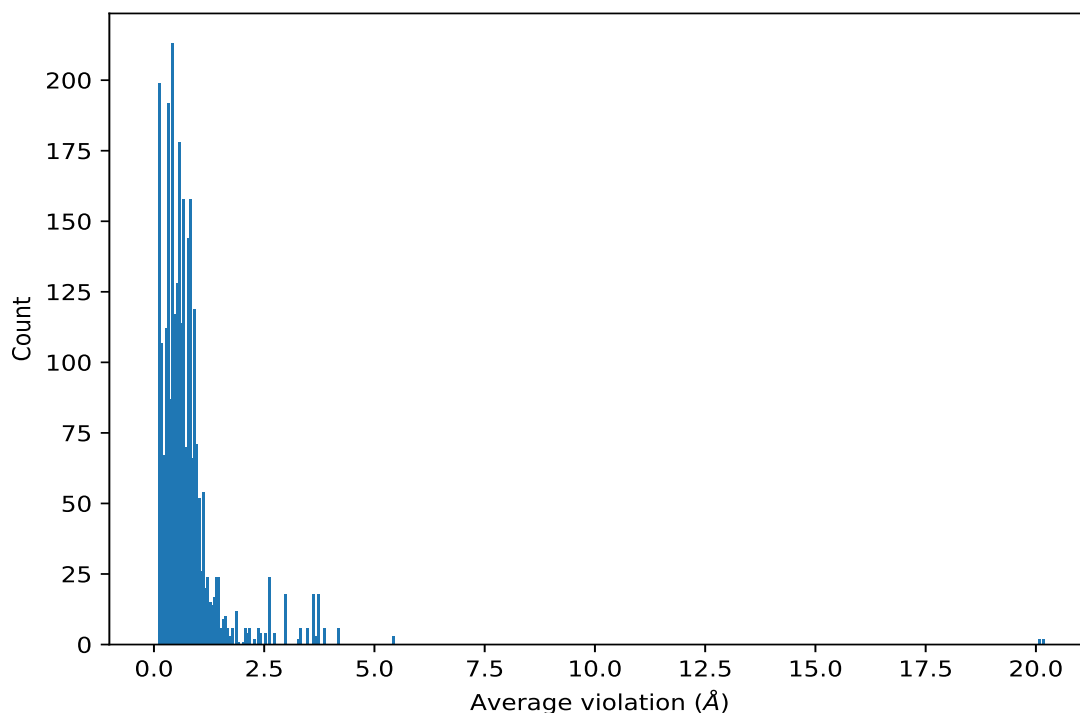
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,662)	1:A:119:GLN:H	1:A:189:PHE:HB2	15	20.17	0.26	20.14
(1,663)	1:A:119:GLN:H	1:A:189:PHE:HB2	15	20.17	0.26	20.14
(1,1906)	1:B:119:GLN:H	1:B:189:PHE:HB2	15	20.05	0.25	20.1
(1,1907)	1:B:119:GLN:H	1:B:189:PHE:HB2	15	20.05	0.25	20.1
(1,2569)	1:B:88:ILE:HD11	1:A:95:ASP:HB2	15	3.85	1.08	3.75
(1,2569)	1:B:88:ILE:HD11	1:A:95:ASP:HB3	15	3.85	1.08	3.75
(1,2569)	1:B:88:ILE:HD12	1:A:95:ASP:HB2	15	3.85	1.08	3.75
(1,2569)	1:B:88:ILE:HD12	1:A:95:ASP:HB3	15	3.85	1.08	3.75
(1,2569)	1:B:88:ILE:HD13	1:A:95:ASP:HB2	15	3.85	1.08	3.75
(1,2569)	1:B:88:ILE:HD13	1:A:95:ASP:HB3	15	3.85	1.08	3.75
(1,2570)	1:B:88:ILE:HD11	1:A:95:ASP:HA	15	3.68	1.44	3.21
(1,2570)	1:B:88:ILE:HD12	1:A:95:ASP:HA	15	3.68	1.44	3.21
(1,2570)	1:B:88:ILE:HD13	1:A:95:ASP:HA	15	3.68	1.44	3.21
(1,2457)	1:B:211:VAL:HG21	1:B:173:HIS:HD1	15	3.47	1.82	3.78
(1,2457)	1:B:211:VAL:HG21	1:B:173:HIS:HD2	15	3.47	1.82	3.78
(1,2457)	1:B:211:VAL:HG22	1:B:173:HIS:HD1	15	3.47	1.82	3.78

