



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2LJD  
BMRB ID : 17930  
Title : monophosphorylated (747pY) beta3 integrin cytoplasmic tail under membrane mimetic conditions  
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
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

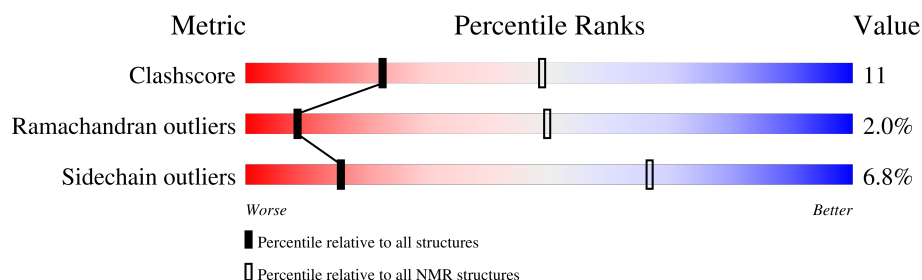
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 87%.

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  $\geq 3$ , 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	67	

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:717-A:746, A:748-A:762 (45)	1.49	1

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, 3, 4, 5, 7, 8, 9, 10, 12, 13, 14, 15
2	2, 6, 11

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 789 atoms, of which 390 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						Trace
1	A	47	Total	C	H	N	O	P	0
			789	250	390	70	78	1	

There are 20 discrepancies between the modelled and reference sequences:

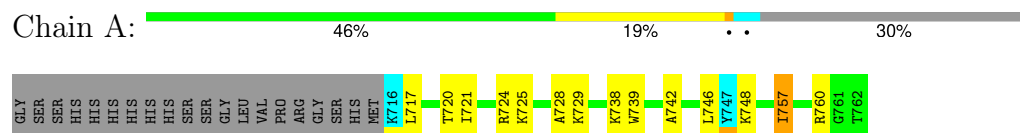
Chain	Residue	Modelled	Actual	Comment	Reference
A	696	GLY	-	expression tag	UNP P05106
A	697	SER	-	expression tag	UNP P05106
A	698	SER	-	expression tag	UNP P05106
A	699	HIS	-	expression tag	UNP P05106
A	700	HIS	-	expression tag	UNP P05106
A	701	HIS	-	expression tag	UNP P05106
A	702	HIS	-	expression tag	UNP P05106
A	703	HIS	-	expression tag	UNP P05106
A	704	HIS	-	expression tag	UNP P05106
A	705	SER	-	expression tag	UNP P05106
A	706	SER	-	expression tag	UNP P05106
A	707	GLY	-	expression tag	UNP P05106
A	708	LEU	-	expression tag	UNP P05106
A	709	VAL	-	expression tag	UNP P05106
A	710	PRO	-	expression tag	UNP P05106
A	711	ARG	-	expression tag	UNP P05106
A	712	GLY	-	expression tag	UNP P05106
A	713	SER	-	expression tag	UNP P05106
A	714	HIS	-	expression tag	UNP P05106
A	715	MET	-	expression tag	UNP P05106

## 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.

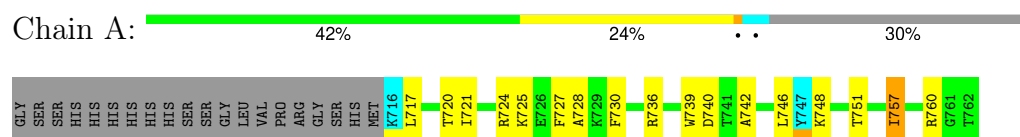
- Molecule 1: Integrin beta-3



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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Integrin beta-3



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry 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
CYANA	structure solution	2.1
CNS	refinement	1.21

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	590
Number of shifts mapped to atoms	590
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR

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	0.79±0.02	0±0/380 ( 0.0± 0.1%)	0.43±0.01	0±0/509 ( 0.0± 0.0%)
All	All	0.79	1/5700 ( 0.0%)	0.43	0/7635 ( 0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	748	LYS	N-CA	-5.17	1.36	1.46	11	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	374	369	368	8±3
All	All	5610	5535	5520	124

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 11.

5 of 53 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:757:ILE:HD13	1:A:760:ARG:HA	0.98	1.33	1	10
1:A:754:PHE:HB2	1:A:757:ILE:HD11	0.76	1.57	13	6
1:A:748:LYS:HG3	1:A:760:ARG:HB3	0.75	1.56	15	1
1:A:739:TRP:HB3	1:A:742:ALA:HB3	0.68	1.64	4	8
1:A:723:ASP:HB3	1:A:727:PHE:HB3	0.67	1.65	3	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	44/67 (66%)	38±1 (86±3%)	5±2 (12±4%)	1±1 (2±2%)	8	50
All	All	660/1005 (66%)	570 (86%)	77 (12%)	13 (2%)	8	50

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)
1	A	746	LEU	10
1	A	761	GLY	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	39/57 (68%)	36±1 (93±2%)	3±1 (7±2%)	16	66
All	All	585/855 (68%)	545 (93%)	40 (7%)	16	66

5 of 11 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	757	ILE	15
1	A	729	LYS	6
1	A	725	LYS	5
1	A	720	THR	3
1	A	734	ARG	3

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	PTR	A	747	1	15,16,17	1.01±0.10	1±1 (9±4%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	PTR	A	747	1	17,22,24	0.75±0.02	0±0 (0±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	747	1	-	0±0,10,11,13	0±0,1,1,1

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	747	PTR	CA-N	2.85	1.40	1.48	7	6
1	A	747	PTR	P-O3P	2.84	1.44	1.54	12	14
1	A	747	PTR	P-OH	2.39	1.55	1.59	8	2

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	747	PTR	O3P-P-O2P	2.08	115.62	107.80	8	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 87% 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 [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	590
Number of shifts mapped to atoms	590
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	46	$0.34 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	45	$0.16 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	43	$0.28 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	45	$0.17 \pm 0.20$	None needed ( $< 0.5$ ppm)

