



wwPDB NMR Structure Validation Summary Report ⓘ

Dec 25, 2024 – 02:40 AM EST

PDB ID : 2RSV
BMRB ID : 11506
Title : Solution structure of human full-length vaccinia related kinase 1 (VRK1)
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Deposited on : 2012-07-12

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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 : 4.02b-467
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) : 2.40

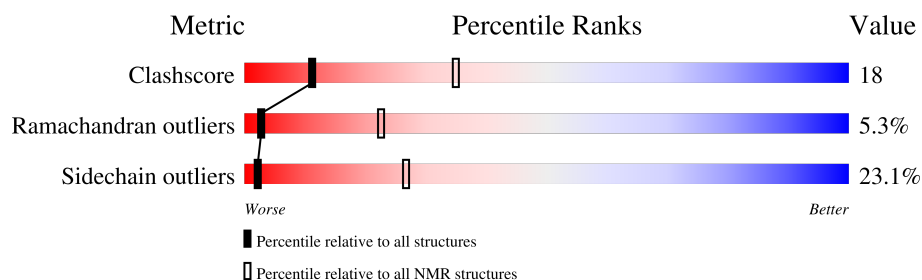
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 52%.

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	403	<div> <div>35%</div> <div>34%</div> <div>.</div> <div>29%</div> </div>

2 Ensemble composition and analysis

This entry contains 18 models. Model 13 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:24-A:44, A:50-A:204, A:223-A:309, A:315-A:336 (285)	1.50	13

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 and 7 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6497 atoms, of which 3260 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Serine/threonine-protein kinase VRK1.

Mol	Chain	Residues	Atoms						Trace
1	A	403	Total	C	H	N	O	S	0
			6497	2043	3260	571	609	14	

There are 7 discrepancies between the modelled and reference sequences:

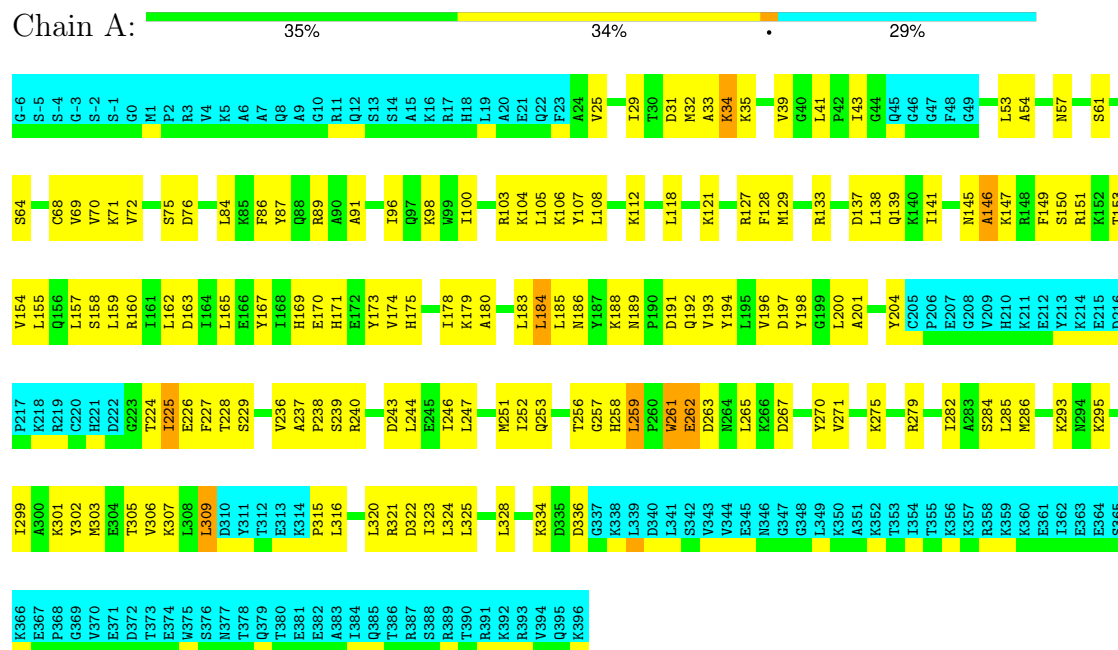
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q99986
A	-5	SER	-	expression tag	UNP Q99986
A	-4	SER	-	expression tag	UNP Q99986
A	-3	GLY	-	expression tag	UNP Q99986
A	-2	SER	-	expression tag	UNP Q99986
A	-1	SER	-	expression tag	UNP Q99986
A	0	GLY	-	expression tag	UNP Q99986

4 Residue-property plots

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.

