

# Full wwPDB NMR Structure Validation Report (i)

### Jun 3, 2023 – 07:04 AM EDT

PDB ID	:	2JVW
BMRB ID	:	15491
Title	:	Solution NMR structure of uncharacterized protein Q5E7H1 from Vibrio fis-
		cheri. Northeast Structural Genomics target VfR117
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		J.; Baran, M.C.; Swapna, G.V.T.; Acton, T.B.; Rost, B.; Montelione, G.T.;
		Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2007-09-26

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

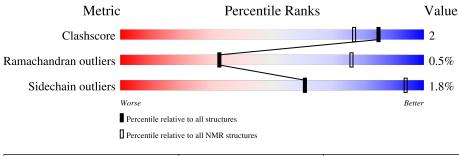
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $SOLUTION\ NMR$ 

The overall completeness of chemical shifts assignment is 95%.

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	NMR archive	
	$(\# { m Entries})$	$(\# { m Entries})$	
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 <=5%

Mol	Chain	Length	Quality of chain		
1	А	88	67%	26%	7%



# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 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:15-A:73 (59)	0.67	8	

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 8 single-model clusters were found.

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



# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1411 atoms, of which 716 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					Trace	
1	Δ	20	Total	С	Η	Ν	0	S	0
	A	02	1411	443	716	124	124	4	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	81	LEU	-	expression tag	UNP Q5E7H1
А	82	GLU	-	expression tag	UNP Q5E7H1
А	83	HIS	-	expression tag	UNP Q5E7H1
А	84	HIS	-	expression tag	UNP Q5E7H1
А	85	HIS	-	expression tag	UNP Q5E7H1
А	86	HIS	-	expression tag	UNP Q5E7H1
А	87	HIS	-	expression tag	UNP Q5E7H1
А	88	HIS	-	expression tag	UNP Q5E7H1



# 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: Uncharacterized protein

Chain A:	67%	26%	7%
M1 A2 153 154 15 15 114 113 113 113 113 113	R74 H75 E77 R77 R77 R77 R78 R18 H1S H1S H1S H1S H1S H1S		

## 4.2 Scores per residue for each member of the ensemble

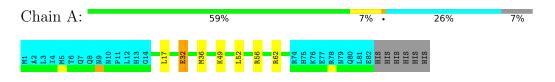
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

• Molecule 1: Uncharacterized protein



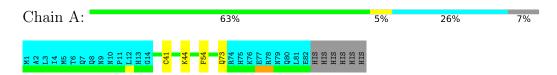
### 4.2.2 Score per residue for model 2





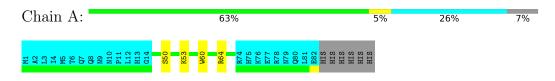
#### 4.2.3 Score per residue for model 3

• Molecule 1: Uncharacterized protein



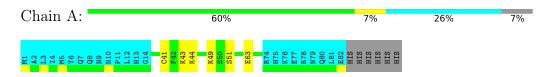
### 4.2.4 Score per residue for model 4

• Molecule 1: Uncharacterized protein



### 4.2.5 Score per residue for model 5

• Molecule 1: Uncharacterized protein

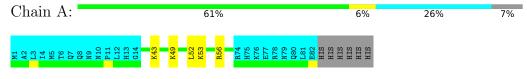


### 4.2.6 Score per residue for model 6

• Molecule 1: Uncharacterized protein



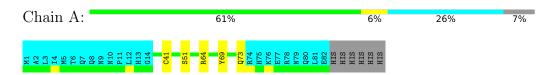
## 4.2.7 Score per residue for model 7





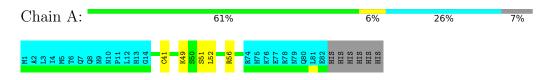
#### 4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: Uncharacterized protein



#### 4.2.9 Score per residue for model 9

• Molecule 1: Uncharacterized protein



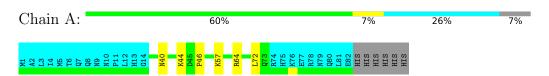
### 4.2.10 Score per residue for model 10