#### 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 87%, i.e. 557 atoms were assigned a chemical shift out of a possible 641. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	221/224 (99%)	90/90 (100%)	87/90 (97%)	44/44 (100%)
Sidechain	292/358 (82%)	198/229 (86%)	91/110 (83%)	3/19 (16%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	44/59 (75%)	22/29 (76%)	21/27 (78%)	1/3 (33%)
Overall	557/641 (87%)	310/348 (89%)	199/227 (88%)	48/66 (73%)

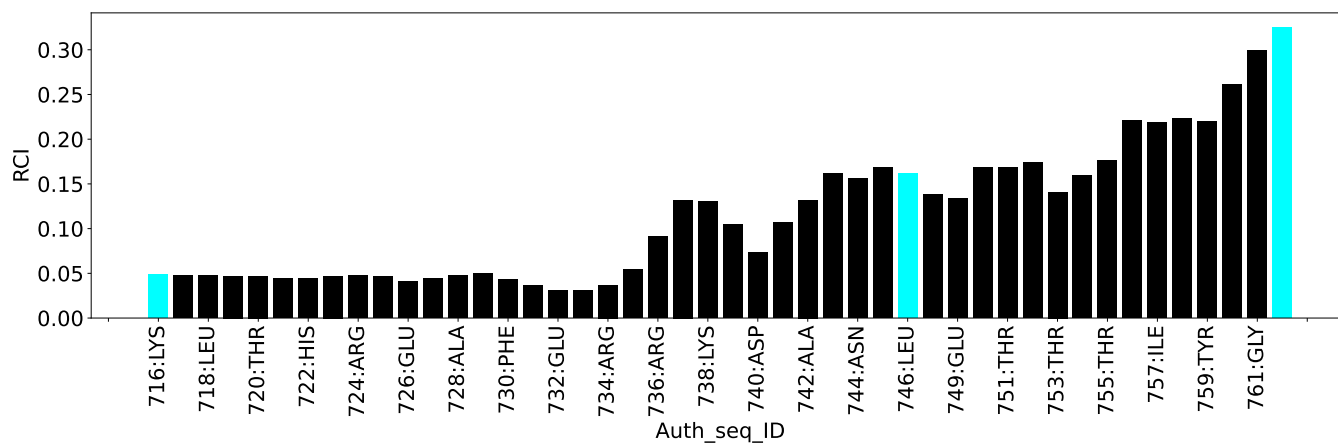
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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	639
Intra-residue ( $ i-j =0$ )	228
Sequential ( $ i-j =1$ )	227
Medium range ( $ i-j >1$ and $ i-j <5$ )	164
Long range ( $ i-j \geq 5$ )	20
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	56
Number of unmapped restraints	0
Number of restraints per residue	10.4
Number of long range restraints per residue <sup>1</sup>	0.3

<sup>1</sup>Long 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)	7.5	0.2
0.2-0.5 (Medium)	3.2	0.49
>0.5 (Large)	0.1	0.51

### 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)	5.5	4.48
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

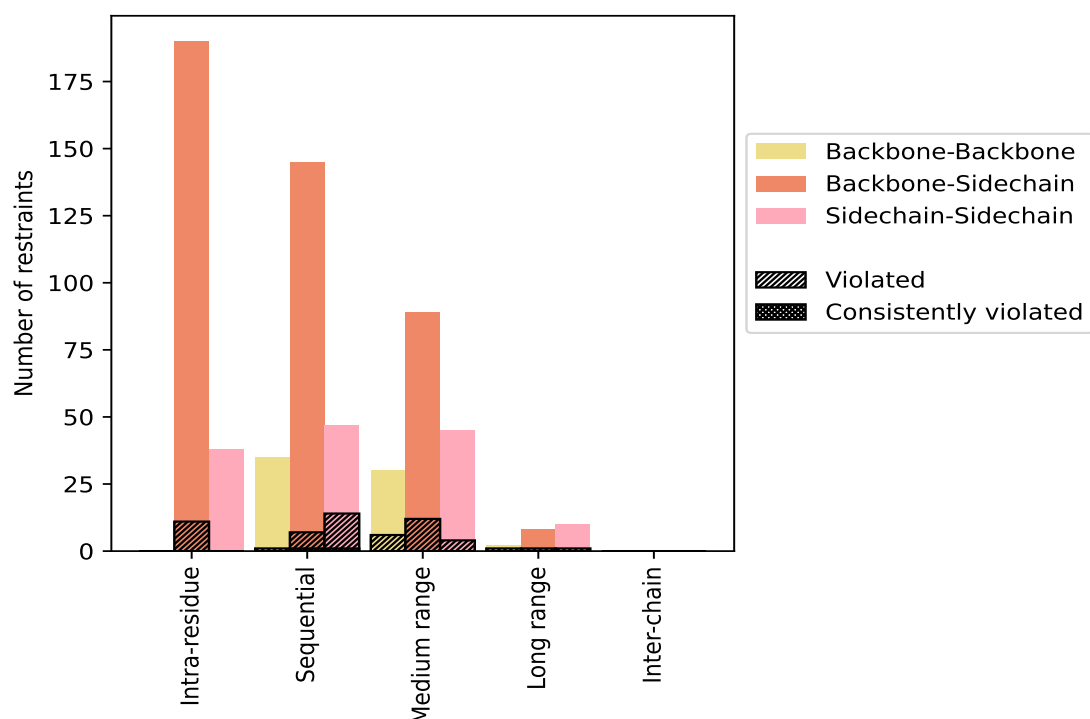
### 9.1 Summary of distance violations ⓘ