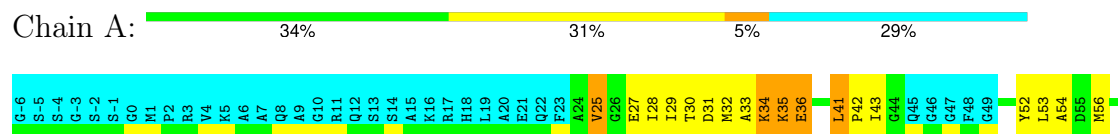
- Molecule 1: Serine/threonine-protein kinase VRK1



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

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Serine/threonine-protein kinase VRK1



S61	T153	C220	E304	P368
	V154	H221	T305	G369
C68	L155	D222	V306	V370
V69			K307	E371
V70	S158	I225	L308	D372
V71	L159	E226	L309	T373
V72	R160	F227	D310	E374
E73		T228	Y311	G375
P74	D163	S229	T312	S376
S75	I164		E313	N377
D76	L165	N234	K314	T378
	E166	G235	P315	Q379
E83	Y167	V236	L316	T380
E84	I168	A237		E381
K85	H169	F238	L320	E382
	E170	S239	R321	A383
Y87	H171		D322	I384
Q88	E172	E245	I323	Q385
R89	Y173	T246	L324	T386
A90	V174	L247	L325	R387
A91	H175	G248		S388
			L328	R389
K98	G176	M251	I331	T390
Y99	D177	I252	G332	R391
I100	K178	Q253	S333	K392
	K179		K334	R393
K104	L183	G257	D335	V394
L105	L184	H258	L336	K396
K106	L185	L259	G337	
Y107	N186	P260	K338	
L108	Y187	E261	L339	
G109	K188	E262	D340	
			L341	
K112	D191	N264	S342	
L118	Q192	L265	V343	
	V193	K266	V344	
	Y194	D267	E345	
R127			M346	
F128	D197	Y270	G347	
M129	Y198	V271	G348	
I130		R272	L349	
	A201		K350	
R133	Y202	Y278	A351	
S136	R203	R279	K352	
D137	Y204		T353	
L138	C205	I282	I354	
Q139	P206	S284	T355	
K140	E207	S284	K356	
G208	G208	L285	K357	
I141	V209	N286	D287	
Y142	H210		R358	
E143	K211		K359	
A144	E212	P291	K360	
N145	Y213	E292	E361	
A146	K214	K293	I362	
K147	E215	N294	E363	
R148	D216		E364	
F149	P217	K301	S365	
S150	K218	Y302	K366	
	R219	M303	E367	

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing*.

Of the 200 calculated structures, 18 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
CNS	structure solution	
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	2601
Number of shifts mapped to atoms	2601
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	52%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

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	2313	2336	2330	83±7
All	All	41634	42048	41940	1486

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 18.

5 of 559 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:309:LEU:HD21	1:A:316:LEU:HD22	0.93	1.40	7	1
1:A:141:ILE:HD11	1:A:185:LEU:HD11	0.91	1.37	1	10
1:A:259:LEU:HD22	1:A:261:TRP:CH2	0.89	2.02	2	18
1:A:278:TYR:CD1	1:A:285:LEU:HD12	0.85	2.06	16	3
1:A:29:ILE:HD12	1:A:128:PHE:CZ	0.84	2.06	9	14

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	285/403 (71%)	237±3 (83±1%)	33±3 (12±1%)	15±3 (5±1%)	3	22
All	All	5130/7254 (71%)	4259 (83%)	600 (12%)	271 (5%)	3	22

5 of 66 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	146	ALA	18
1	A	261	TRP	18
1	A	197	ASP	14
1	A	257	GLY	13
1	A	191	ASP	12

6.3.2 Protein sidechains ⓘ

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	250/349 (72%)	192±6 (77±2%)	58±6 (23±2%)	2	27
All	All	4500/6282 (72%)	3459 (77%)	1041 (23%)	2	27

5 of 169 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	259	LEU	18
1	A	251	MET	15
1	A	184	LEU	14
1	A	309	LEU	13
1	A	32	MET	12

6.3.3 RNA ⓘ

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 52% for the well-defined parts and 46% 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	2601
Number of shifts mapped to atoms	2601
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	363	0.12 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	325	1.09 ± 0.09	Should be checked
$^{13}\text{C}'$	363	-0.01 ± 0.09	None needed (< 0.5 ppm)
^{15}N	343	-0.15 ± 0.11	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 52%, i.e. 2114 atoms were assigned a chemical shift out of a possible 4029. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1092/1419 (77%)	266/577 (46%)	560/570 (98%)	266/272 (98%)
Sidechain	896/2270 (39%)	474/1471 (32%)	422/707 (60%)	0/92 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	126/340 (37%)	63/161 (39%)	58/162 (36%)	5/17 (29%)
Overall	2114/4029 (52%)	803/2209 (36%)	1040/1439 (72%)	271/381 (71%)