• Molecule 1: Uncharacterized protein

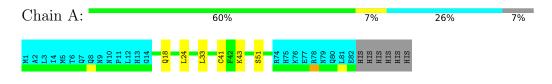
Chain A:	61%	6%	26%	7%
M1 A2 133 46 76 47 41 7110 7110 7111 7111 7111 7113 714 7113 714 7113 714	I 48 152 152 152 168 168 175 175 175 180 180			

### 4.2.11 Score per residue for model 11

• Molecule 1: Uncharacterized protein



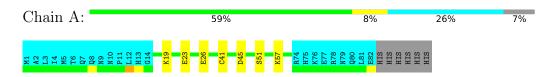
### 4.2.12 Score per residue for model 12





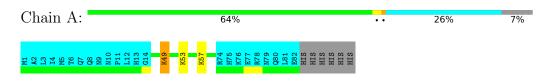
#### 4.2.13 Score per residue for model 13

• Molecule 1: Uncharacterized protein



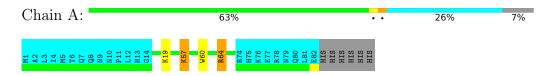
### 4.2.14 Score per residue for model 14

• Molecule 1: Uncharacterized protein



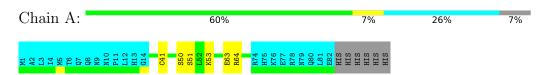
### 4.2.15 Score per residue for model 15

• Molecule 1: Uncharacterized protein

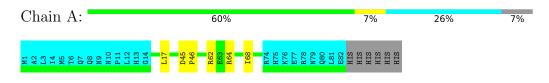


### 4.2.16 Score per residue for model 16

• Molecule 1: Uncharacterized protein



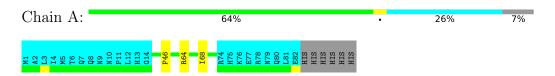
### 4.2.17 Score per residue for model 17





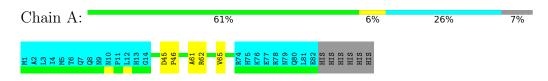
#### 4.2.18 Score per residue for model 18

• Molecule 1: Uncharacterized protein



#### 4.2.19 Score per residue for model 19

• Molecule 1: Uncharacterized protein



#### 4.2.20 Score per residue for model 20

Chain A:	61%	6%	26%	7%
M1 A2 L3 L3 L3 M5 M5 Q7 Q7 N10 N10 N110 N112 C114 C114 C114	K19 M36 M36 L62 L62 K74 H75 K75 K76 K76 K76 K76 K76 K76 K76 K76 K76 K76	NIN NIN NIN NIN NIN NIN		



# 5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	2.1
CNS	refinement	1.1

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	1124
Number of shifts mapped to atoms	1124
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	95%



# 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	А	504	521	520	2±1
All	All	10080	10420	10400	46

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Mod	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:32:GLU:O	1:A:36:MET:SD	0.57	2.63	2	1
1:A:63:GLU:HG3	1:A:64:ARG:HG3	0.55	1.77	16	1
1:A:41:CYS:SG	1:A:51:SER:HA	0.55	2.42	13	6
1:A:45:ASP:N	1:A:46:PRO:HD3	0.54	2.18	17	1
1:A:39:ILE:HD12	1:A:41:CYS:SG	0.51	2.45	6	1
1:A:36:MET:SD	1:A:71:LYS:NZ	0.50	2.77	20	2
1:A:52:LEU:O	1:A:56:ARG:HG2	0.50	2.07	7	2
1:A:17:LEU:HD13	1:A:62:ARG:NH1	0.49	2.23	2	2
1:A:50:SER:HA	1:A:53:LYS:HE3	0.49	1.83	4	2
1:A:60:TRP:O	1:A:64:ARG:HG2	0.48	2.09	4	2
1:A:41:CYS:SG	1:A:54:PHE:CG	0.47	3.08	3	1
1:A:57:LYS:HB3	1:A:57:LYS:NZ	0.47	2.25	15	1
1:A:41:CYS:SG	1:A:54:PHE:CB	0.46	3.04	3	1
1:A:49:LYS:O	1:A:53:LYS:HD3	0.46	2.11	7	2

All unique clashes are listed below, sorted by their clash magnitude.