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>228</b>	<b>35.7</b>	<b>11</b>	<b>4.8</b>	<b>1.7</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	190	29.7	11	5.8	1.7	0	0.0	0.0
Sidechain-Sidechain	38	5.9	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>227</b>	<b>35.5</b>	<b>22</b>	<b>9.7</b>	<b>3.4</b>	<b>2</b>	<b>0.9</b>	<b>0.3</b>
Backbone-Backbone	35	5.5	1	2.9	0.2	0	0.0	0.0
Backbone-Sidechain	145	22.7	7	4.8	1.1	1	0.7	0.2
Sidechain-Sidechain	47	7.4	14	29.8	2.2	1	2.1	0.2
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>164</b>	<b>25.7</b>	<b>22</b>	<b>13.4</b>	<b>3.4</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	30	4.7	6	20.0	0.9	0	0.0	0.0
Backbone-Sidechain	89	13.9	12	13.5	1.9	0	0.0	0.0
Sidechain-Sidechain	45	7.0	4	8.9	0.6	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>20</b>	<b>3.1</b>	<b>3</b>	<b>15.0</b>	<b>0.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	2	0.3	1	50.0	0.2	0	0.0	0.0
Backbone-Sidechain	8	1.3	1	12.5	0.2	0	0.0	0.0
Sidechain-Sidechain	10	1.6	1	10.0	0.2	0	0.0	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Hydrogen bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>639</b>	<b>100.0</b>	<b>58</b>	<b>9.1</b>	<b>9.1</b>	<b>2</b>	<b>0.3</b>	<b>0.3</b>
Backbone-Backbone	67	10.5	8	11.9	1.3	0	0.0	0.0
Backbone-Sidechain	432	67.6	31	7.2	4.9	1	0.2	0.2
Sidechain-Sidechain	140	21.9	19	13.6	3.0	1	0.7	0.2

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	1	3	6	0	0	10	0.16	0.3	0.06	0.12
2	4	6	5	1	0	16	0.17	0.51	0.1	0.13
3	0	8	2	0	0	10	0.17	0.29	0.07	0.13
4	3	8	1	0	0	12	0.19	0.42	0.1	0.14
5	2	7	3	1	0	13	0.15	0.3	0.06	0.14
6	1	4	4	0	0	9	0.17	0.28	0.06	0.15
7	5	6	6	0	0	17	0.18	0.37	0.08	0.14
8	3	6	4	0	0	13	0.17	0.49	0.11	0.12
9	3	5	2	1	0	11	0.14	0.25	0.05	0.12
10	1	7	2	0	0	10	0.16	0.34	0.08	0.12

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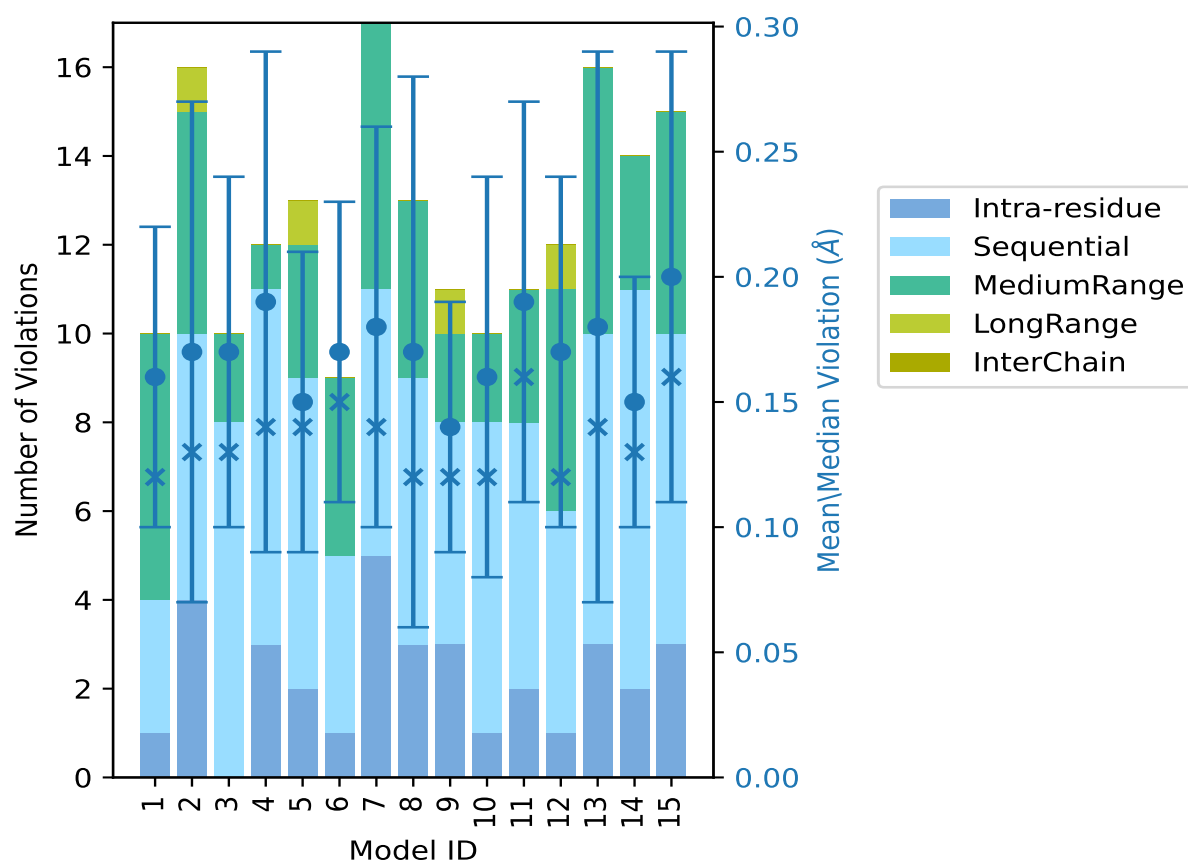


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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	2	6	3	0	0	11	0.19	0.4	0.08	0.16
12	1	5	5	1	0	12	0.17	0.33	0.07	0.12
13	3	7	6	0	0	16	0.18	0.49	0.11	0.14
14	2	9	3	0	0	14	0.15	0.26	0.05	0.13
15	3	7	5	0	0	15	0.2	0.4	0.09	0.16