7.1.4 Statistically unusual chemical shifts [i](#)

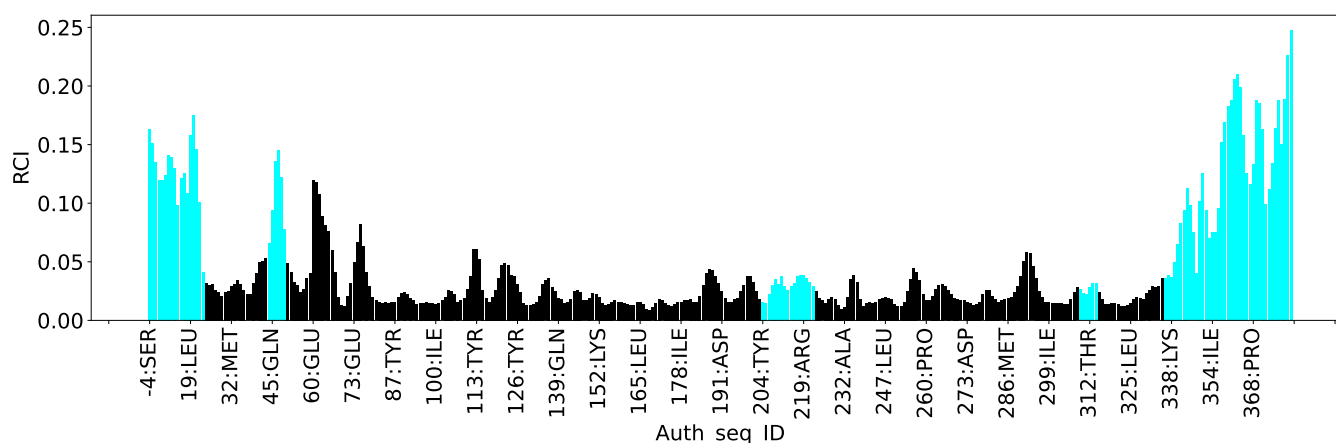
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	29	ILE	HG21	-0.64	-0.56 – 2.11	-5.3
1	A	29	ILE	HG22	-0.64	-0.56 – 2.11	-5.3
1	A	29	ILE	HG23	-0.64	-0.56 – 2.11	-5.3
1	A	29	ILE	HD11	-0.81	-0.72 – 2.09	-5.3
1	A	29	ILE	HD12	-0.81	-0.72 – 2.09	-5.3
1	A	29	ILE	HD13	-0.81	-0.72 – 2.09	-5.3

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	3061
Intra-residue ($ i-j =0$)	440
Sequential ($ i-j =1$)	710
Medium range ($ i-j >1$ and $ i-j <5$)	599
Long range ($ i-j \geq 5$)	1224
Inter-chain	0
Hydrogen bond restraints	88
Disulfide bond restraints	0
Total dihedral-angle restraints	322
Number of unmapped restraints	0
Number of restraints per residue	8.4
Number of long range restraints per residue ¹	3.1

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)	0.8	0.14
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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)	0.1	1.13
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis [i](#)

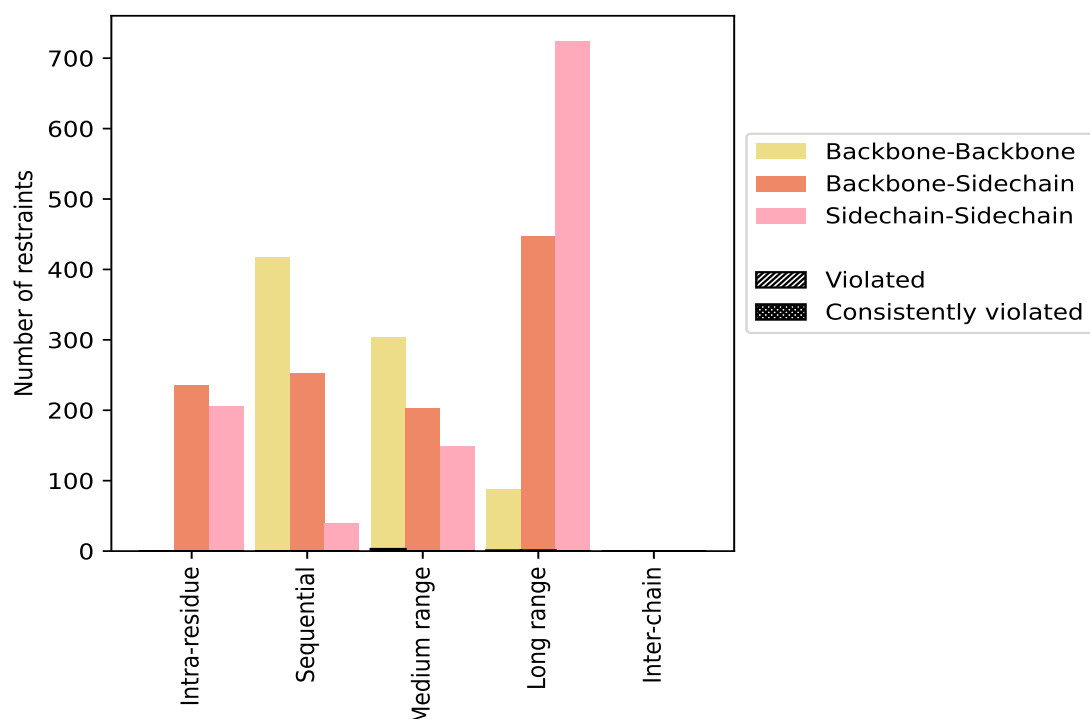
9.1 Summary of distance violations [i](#)