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:41:CYS:SG	1:A:54:PHE:CD2	0.46	3.09	3	1
1:A:19:LYS:O	1:A:23:GLU:HG2	0.45	2.12	13	1
1:A:60:TRP:O	1:A:64:ARG:HD2	0.45	2.12	15	1
1:A:40:ASN:O	1:A:44:LYS:HG2	0.44	2.12	11	1
1:A:43:LYS:HE2	1:A:43:LYS:HA	0.43	1.91	7	1
1:A:69:TYR:O	1:A:73:GLN:HG2	0.42	2.14	8	2
1:A:64:ARG:O	1:A:68:ILE:HG13	0.42	2.14	6	4
1:A:64:ARG:NE	1:A:64:ARG:HA	0.42	2.30	10	1
1:A:48:ILE:O	1:A:52:LEU:HG	0.42	2.15	10	2
1:A:41:CYS:SG	1:A:54:PHE:HB3	0.42	2.55	3	1
1:A:73:GLN:OE1	1:A:73:GLN:HA	0.42	2.15	3	1
1:A:43:LYS:NZ	1:A:43:LYS:HB3	0.41	2.31	12	1
1:A:64:ARG:HA	1:A:64:ARG:NE	0.41	2.30	11	1
1:A:24:LEU:HB3	1:A:33:LEU:HD21	0.41	1.92	12	1
1:A:61:ALA:O	1:A:65:VAL:HG23	0.41	2.16	19	1
1:A:52:LEU:O	1:A:56:ARG:HG3	0.40	2.17	2	1

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## 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	А	59/88~(67%)	$54\pm1$ (92 $\pm2\%$ )	$4\pm1~(7\pm2\%)$	0±1 (1±1%)	32 76
All	All	1180/1760~(67%)	1087~(92%)	87 (7%)	6 (1%)	32 76

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	А	46	PRO	4
1	А	45	ASP	2



#### 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	Percen	tiles
1	А	57/84~(68%)	$56\pm1 (98\pm2\%)$	$1\pm1~(2\pm2\%)$	61	94
All	All	1140/1680 (68%)	1119 (98%)	21 (2%)	61	94

All 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	А	57	LYS	5
1	А	49	LYS	4
1	А	44	LYS	2
1	А	64	ARG	2
1	А	19	LYS	2
1	А	32	GLU	1
1	А	43	LYS	1
1	А	63	GLU	1
1	А	18	GLN	1
1	А	26	GLU	1
1	А	62	ARG	1

### 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 95% for the well-defined parts and 91% 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	1124
Number of shifts mapped to atoms	1124
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\rm Correction}\pm{\rm precision},ppm$	Suggested action
$^{13}C_{\alpha}$	81	$-0.62 \pm 0.22$	Should be checked
$^{13}C_{\beta}$	79	$0.49 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}C'$	81	$-0.35 \pm 0.13$	None needed ( $< 0.5$ ppm)
<sup>15</sup> N	78	$0.32 \pm 0.18$	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 95%, i.e. 841 atoms were assigned a chemical shift out of a possible 888. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	294/294~(100%)	118/118~(100%)	118/118 (100%)	58/58~(100%)
Sidechain	479/515~(93%)	321/333~(96%)	150/161~(93%)	8/21~(38%)

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	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Aromatic	68/79~(86%)	34/38~(89%)	32/37~(86%)	2/4~(50%)
Overall	841/888~(95%)	473/489~(97%)	300/316~(95%)	68/83~(82%)