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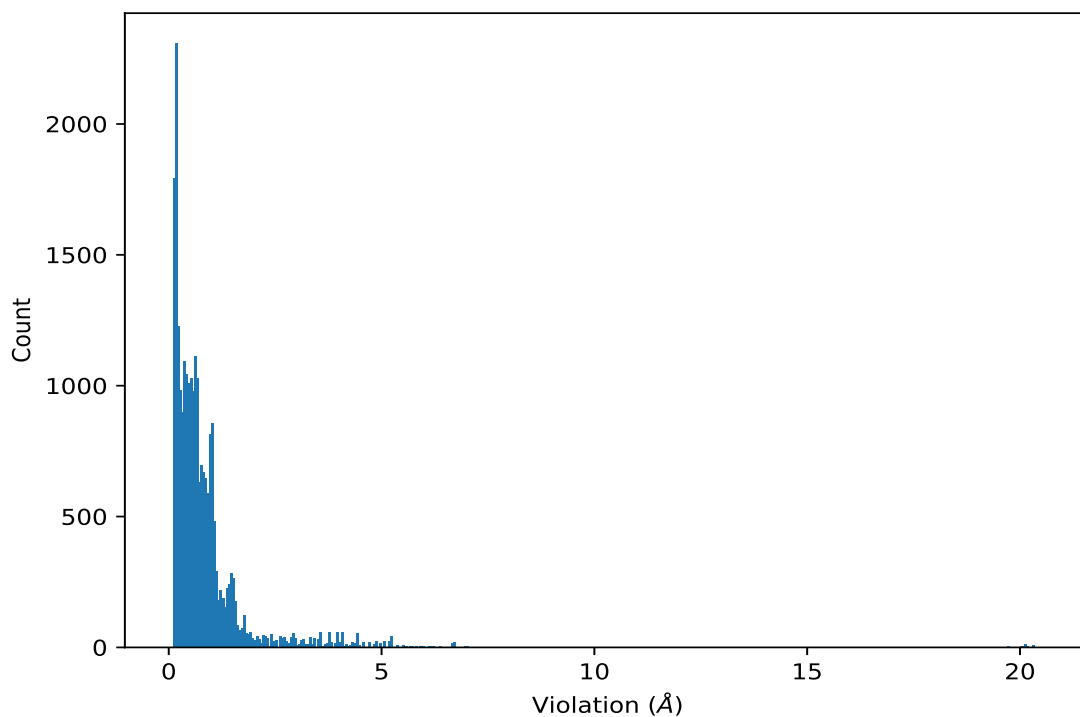
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2457)	1:B:211:VAL:HG22	1:B:173:HIS:HD2	15	3.47	1.82	3.78
(1,2457)	1:B:211:VAL:HG23	1:B:173:HIS:HD1	15	3.47	1.82	3.78
(1,2457)	1:B:211:VAL:HG23	1:B:173:HIS:HD2	15	3.47	1.82	3.78
(1,1213)	1:A:211:VAL:HG21	1:A:173:HIS:HD1	15	3.33	1.86	3.56
(1,1213)	1:A:211:VAL:HG21	1:A:173:HIS:HD2	15	3.33	1.86	3.56
(1,1213)	1:A:211:VAL:HG22	1:A:173:HIS:HD1	15	3.33	1.86	3.56
(1,1213)	1:A:211:VAL:HG22	1:A:173:HIS:HD2	15	3.33	1.86	3.56
(1,1213)	1:A:211:VAL:HG23	1:A:173:HIS:HD1	15	3.33	1.86	3.56
(1,1213)	1:A:211:VAL:HG23	1:A:173:HIS:HD2	15	3.33	1.86	3.56
(1,2610)	2:C:25:LEU:HG	1:A:66:LYS:H	15	3.25	1.05	3.36
(1,2610)	2:C:25:LEU:HG	1:B:66:LYS:H	15	3.25	1.05	3.36
(1,1355)	1:B:27:LYS:H	1:B:27:LYS:HE2	15	2.02	0.62	1.86