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)	440	14.4	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	235	7.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	205	6.7	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	710	23.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	417	13.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	253	8.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	40	1.3	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	599	19.6	3	0.5	0.1	0	0.0	0.0
Backbone-Backbone	303	9.9	3	1.0	0.1	0	0.0	0.0
Backbone-Sidechain	148	4.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	148	4.8	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	1224	40.0	2	0.2	0.1	0	0.0	0.0
Backbone-Backbone	87	2.8	1	1.1	0.0	0	0.0	0.0
Backbone-Sidechain	413	13.5	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	724	23.7	0	0.0	0.0	0	0.0	0.0
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	88	2.9	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	3061	100.0	5	0.2	0.2	0	0.0	0.0
Backbone-Backbone	807	26.4	4	0.5	0.1	0	0.0	0.0
Backbone-Sidechain	1137	37.1	1	0.1	0.0	0	0.0	0.0
Sidechain-Sidechain	1117	36.5	0	0.0	0.0	0	0.0	0.0

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and 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	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	1	1	0	2	0.1	0.1	0.0	0.1
3	0	0	1	0	0	1	0.1	0.1	0.0	0.1
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	1	0	0	1	0.13	0.13	0.0	0.13
6	0	0	1	0	0	1	0.12	0.12	0.0	0.12
7	0	0	1	1	0	2	0.12	0.12	0.0	0.12
8	0	0	1	0	0	1	0.11	0.11	0.0	0.11
9	0	0	1	0	0	1	0.13	0.13	0.0	0.13
10	0	0	2	0	0	2	0.12	0.13	0.01	0.12

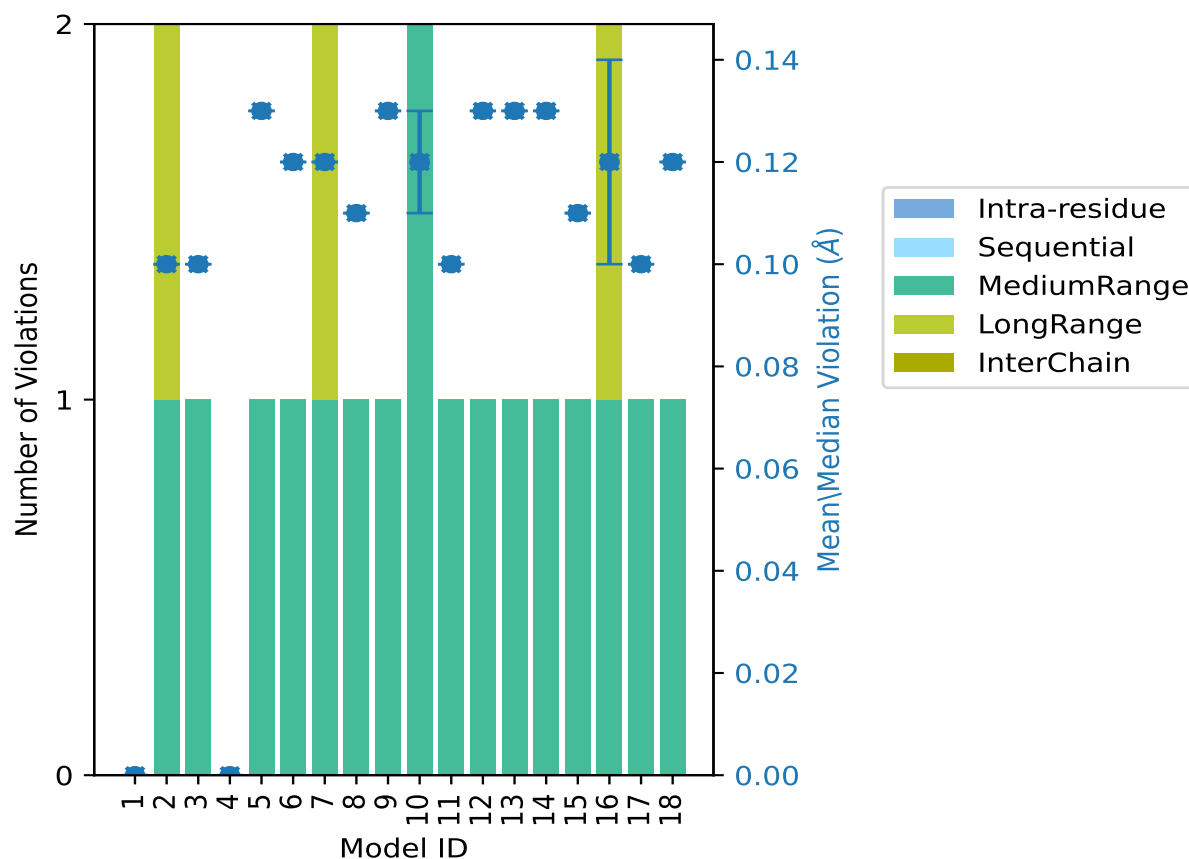
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	1	0	0	1	0.1	0.1	0.0	0.1
12	0	0	1	0	0	1	0.13	0.13	0.0	0.13
13	0	0	1	0	0	1	0.13	0.13	0.0	0.13
14	0	0	1	0	0	1	0.13	0.13	0.0	0.13
15	0	0	1	0	0	1	0.11	0.11	0.0	0.11
16	0	0	1	1	0	2	0.12	0.14	0.02	0.12
17	0	0	1	0	0	1	0.1	0.1	0.0	0.1
18	0	0	1	0	0	1	0.12	0.12	0.0	0.12