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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1124 atoms were assigned a chemical shift out of a possible 1229. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}$ N
Backbone	401/408~(98%)	161/164~(98%)	162/164~(99%)	78/80~(98%)
Sidechain	655/726~(90%)	436/468~(93%)	205/224~(92%)	14/34~(41%)
Aromatic	68/95~(72%)	34/46~(74%)	32/41~(78%)	2/8~(25%)
Overall	1124/1229~(91%)	631/678~(93%)	399/429~(93%)	94/122~(77%)

### 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.

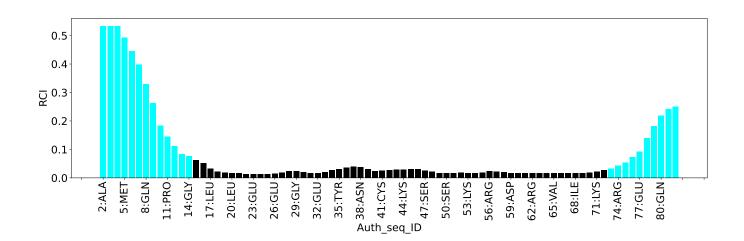
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	А	46	PRO	HB3	-0.58	0.25 - 3.76	-7.4

### 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 (i)

# 8.1 Conformationally restricting restraints (i)

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	1537
Intra-residue ( i-j =0)	551
Sequential ( i-j =1)	385
Medium range ( $ i-j >1$ and $ i-j <5$ )	285
Long range $( i-j  \ge 5)$	270
Inter-chain	0
Hydrogen bond restraints	46
Disulfide bond restraints	0
Total dihedral-angle restraints	88
Number of unmapped restraints	0
Number of restraints per residue	18.5
Number of long range restraints per residue <sup>1</sup>	3.1

<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 (i)

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 (i)

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)	1.0	0.2
0.2-0.5 (Medium)	0.1	0.32
>0.5 (Large)	None	None



### 8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation.

Bins $(^{\circ})$	Average number of violations per model	Max ( $^{\circ}$ )
1.0-10.0 (Small)	0.1	1.2
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None



# 9 Distance violation analysis (i)

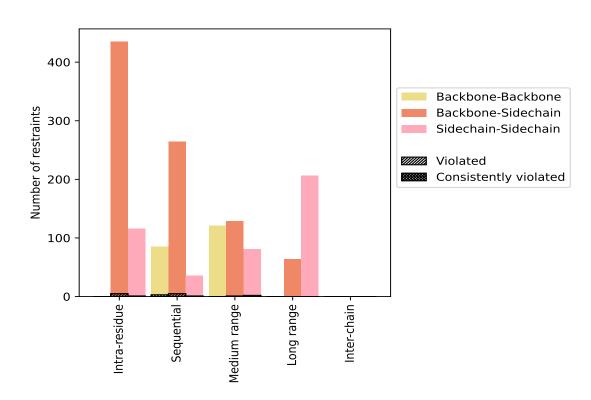
# 9.1 Summary of distance violations (i)

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.