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble ⓘ

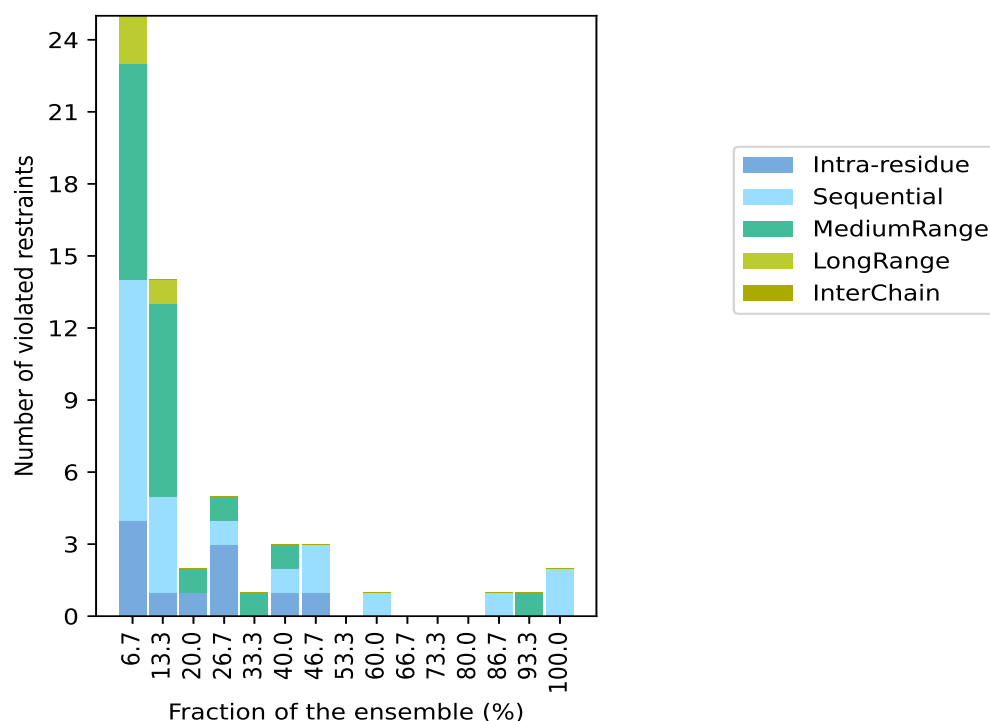
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 581(IR:217, SQ:205, MR:142, LR:17, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
4	10	9	2	0	25	1	6.7
1	4	8	1	0	14	2	13.3
1	0	1	0	0	2	3	20.0
3	1	1	0	0	5	4	26.7
0	0	1	0	0	1	5	33.3
1	1	1	0	0	3	6	40.0
1	2	0	0	0	3	7	46.7
0	0	0	0	0	0	8	53.3
0	1	0	0	0	1	9	60.0
0	0	0	0	0	0	10	66.7
0	0	0	0	0	0	11	73.3
0	0	0	0	0	0	12	80.0
0	1	0	0	0	1	13	86.7
0	0	1	0	0	1	14	93.3
0	2	0	0	0	2	15	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

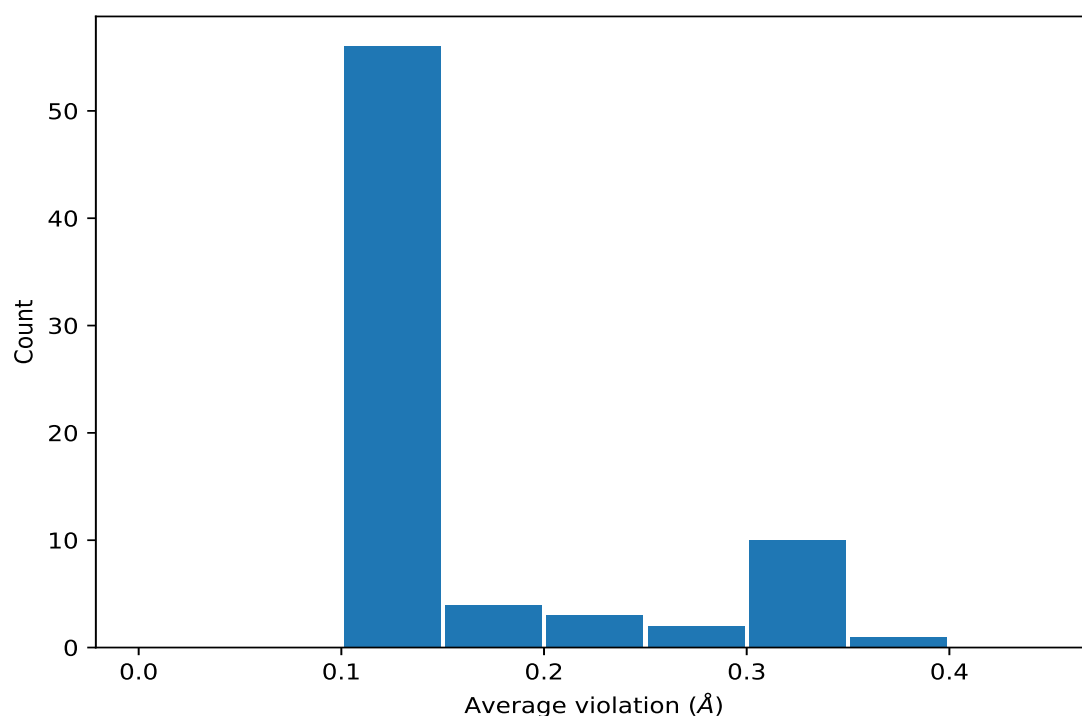
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,447)	1:747:A:PTR:HB2	1:748:A:LYS:HB2	15	0.27	0.03	0.27
(1,447)	1:747:A:PTR:HB2	1:748:A:LYS:HB3	15	0.27	0.03	0.27
(1,342)	1:738:A:LYS:HA	1:739:A:TRP:HE1	15	0.23	0.03	0.23
(1,43)	1:717:A:LEU:HG	1:720:A:THR:H	14	0.12	0.01	0.12
(1,237)	1:730:A:PHE:HB2	1:731:A:GLU:HB2	13	0.15	0.03	0.16
(1,237)	1:730:A:PHE:HB2	1:731:A:GLU:HB3	13	0.15	0.03	0.16
(1,59)	1:718:A:LEU:HD11	1:719:A:ILE:HG12	9	0.32	0.11	0.28
(1,59)	1:718:A:LEU:HD11	1:719:A:ILE:HG13	9	0.32	0.11	0.28
(1,59)	1:718:A:LEU:HD12	1:719:A:ILE:HG12	9	0.32	0.11	0.28
(1,59)	1:718:A:LEU:HD12	1:719:A:ILE:HG13	9	0.32	0.11	0.28
(1,59)	1:718:A:LEU:HD13	1:719:A:ILE:HG12	9	0.32	0.11	0.28
(1,59)	1:718:A:LEU:HD13	1:719:A:ILE:HG13	9	0.32	0.11	0.28
(1,449)	1:747:A:PTR:HB2	1:748:A:LYS:HD2	7	0.14	0.02	0.14
(1,449)	1:747:A:PTR:HB2	1:748:A:LYS:HD3	7	0.14	0.02	0.14
(1,439)	1:746:A:LEU:HA	1:747:A:PTR:HB3	7	0.13	0.03	0.13
(1,366)	1:740:A:ASP:H	1:740:A:ASP:HB2	7	0.1	0.0	0.1