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

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)
(1,663)	1:A:119:GLN:H	1:A:189:PHE:HB2	7	20.64
(1,662)	1:A:119:GLN:H	1:A:189:PHE:HB2	7	20.64
(1,663)	1:A:119:GLN:H	1:A:189:PHE:HB2	13	20.54
(1,662)	1:A:119:GLN:H	1:A:189:PHE:HB2	13	20.54
(1,1907)	1:B:119:GLN:H	1:B:189:PHE:HB2	7	20.48
(1,1906)	1:B:119:GLN:H	1:B:189:PHE:HB2	7	20.48
(1,663)	1:A:119:GLN:H	1:A:189:PHE:HB2	3	20.42
(1,662)	1:A:119:GLN:H	1:A:189:PHE:HB2	3	20.42
(1,663)	1:A:119:GLN:H	1:A:189:PHE:HB2	2	20.34
(1,662)	1:A:119:GLN:H	1:A:189:PHE:HB2	2	20.34

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

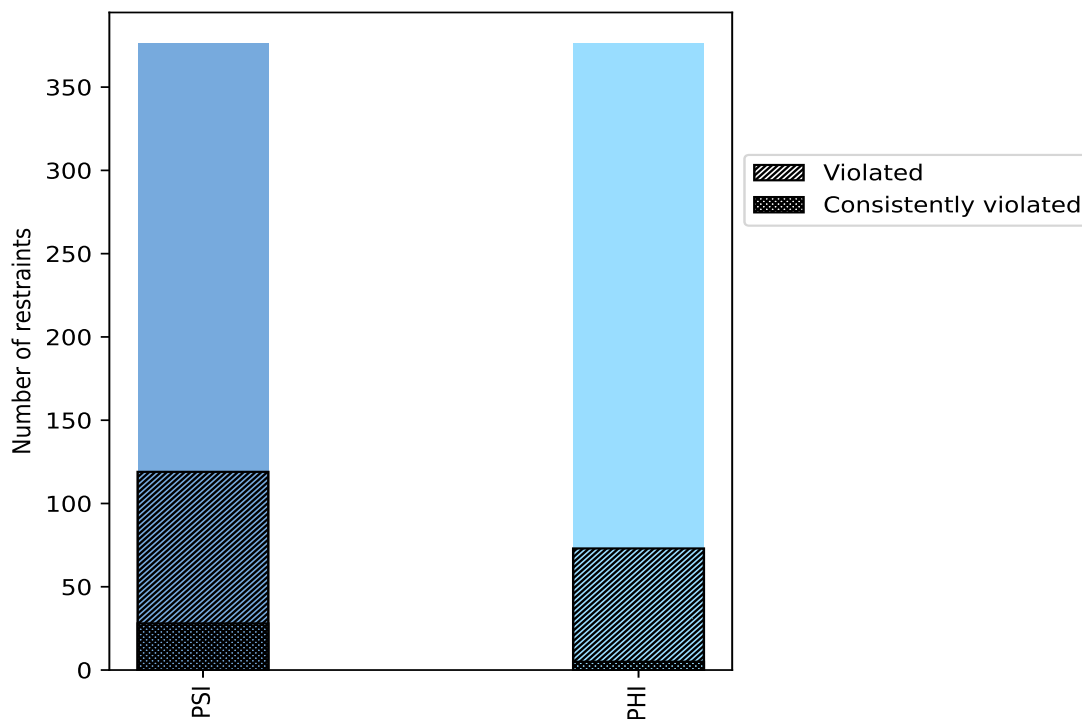
10.1 Summary of dihedral-angle violations [i](#)