Destroints type	Count	$\%^1$	Vio	lated	3	Consis	tently	$^{\prime}$ Violated <sup>4</sup>
Restraints type	$\operatorname{Count}$	701	Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
Intra-residue ( i-j =0)	551	35.8	6	1.1	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	435	28.3	5	1.1	0.3	0	0.0	0.0
Sidechain-Sidechain	116	7.5	1	0.9	0.1	0	0.0	0.0
Sequential ( i-j =1)	385	25.0	9	2.3	0.6	0	0.0	0.0
Backbone-Backbone	85	5.5	3	3.5	0.2	0	0.0	0.0
Backbone-Sidechain	264	17.2	5	1.9	0.3	0	0.0	0.0
Sidechain-Sidechain	36	2.3	1	2.8	0.1	0	0.0	0.0
Medium range ( $ i-j  > 1 \&  i-j  < 5$ )	285	18.5	3	1.1	0.2	0	0.0	0.0
Backbone-Backbone	75	4.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	129	8.4	1	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	81	5.3	2	2.5	0.1	0	0.0	0.0
Long range $( i-j  \ge 5)$	270	17.6	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	64	4.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	206	13.4	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	46	3.0	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	1537	100.0	18	1.2	1.2	0	0.0	0.0
Backbone-Backbone	206	13.4	3	1.5	0.2	0	0.0	0.0
Backbone-Sidechain	892	58.0	11	1.2	0.7	0	0.0	0.0
Sidechain-Sidechain	439	28.6	4	0.9	0.3	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		Nun	nber o	f viola	ations	5	Maan (Å)	Morr (Å)	$SD^6$ (Å)	Median (Å)
Model ID	$IR^1$	$SQ^2$	$MR^3$	$LR^4$	$  IC^5  $	Total	Mean (Å)	Max (Å)	$SD^{*}(A)$	Median (A)
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	1	0	0	0	1	0.12	0.12	0.0	0.12
3	2	0	0	0	0	2	0.22	0.32	0.1	0.22
4	0	2	0	0	0	2	0.13	0.15	0.02	0.13
5	0	3	1	0	0	4	0.15	0.17	0.02	0.14
6	1	0	0	0	0	1	0.2	0.2	0.0	0.2
7	0	1	0	0	0	1	0.13	0.13	0.0	0.13
8	0	0	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	0.0
10	1	0	0	0	0	1	0.14	0.14	0.0	0.14
11	1	1	2	0	0	4	0.12	0.14	0.01	0.12

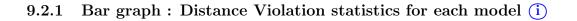
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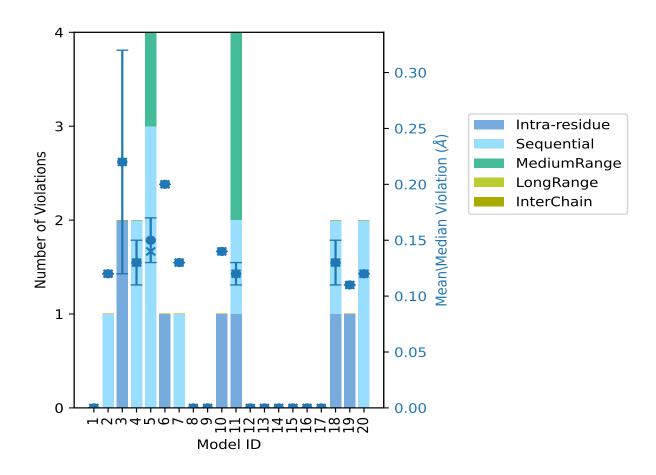


			nber o		ations	5				
Model ID	$\mathrm{IR}^{1}$	$SQ^2$	$MR^3$	$LR^4$	$  IC^5 $	Total	Mean (Å)	Max (Å)	$\mathbf{SD}^{6}$ (Å)	Median (Å)
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	1	1	0	0	0	2	0.13	0.15	0.02	0.13
19	1	0	0	0	0	1	0.11	0.11	0.0	0.11
20	0	2	0	0	0	2	0.12	0.12	0.0	0.12

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 $^1$ Intra-residue restraints,  $^2$ Sequential restraints,  $^3$ Medium range restraints,  $^4$ Long range restraints,  $^5$ Inter-chain restraints,  $^6$ Standard deviation





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



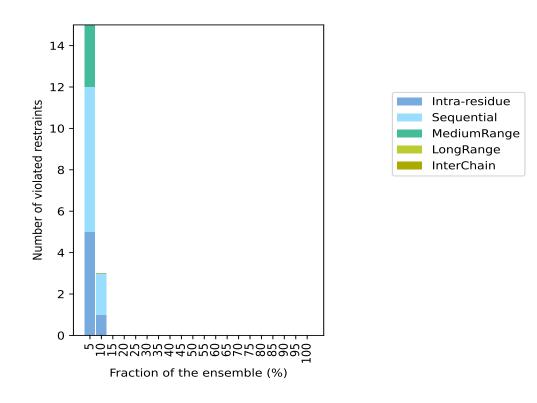
## 9.3 Distance violation statistics for the ensemble (i)

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, 1473(IR:545, SQ:376, MR:282, LR:270, IC:0) restraints are not violated in the ensemble.