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](#)

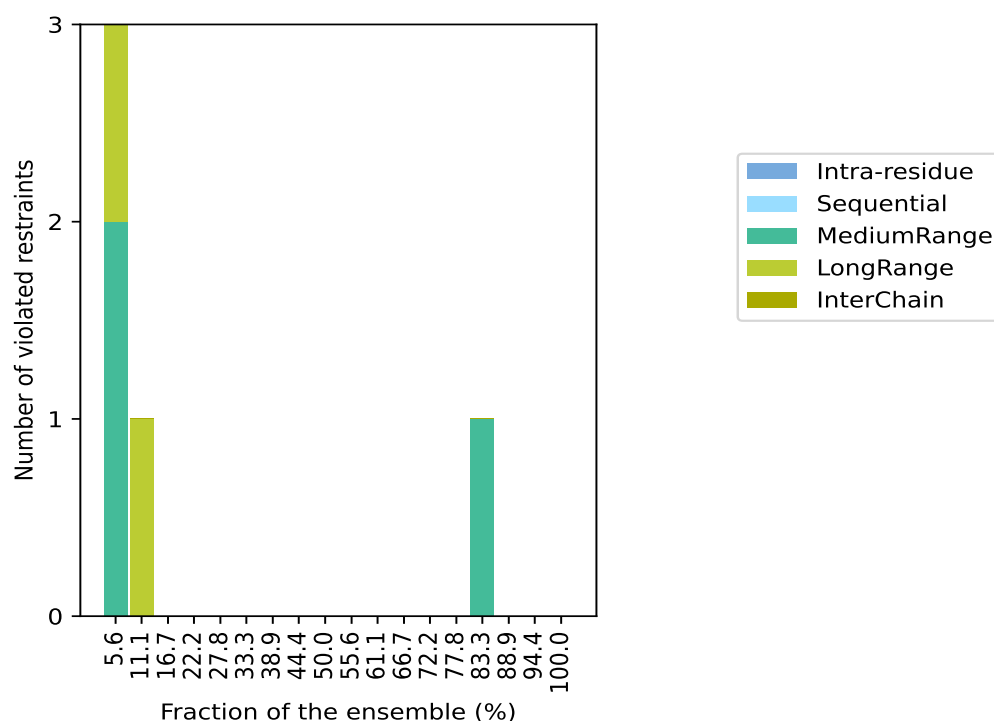
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2968(IR:440, SQ:710, MR:596, LR:1222, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	2	1	0	3	1	5.6
0	0	0	1	0	1	2	11.1
0	0	0	0	0	0	3	16.7
0	0	0	0	0	0	4	22.2
0	0	0	0	0	0	5	27.8
0	0	0	0	0	0	6	33.3
0	0	0	0	0	0	7	38.9
0	0	0	0	0	0	8	44.4
0	0	0	0	0	0	9	50.0
0	0	0	0	0	0	10	55.6
0	0	0	0	0	0	11	61.1
0	0	0	0	0	0	12	66.7
0	0	0	0	0	0	13	72.2
0	0	0	0	0	0	14	77.8
0	0	1	0	0	1	15	83.3
0	0	0	0	0	0	16	88.9
0	0	0	0	0	0	17	94.4
0	0	0	0	0	0	18	100.0