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	376	50.0	119	31.6	15.8	28	7.4	3.7
PHI	376	50.0	73	19.4	9.7	5	1.3	0.7
Total	752	100.0	192	25.5	25.5	33	4.4	4.4

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

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



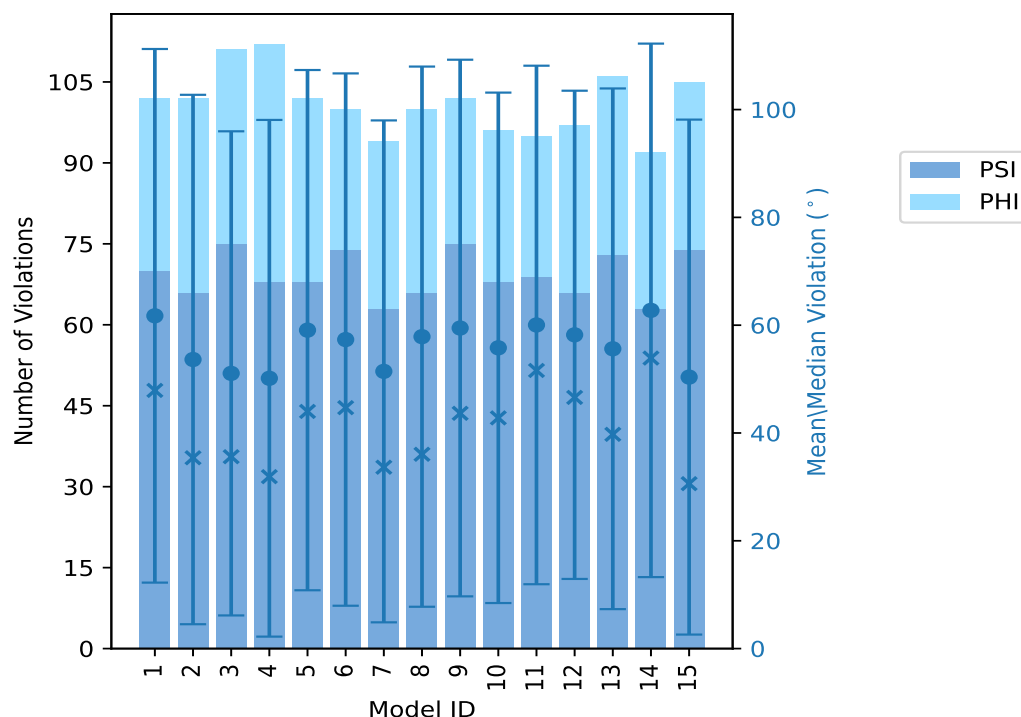
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [\(i\)](#)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	70	32	102	61.74	157.2	49.5	47.9
2	66	36	102	53.63	146.8	49.11	35.4
3	75	36	111	51.06	152.3	44.91	35.6
4	68	44	112	50.15	153.9	47.93	31.9
5	68	34	102	59.08	152.2	48.26	44.0
6	74	26	100	57.33	144.0	49.38	44.7
7	63	31	94	51.43	148.1	46.56	33.65
8	66	34	100	57.87	151.3	50.11	36.05
9	75	27	102	59.47	154.3	49.78	43.65
10	68	28	96	55.8	151.8	47.35	42.8
11	69	26	95	60.04	149.9	48.1	51.6
12	66	31	97	58.21	148.7	45.29	46.6
13	73	33	106	55.62	148.3	48.3	39.75
14	63	29	92	62.75	149.3	49.49	53.9
15	74	31	105	50.37	149.2	47.77	30.6