Nu	mber	of vio	lated	restra	aints	Fractio	n of the ensemble
$IR^1$	$SQ^2$	$MR^3$	LR <sup>4</sup>	IC <sup>5</sup>	Total	$\operatorname{Count}^6$	%
5	7	3	0	0	15	1	5.0
1	2	0	0	0	3	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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





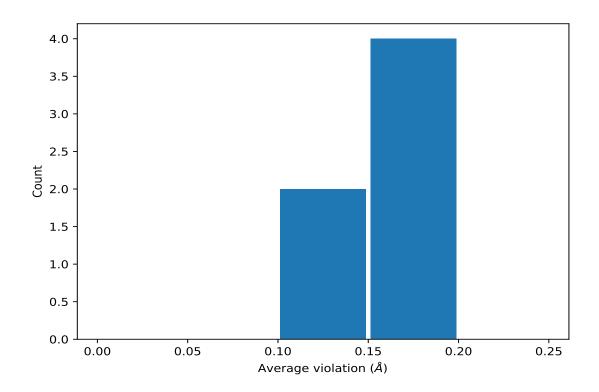
### 9.3.1 Bar graph : Distance violation statistics for the ensemble (i)

### 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)
(1,1362)	1:A:44:LYS:HB2	1:A:44:LYS:HD2	2	0.16	0.04	0.16
(1,1362)	1:A:44:LYS:HB2	1:A:44:LYS:HD3	2	0.16	0.04	0.16
(1,1362)	1:A:44:LYS:HB3	1:A:44:LYS:HD2	2	0.16	0.04	0.16
(1,1362)	1:A:44:LYS:HB3	1:A:44:LYS:HD3	2	0.16	0.04	0.16
(1,845)	1:A:44:LYS:HA	1:A:45:ASP:H	2	0.14	0.01	0.14
(1,1126)	1:A:78:ARG:HB2	1:A:79:ASN:H	2	0.12	0.01	0.12