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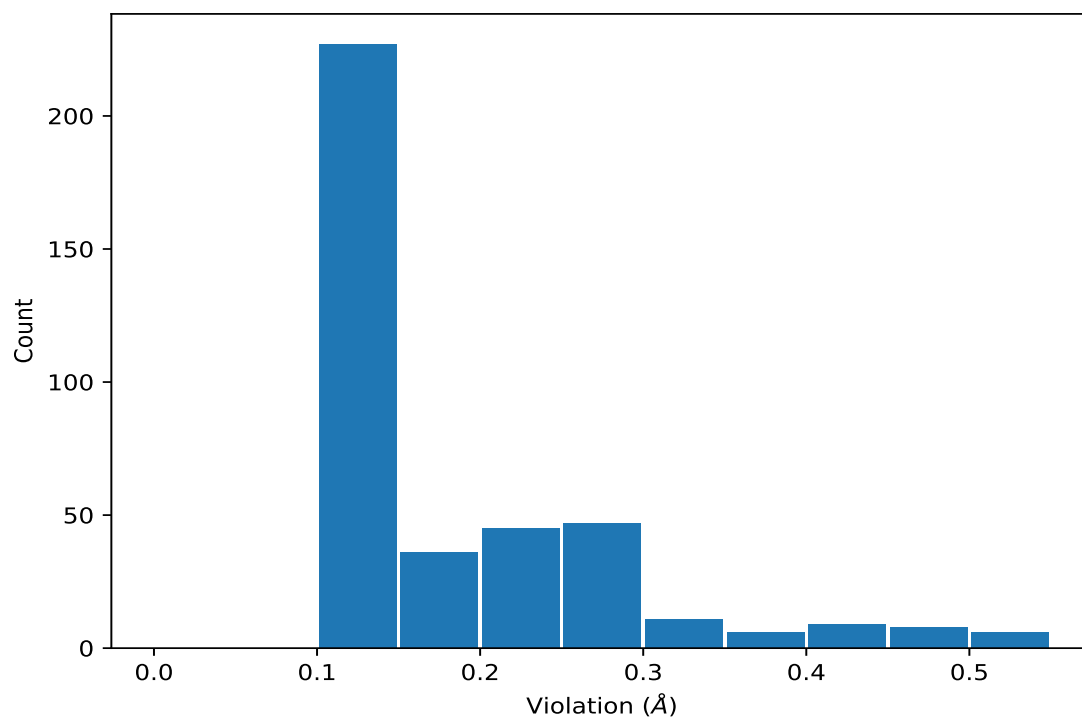
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5)	1:716:A:LYS:H	1:716:A:LYS:HD2	6	0.32	0.09	0.31
(1,5)	1:716:A:LYS:H	1:716:A:LYS:HD3	6	0.32	0.09	0.31
(1,612)	1:759:A:TYR:HA	1:762:A:THR:H	6	0.13	0.02	0.14

<sup>1</sup>Number of violated models, <sup>2</sup>Standard 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)
(1,59)	1:718:A:LEU:HD11	1:719:A:ILE:HG12	2	0.51
(1,59)	1:718:A:LEU:HD11	1:719:A:ILE:HG13	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:718:A:LEU:HD12	1:719:A:ILE:HG12	2	0.51
(1,59)	1:718:A:LEU:HD12	1:719:A:ILE:HG13	2	0.51
(1,59)	1:718:A:LEU:HD13	1:719:A:ILE:HG12	2	0.51
(1,59)	1:718:A:LEU:HD13	1:719:A:ILE:HG13	2	0.51
(1,59)	1:718:A:LEU:HD11	1:719:A:ILE:HG12	8	0.49
(1,59)	1:718:A:LEU:HD11	1:719:A:ILE:HG13	8	0.49
(1,59)	1:718:A:LEU:HD12	1:719:A:ILE:HG12	8	0.49
(1,59)	1:718:A:LEU:HD12	1:719:A:ILE:HG13	8	0.49
(1,59)	1:718:A:LEU:HD13	1:719:A:ILE:HG12	8	0.49
(1,59)	1:718:A:LEU:HD13	1:719:A:ILE:HG13	8	0.49
(1,5)	1:716:A:LYS:H	1:716:A:LYS:HD2	13	0.49
(1,5)	1:716:A:LYS:H	1:716:A:LYS:HD3	13	0.49
(1,11)	1:716:A:LYS:H	1:716:A:LYS:HG2	4	0.42
(1,11)	1:716:A:LYS:H	1:716:A:LYS:HG3	4	0.42
(1,59)	1:718:A:LEU:HD11	1:719:A:ILE:HG12	11	0.4
(1,59)	1:718:A:LEU:HD11	1:719:A:ILE:HG13	11	0.4
(1,59)	1:718:A:LEU:HD12	1:719:A:ILE:HG12	11	0.4
(1,59)	1:718:A:LEU:HD12	1:719:A:ILE:HG13	11	0.4
(1,59)	1:718:A:LEU:HD13	1:719:A:ILE:HG12	11	0.4
(1,59)	1:718:A:LEU:HD13	1:719:A:ILE:HG13	11	0.4
(1,20)	1:716:A:LYS:H	1:718:A:LEU:H	15	0.4
(1,4)	1:716:A:LYS:H	1:716:A:LYS:HE2	7	0.37
(1,4)	1:716:A:LYS:H	1:716:A:LYS:HE3	7	0.37
(1,4)	1:716:A:LYS:H	1:716:A:LYS:HE2	13	0.37
(1,4)	1:716:A:LYS:H	1:716:A:LYS:HE3	13	0.37
(1,5)	1:716:A:LYS:H	1:716:A:LYS:HD2	15	0.36
(1,5)	1:716:A:LYS:H	1:716:A:LYS:HD3	15	0.36
(1,4)	1:716:A:LYS:H	1:716:A:LYS:HE2	4	0.35