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

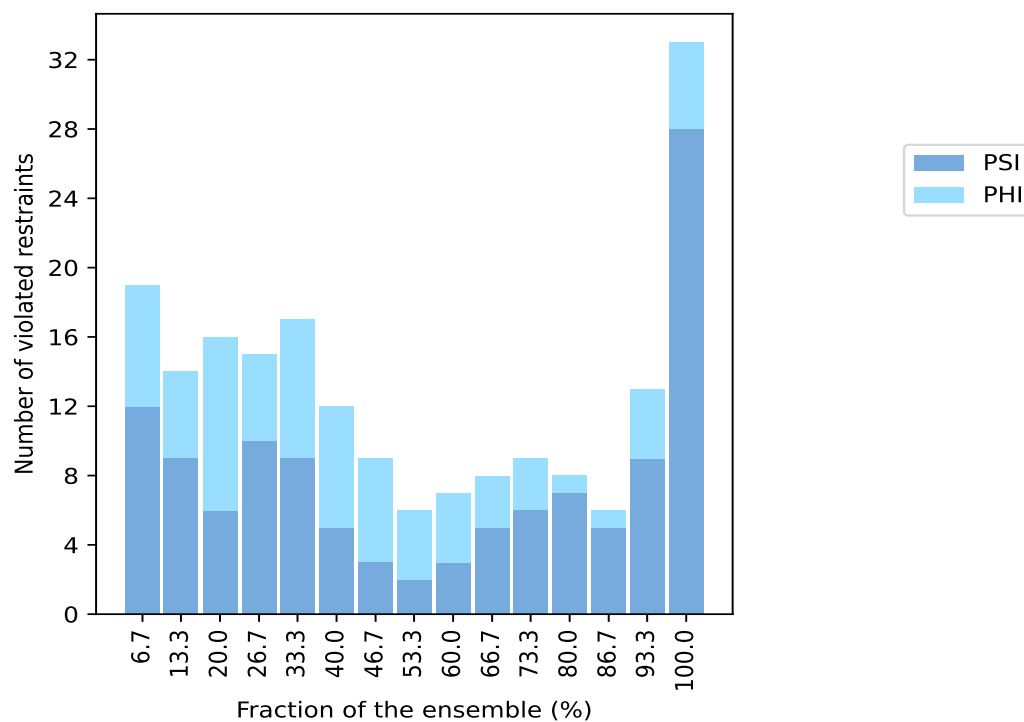
10.3 Dihedral-angle violation statistics for the ensemble

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	%
12	7	19	1	6.7
9	5	14	2	13.3
6	10	16	3	20.0
10	5	15	4	26.7
9	8	17	5	33.3
5	7	12	6	40.0
3	6	9	7	46.7
2	4	6	8	53.3
3	4	7	9	60.0
5	3	8	10	66.7
6	3	9	11	73.3
7	1	8	12	80.0
5	1	6	13	86.7
9	4	13	14	93.3
28	5	33	15	100.0