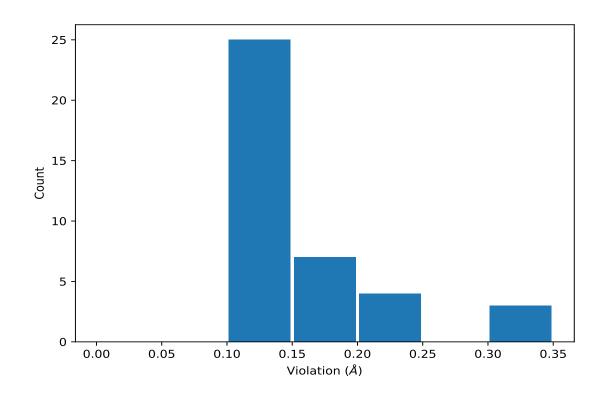
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 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 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. 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)
(1,296)	1:A:12:LEU:HA	1:A:12:LEU:HD21	3	0.32
(1,296)	1:A:12:LEU:HA	1:A:12:LEU:HD22	3	0.32
(1,296)	1:A:12:LEU:HA	1:A:12:LEU:HD23	3	0.32
(1,1362)	1:A:44:LYS:HB2	1:A:44:LYS:HD2	6	0.2
(1,1362)	1:A:44:LYS:HB2	1:A:44:LYS:HD3	6	0.2
(1,1362)	1:A:44:LYS:HB3	1:A:44:LYS:HD2	6	0.2
(1,1362)	1:A:44:LYS:HB3	1:A:44:LYS:HD3	6	0.2
(1,1223)	1:A:9:ASN:HB2	1:A:10:ASN:H	5	0.17
(1,1223)	1:A:9:ASN:HB3	1:A:10:ASN:H	5	0.17
(1,845)	1:A:44:LYS:HA	1:A:45:ASP:H	4	0.15
(1,1462)	1:A:74:ARG:HG2	1:A:75:HIS:HA	5	0.15
(1,1462)	1:A:74:ARG:HG3	1:A:75:HIS:HA	5	0.15
(1,1460)	1:A:74:ARG:H	1:A:74:ARG:HG2	18	0.15
(1,1460)	1:A:74:ARG:H	1:A:74:ARG:HG3	18	0.15
(1,764)	1:A:13:HIS:H	1:A:13:HIS:HB3	10	0.14
(1,1266)	1:A:19:LYS:HA	1:A:19:LYS:HD2	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1266)	1:A:19:LYS:HA	1:A:19:LYS:HD3	11	0.14
(1,845)	1:A:44:LYS:HA	1:A:45:ASP:H	7	0.13
(1,592)	1:A:73:GLN:HA	1:A:76:LYS:HE2	5	0.13
(1,592)	1:A:73:GLN:HA	1:A:76:LYS:HE3	5	0.13
(1,577)	1:A:28:TYR:HB2	1:A:32:GLU:HB3	11	0.13
(1,1362)	1:A:44:LYS:HB2	1:A:44:LYS:HD2	3	0.13
(1,1362)	1:A:44:LYS:HB2	1:A:44:LYS:HD3	3	0.13
(1,1362)	1:A:44:LYS:HB3	1:A:44:LYS:HD2	3	0.13
(1,1362)	1:A:44:LYS:HB3	1:A:44:LYS:HD3	3	0.13
(1,1126)	1:A:78:ARG:HB2	1:A:79:ASN:H	5	0.13
(1,809)	1:A:12:LEU:H	1:A:13:HIS:H	20	0.12
(1,679)	1:A:72:LEU:HD21	1:A:73:GLN:HE22	20	0.12
(1,679)	1:A:72:LEU:HD22	1:A:73:GLN:HE22	20	0.12
(1,679)	1:A:72:LEU:HD23	1:A:73:GLN:HE22	20	0.12
(1,576)	1:A:28:TYR:HB2	1:A:32:GLU:HB2	11	0.12
(1,10)	1:A:35:TYR:HD1	1:A:36:MET:HA	2	0.12
(1,10)	1:A:35:TYR:HD2	1:A:36:MET:HA	2	0.12
(1,964)	1:A:45:ASP:H	1:A:46:PRO:HD2	11	0.11
(1,926)	1:A:12:LEU:H	1:A:12:LEU:HD21	19	0.11
(1,926)	1:A:12:LEU:H	1:A:12:LEU:HD22	19	0.11
(1,926)	1:A:12:LEU:H	1:A:12:LEU:HD23	19	0.11
(1,1126)	1:A:78:ARG:HB2	1:A:79:ASN:H	4	0.11
(1,1012)	1:A:14:GLY:H	1:A:15:ILE:H	18	0.11

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# 10 Dihedral-angle violation analysis (i)

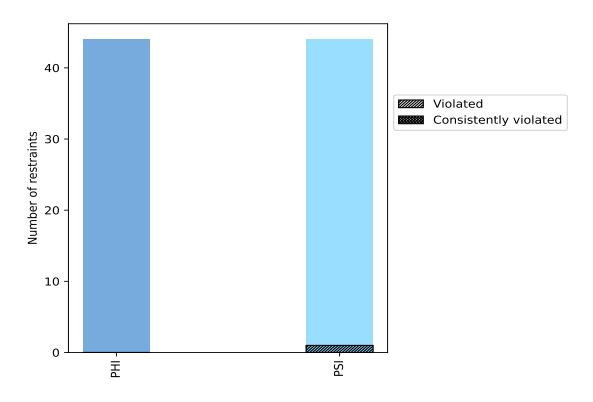
# 10.1 Summary of dihedral-angle violations (i)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than  $1^{\circ}$  are not included in the calculation.