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

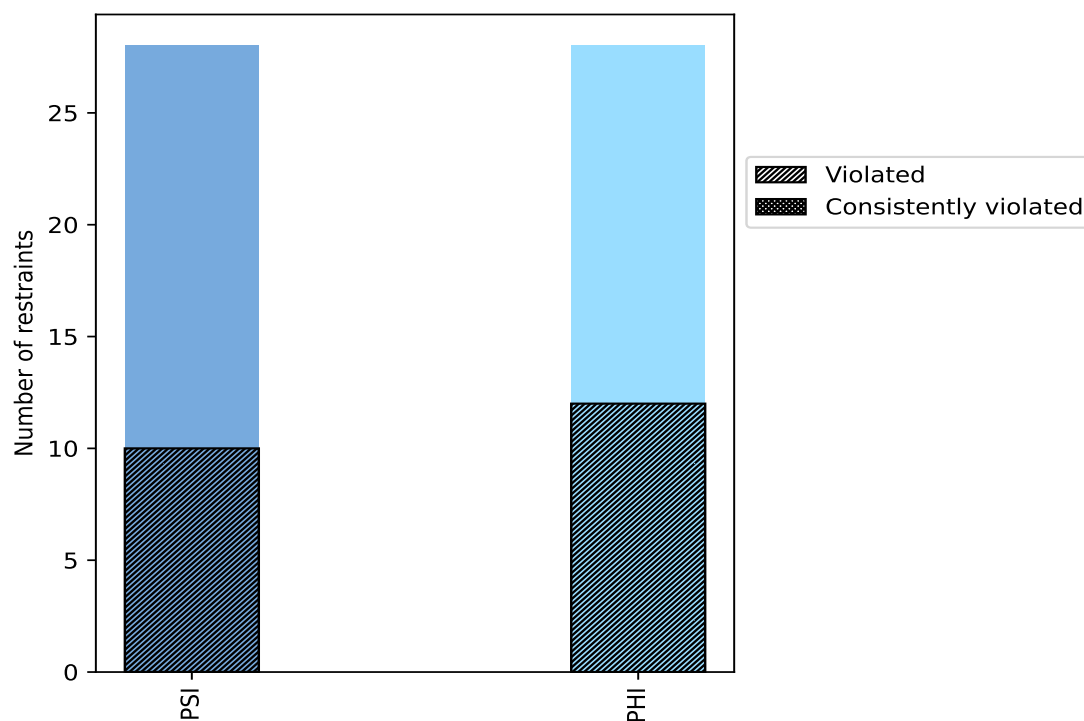
### 10.1 Summary of dihedral-angle violations [i](#)

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PSI	28	50.0	10	35.7	17.9	0	0.0	0.0
PHI	28	50.0	12	42.9	21.4	0	0.0	0.0
Total	56	100.0	22	39.3	39.3	0	0.0	0.0

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

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



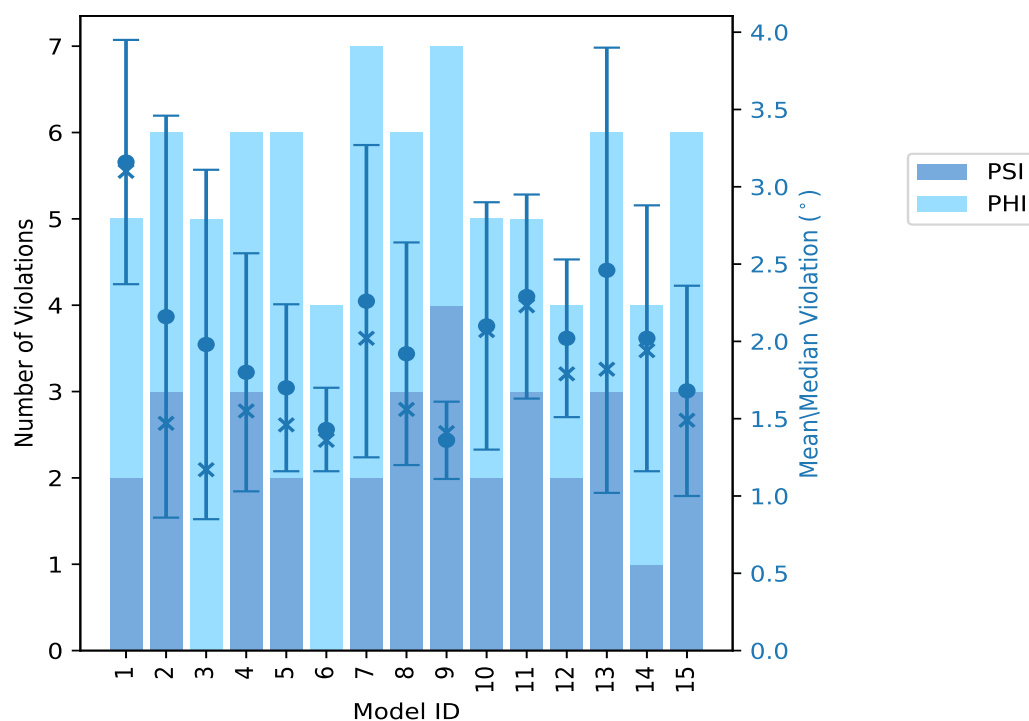
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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	2	3	5	3.16	4.15	0.79	3.1
2	3	3	6	2.16	4.48	1.3	1.47
3	0	5	5	1.98	3.64	1.13	1.17
4	3	3	6	1.8	3.41	0.77	1.55
5	2	4	6	1.7	2.43	0.54	1.46
6	0	4	4	1.43	1.83	0.27	1.36
7	2	5	7	2.26	3.88	1.01	2.02
8	3	3	6	1.92	3.05	0.72	1.56
9	4	3	7	1.36	1.61	0.25	1.41
10	2	3	5	2.1	3.54	0.8	2.07
11	3	2	5	2.29	2.99	0.66	2.23
12	2	2	4	2.02	2.89	0.51	1.79
13	3	3	6	2.46	4.46	1.44	1.82
14	1	3	4	2.02	3.11	0.86	1.94
15	3	3	6	1.68	3.08	0.68	1.49