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

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

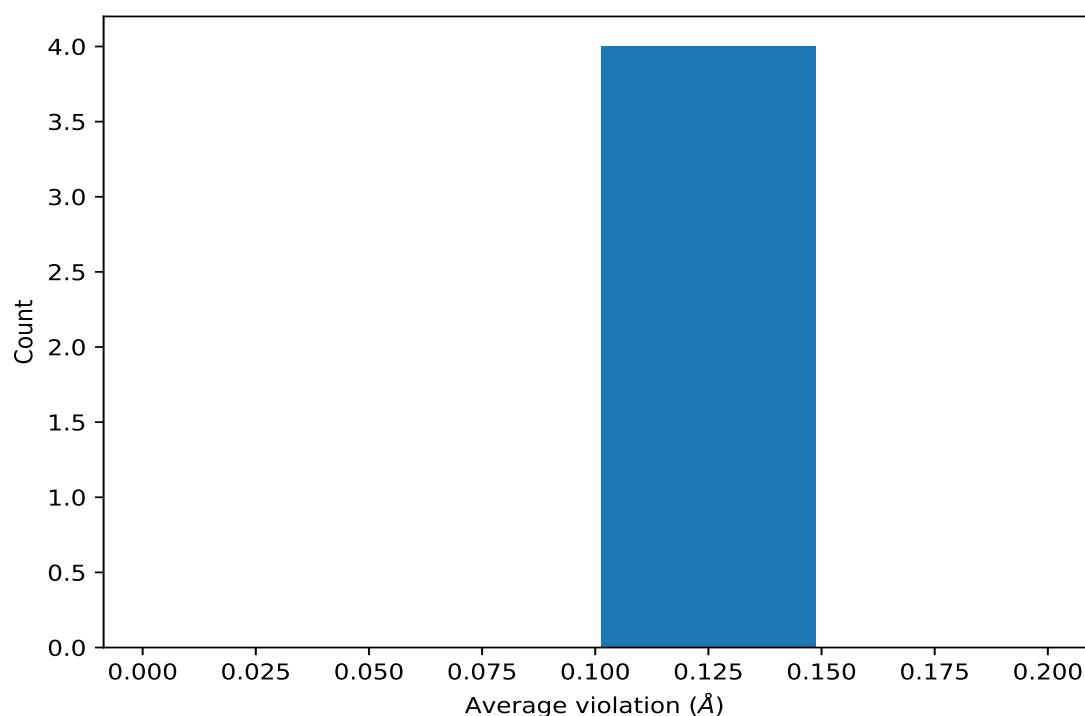
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 violation for each restraint sorted by number of violated models and the mean 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.

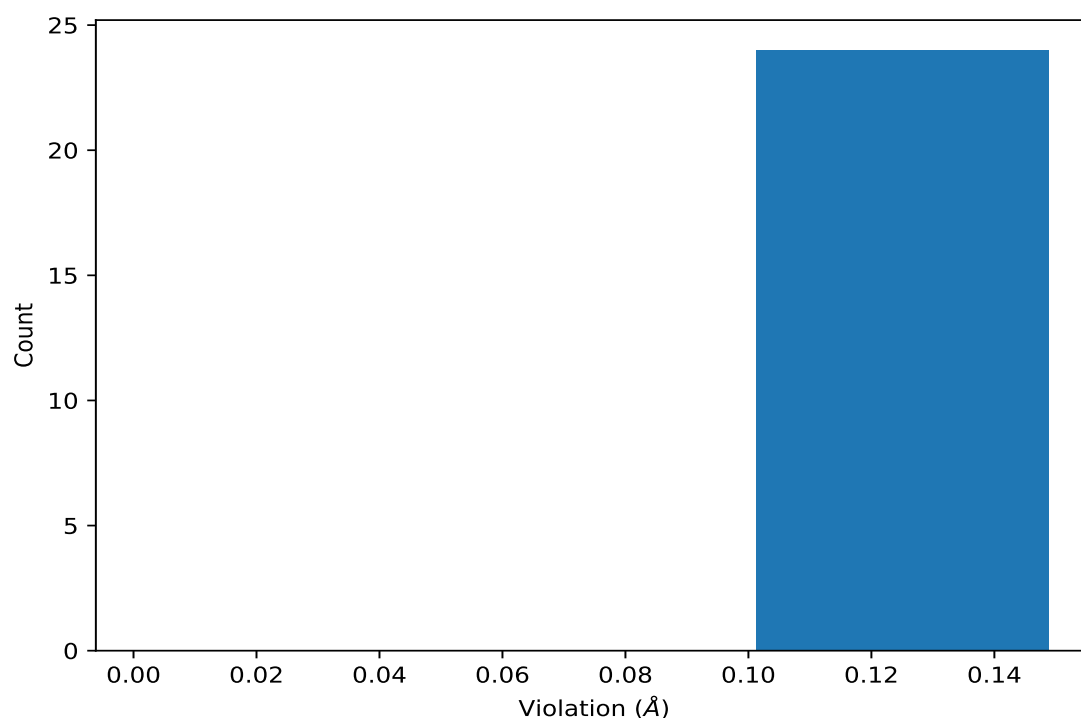
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	15	0.12	0.01	0.12
(1,1335)	1:138:A:LEU:HD11	1:194:A:TYR:H	2	0.11	0.0	0.11
(1,1335)	1:138:A:LEU:HD12	1:194:A:TYR:H	2	0.11	0.0	0.11
(1,1335)	1:138:A:LEU:HD13	1:194:A:TYR:H	2	0.11	0.0	0.11