	Count	071	$\%^1$ Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
Angle type	Count	70-	Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
PHI	44	50.0	0	0.0	0.0	0	0.0	0.0
PSI	44	50.0	1	2.3	1.1	0	0.0	0.0
Total	88	100.0	1	1.1	1.1	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



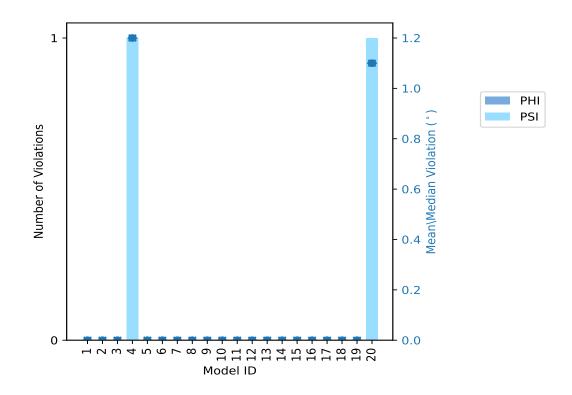
# 10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than  $1^{\circ}$  are not included in the statistics.

Model ID	Number of violations		Mean (°)	$M_{ov}$ (°)	SD (°)	Median (°)	
Model ID	PHI	PSI	Total	Mean ()	$Max (^{\circ})$	$SD(^{\circ})$	Median ()
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	1	1	1.2	1.2	0.0	1.2
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0.0	0.0	0.0	0.0
20	0	1	1	1.1	1.1	0.0	1.1



#### 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.

Num	ber o	f violated restraints	Fractio	n of the ensemble
PHI	PSI	Total	$\operatorname{Count}^1$	%
0	0	0	1	5.0
0	1	1	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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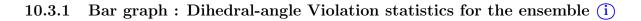
PHI

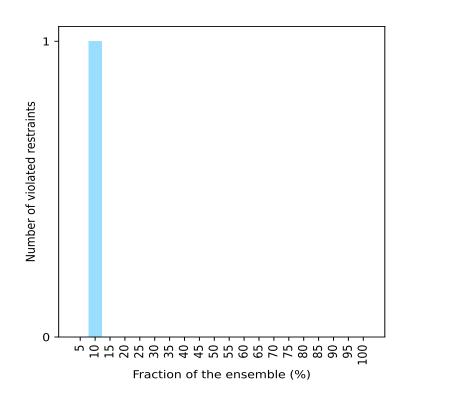
PSI

Num	iber o	of violated restraints	Fraction of the ensemble						
PHI	PSI	Total	$\operatorname{Count}^1$	%					
0	0	0	12	60.0					
0	0	0	13	65.0					
0	0	0	14	70.0					
0	0	0	15	75.0					
0	0	0	16	80.0					
0	0	0	17	85.0					
0	0	0	18	90.0					
0	0	0	19	95.0					
0	0	0	20	100.0					

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 $^{1}$  Number of models with violations





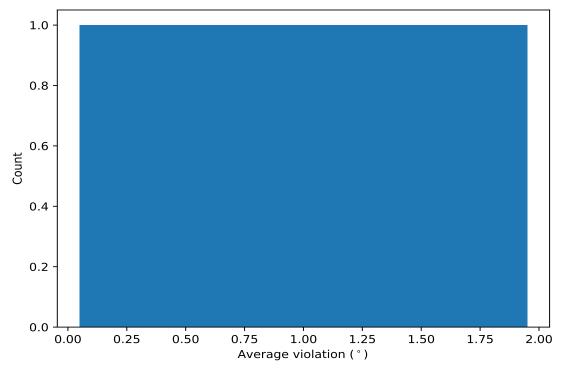
# 10.4 Most violated dihedral-angle restraints in the ensemble (i)

## 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 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	$Models^1$	Mean	$SD^2$	Median
(1,24)	1:A:28:TYR:N	1:A:28:TYR:CA	1:A:28:TYR:C	1:A:29:GLY:N	2	1.15	0.05	1.15

<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.

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 ( $^{\circ}$ )
(1,24)	1:A:28:TYR:N	1:A:28:TYR:CA	1:A:28:TYR:C	1:A:29:GLY:N	4	1.2
(1,24)	1:A:28:TYR:N	1:A:28:TYR:CA	1:A:28:TYR:C	1:A:29:GLY:N	20	1.1