### 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

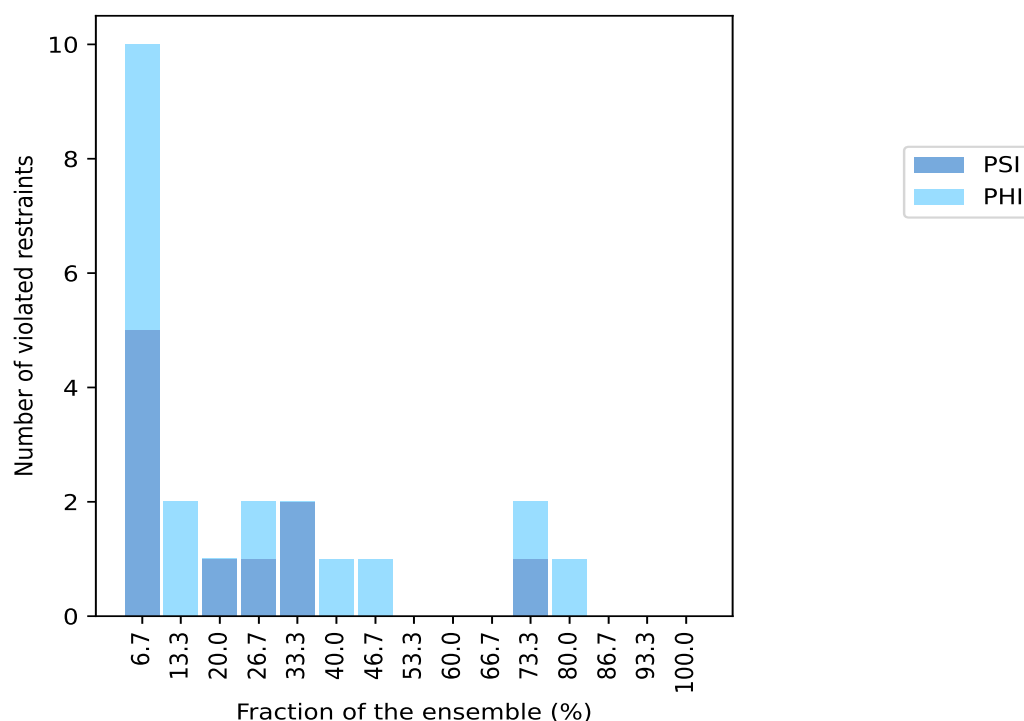
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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 <sup>1</sup>	%
5	5	10	1	6.7
0	2	2	2	13.3
1	0	1	3	20.0
1	1	2	4	26.7
2	0	2	5	33.3
0	1	1	6	40.0
0	1	1	7	46.7
0	0	0	8	53.3
0	0	0	9	60.0
0	0	0	10	66.7
1	1	2	11	73.3
0	1	1	12	80.0
0	0	0	13	86.7
0	0	0	14	93.3
0	0	0	15	100.0

<sup>1</sup> Number of models with violations

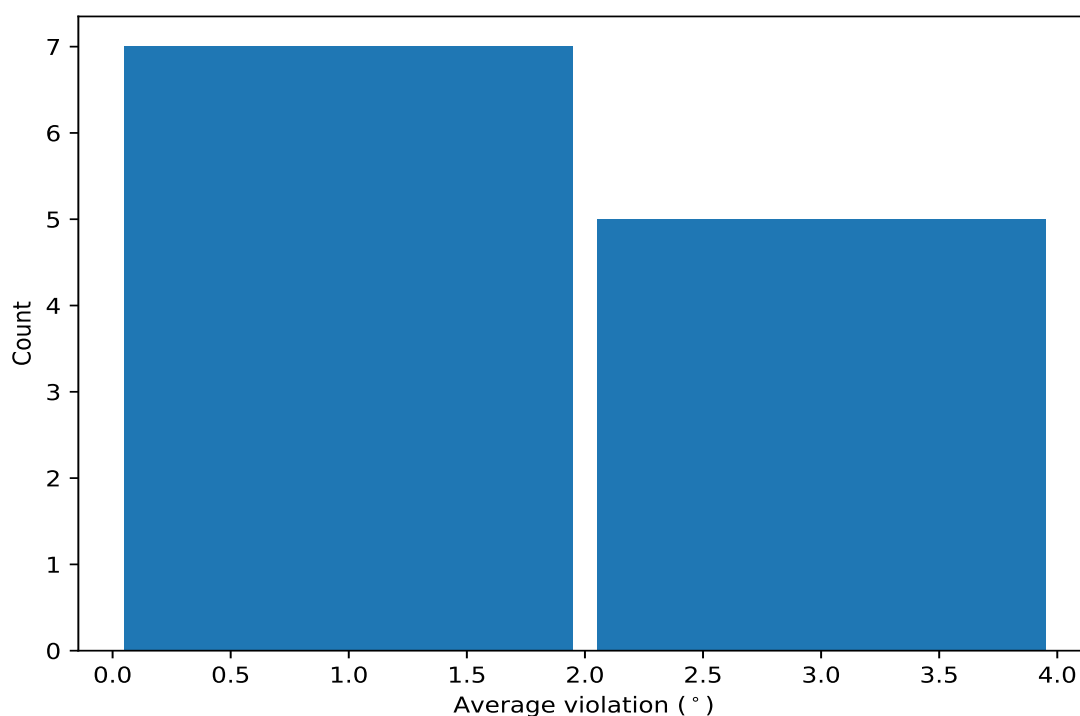
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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.