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)
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	16	0.14
(1,1089)	1:121:A:LYS:H	1:123:A:GLY:H	12	0.13
(1,818)	1:189:A:ASN:H	1:187:A:TYR:H	10	0.13
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	5	0.13
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	9	0.13
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	13	0.13
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	14	0.13
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	6	0.12
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	7	0.12
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	10	0.12

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

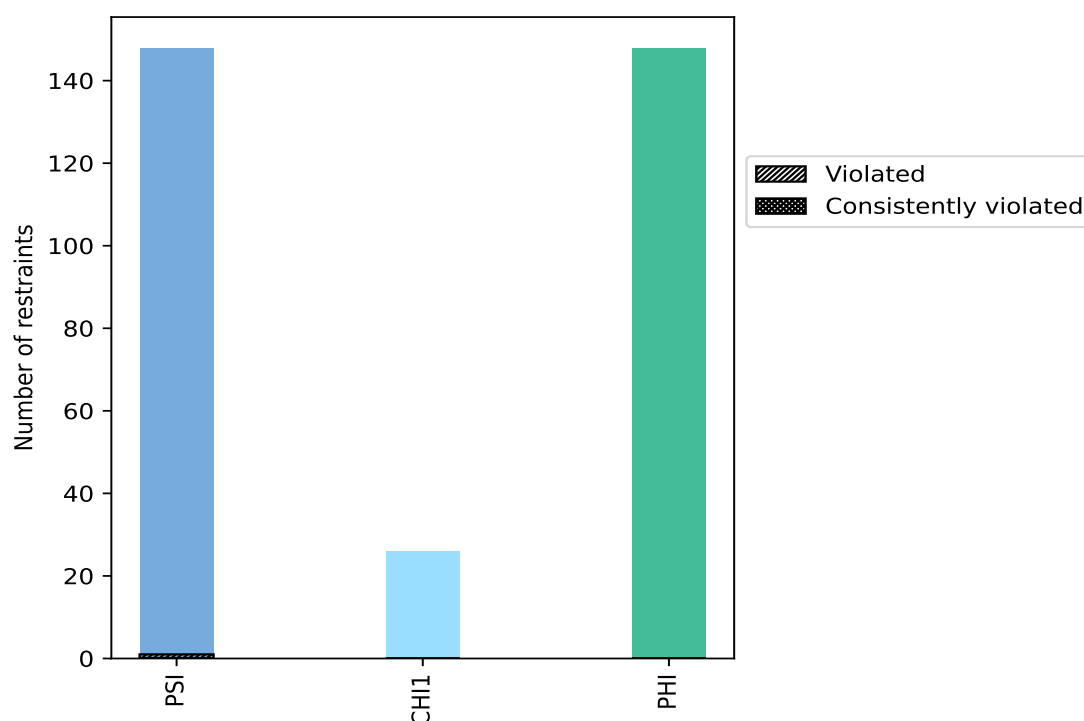
10.1 Summary of dihedral-angle violations [i](#)

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	148	46.0	1	0.7	0.3	0	0.0	0.0
CHI1	26	8.1	0	0.0	0.0	0	0.0	0.0
PHI	148	46.0	0	0.0	0.0	0	0.0	0.0
Total	322	100.0	1	0.3	0.3	0	0.0	0.0

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](#)