¹ Number of models with violations

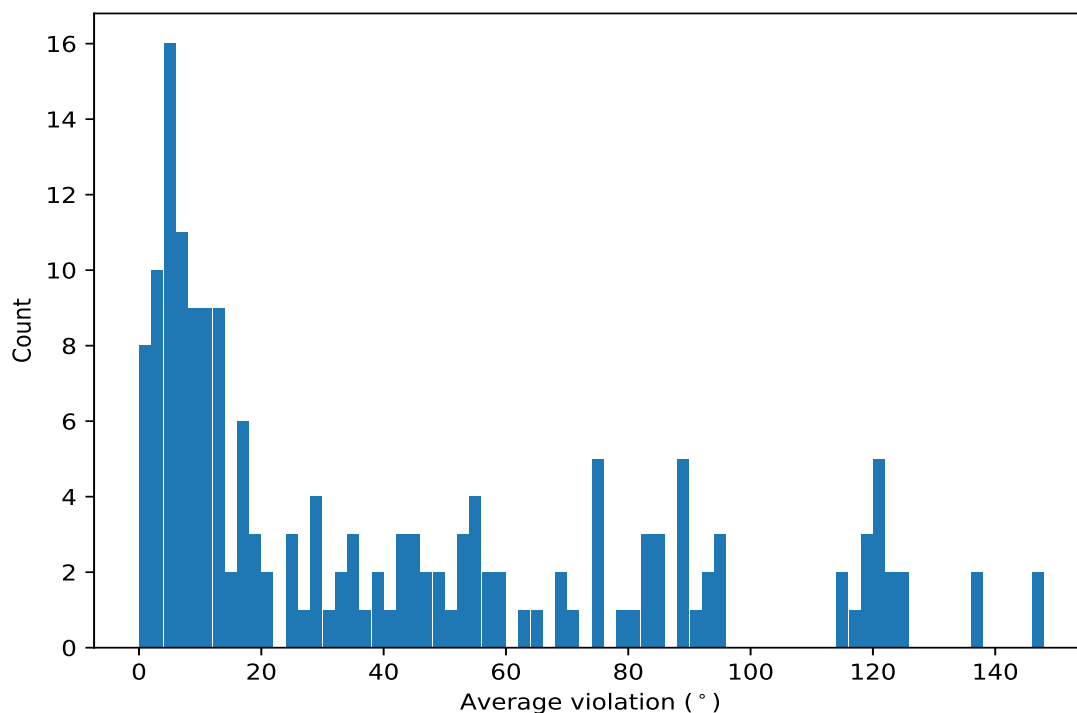
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