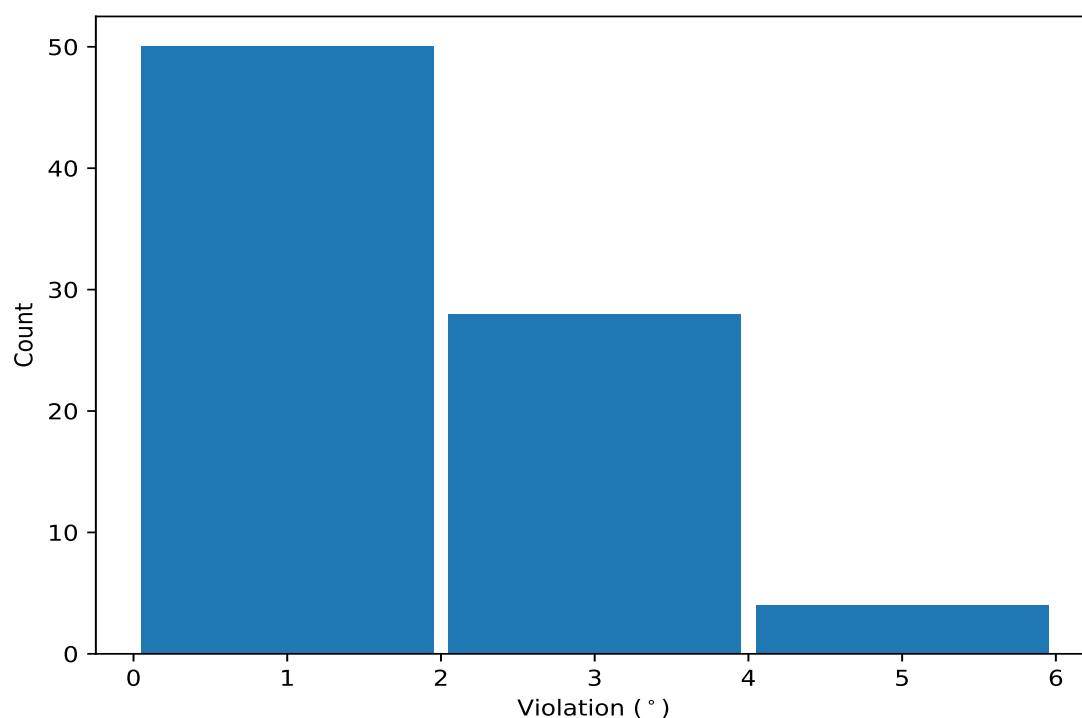
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,19)	1:725:A:LYS:C	1:726:A:GLU:N	1:726:A:GLU:CA	1:726:A:GLU:C	12	2.44	0.78	2.5
(1,35)	1:733:A:GLU:C	1:734:A:ARG:N	1:734:A:ARG:CA	1:734:A:ARG:C	11	2.29	0.78	2.42
(1,20)	1:726:A:GLU:N	1:726:A:GLU:CA	1:726:A:GLU:C	1:727:A:PHE:N	11	1.89	0.75	1.54
(1,17)	1:724:A:ARG:C	1:725:A:LYS:N	1:725:A:LYS:CA	1:725:A:LYS:C	7	3.04	1.19	3.41
(1,21)	1:726:A:GLU:C	1:727:A:PHE:N	1:727:A:PHE:CA	1:727:A:PHE:C	6	2.46	1.16	2.24
(1,52)	1:750:A:ALA:N	1:750:A:ALA:CA	1:750:A:ALA:C	1:751:A:THR:N	5	2.43	1.32	1.57
(1,30)	1:731:A:GLU:N	1:731:A:GLU:CA	1:731:A:GLU:C	1:732:A:GLU:N	5	1.36	0.36	1.15
(1,14)	1:723:A:ASP:N	1:723:A:ASP:CA	1:723:A:ASP:C	1:724:A:ARG:N	4	1.61	0.41	1.56
(1,7)	1:719:A:ILE:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	4	1.32	0.19	1.27
(1,44)	1:741:A:THR:N	1:741:A:THR:CA	1:741:A:THR:C	1:742:A:ALA:N	3	1.64	0.06	1.67

<sup>1</sup> Number of violated models, <sup>2</sup>Standard 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 (°)
(1,17)	1:724:A:ARG:C	1:725:A:LYS:N	1:725:A:LYS:CA	1:725:A:LYS:C	2	4.48
(1,52)	1:750:A:ALA:N	1:750:A:ALA:CA	1:750:A:ALA:C	1:751:A:THR:N	13	4.46
(1,17)	1:724:A:ARG:C	1:725:A:LYS:N	1:725:A:LYS:CA	1:725:A:LYS:C	13	4.4
(1,21)	1:726:A:GLU:C	1:727:A:PHE:N	1:727:A:PHE:CA	1:727:A:PHE:C	1	4.15
(1,20)	1:726:A:GLU:N	1:726:A:GLU:CA	1:726:A:GLU:C	1:727:A:PHE:N	1	3.94
(1,19)	1:725:A:LYS:C	1:726:A:GLU:N	1:726:A:GLU:CA	1:726:A:GLU:C	7	3.88
(1,17)	1:724:A:ARG:C	1:725:A:LYS:N	1:725:A:LYS:CA	1:725:A:LYS:C	3	3.64
(1,21)	1:726:A:GLU:C	1:727:A:PHE:N	1:727:A:PHE:CA	1:727:A:PHE:C	7	3.62
(1,52)	1:750:A:ALA:N	1:750:A:ALA:CA	1:750:A:ALA:C	1:751:A:THR:N	10	3.54
(1,17)	1:724:A:ARG:C	1:725:A:LYS:N	1:725:A:LYS:CA	1:725:A:LYS:C	4	3.41