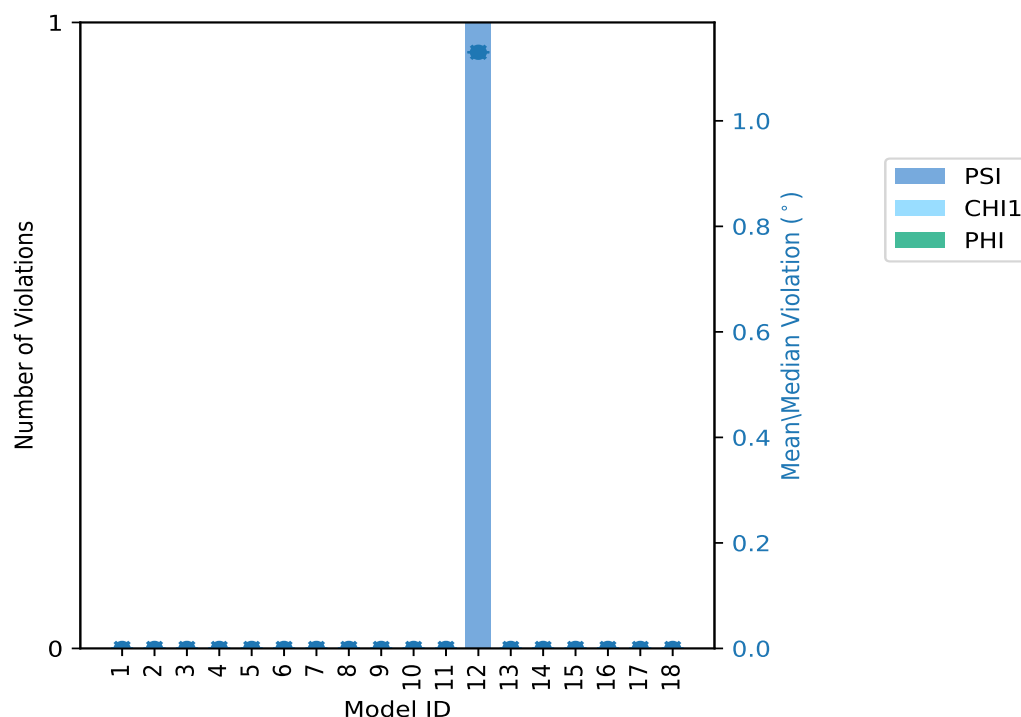
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	CHI1	PHI	Total				
1	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0.0	0.0	0.0	0.0
12	1	0	0	1	1.13	1.13	0.0	1.13
13	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0.0	0.0	0.0	0.0

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



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

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

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

Number of violated restraints				Fraction of the ensemble	
PSI	CHI1	PHI	Total	Count ¹	%
1	0	0	1	1	5.6
0	0	0	0	2	11.1
0	0	0	0	3	16.7
0	0	0	0	4	22.2
0	0	0	0	5	27.8
0	0	0	0	6	33.3
0	0	0	0	7	38.9
0	0	0	0	8	44.4
0	0	0	0	9	50.0
0	0	0	0	10	55.6
0	0	0	0	11	61.1

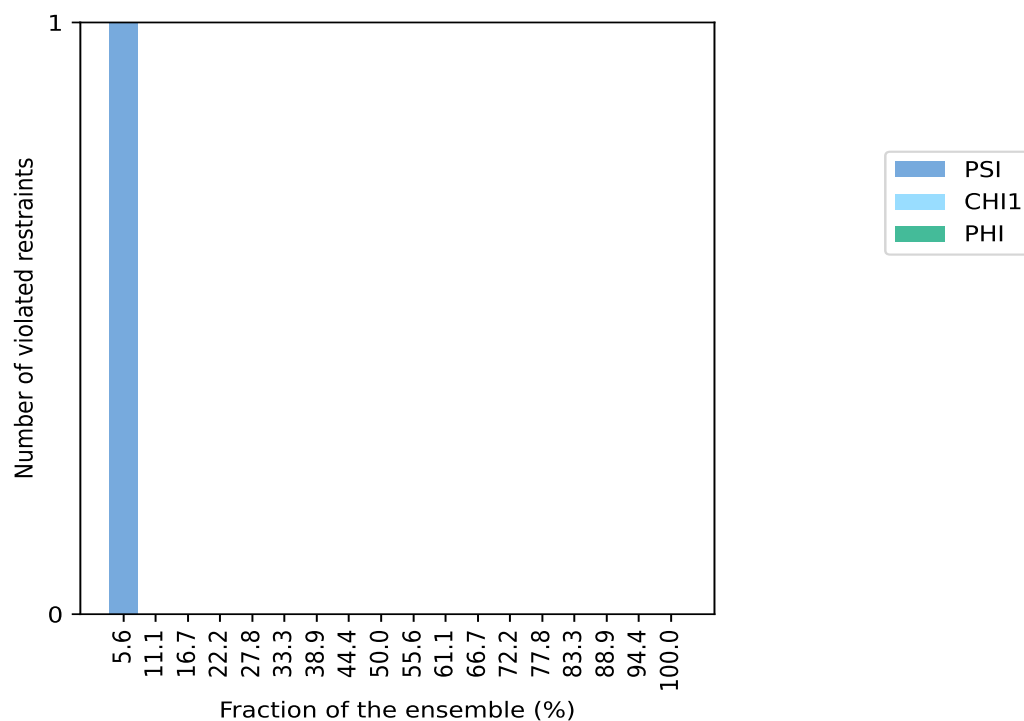
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Number of violated restraints				Fraction of the ensemble	
PSI	CHI1	PHI	Total	Count ¹	%
0	0	0	0	12	66.7
0	0	0	0	13	72.2
0	0	0	0	14	77.8
0	0	0	0	15	83.3
0	0	0	0	16	88.9
0	0	0	0	17	94.4
0	0	0	0	18	100.0

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](#)

No violations found

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.

Data insufficient to plot histogram

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

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its 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 (°)
(1,82)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:ASN:N	12	1.13