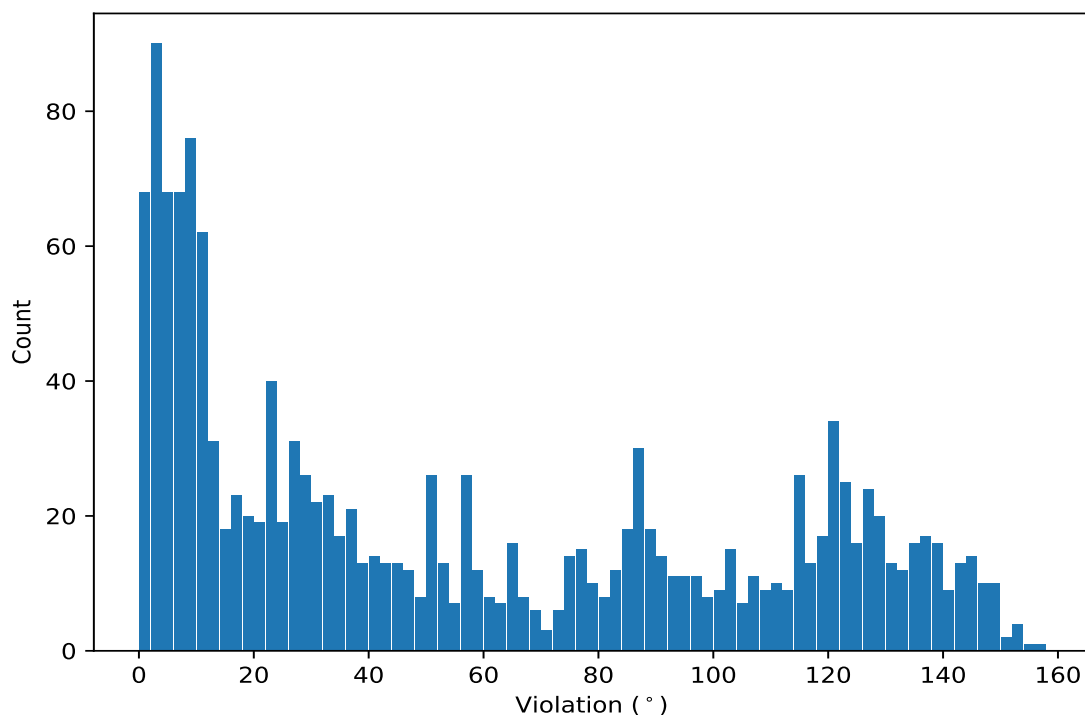
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,38)	1:A:26:PRO:N	1:A:26:PRO:CA	1:A:26:PRO:C	1:A:27:LYS:N	15	147.07	3.62	146.7
(1,414)	1:B:26:PRO:N	1:B:26:PRO:CA	1:B:26:PRO:C	1:B:27:LYS:N	15	146.71	4.62	148.7
(1,438)	1:B:39:PRO:N	1:B:39:PRO:CA	1:B:39:PRO:C	1:B:40:ASN:N	15	136.64	8.25	137.4
(1,62)	1:A:39:PRO:N	1:A:39:PRO:CA	1:A:39:PRO:C	1:A:40:ASN:N	15	136.29	10.77	137.8
(1,470)	1:B:60:PRO:N	1:B:60:PRO:CA	1:B:60:PRO:C	1:B:61:LEU:N	15	124.22	11.91	126.6
(1,584)	1:B:123:ASN:N	1:B:123:ASN:CA	1:B:123:ASN:C	1:B:124:ILE:N	15	123.29	4.74	124.9
(1,94)	1:A:60:PRO:N	1:A:60:PRO:CA	1:A:60:PRO:C	1:A:61:LEU:N	15	122.55	9.58	124.6
(1,336)	1:A:198:MET:N	1:A:198:MET:CA	1:A:198:MET:C	1:A:199:GLY:N	15	121.33	1.43	120.8
(1,614)	1:B:141:ILE:N	1:B:141:ILE:CA	1:B:141:ILE:C	1:B:142:THR:N	15	121.2	14.55	122.1
(1,712)	1:B:198:MET:N	1:B:198:MET:CA	1:B:198:MET:C	1:B:199:GLY:N	15	121.08	0.71	120.8

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 (°)
(1,62)	1:A:39:PRO:N	1:A:39:PRO:CA	1:A:39:PRO:C	1:A:40:ASN:N	1	157.2
(1,438)	1:B:39:PRO:N	1:B:39:PRO:CA	1:B:39:PRO:C	1:B:40:ASN:N	9	154.3
(1,38)	1:A:26:PRO:N	1:A:26:PRO:CA	1:A:26:PRO:C	1:A:27:LYS:N	4	153.9
(1,414)	1:B:26:PRO:N	1:B:26:PRO:CA	1:B:26:PRO:C	1:B:27:LYS:N	4	153.1
(1,38)	1:A:26:PRO:N	1:A:26:PRO:CA	1:A:26:PRO:C	1:A:27:LYS:N	3	152.3
(1,414)	1:B:26:PRO:N	1:B:26:PRO:CA	1:B:26:PRO:C	1:B:27:LYS:N	5	152.2
(1,38)	1:A:26:PRO:N	1:A:26:PRO:CA	1:A:26:PRO:C	1:A:27:LYS:N	10	151.8
(1,414)	1:B:26:PRO:N	1:B:26:PRO:CA	1:B:26:PRO:C	1:B:27:LYS:N	8	151.3
(1,414)	1:B:26:PRO:N	1:B:26:PRO:CA	1:B:26:PRO:C	1:B:27:LYS:N	11	149.9
(1,414)	1:B:26:PRO:N	1:B:26:PRO:CA	1:B:26:PRO:C	1:B:27:LYS:N	9	149.5