

# wwPDB NMR Structure Validation Summary Report (i)

Sep 28, 2023 – 01:15 pm BST

PDB ID : 8B4S BMRB ID : 34757

Title: Antimicrobial peptide capitellacin from polychaeta Capitella teleta in DPC (

dodecylphosphocholine) micelles, dimeric form

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Deposited on : 2022-09-21

This is a wwPDB NMR Structure Validation Summary 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)

 $\begin{array}{ccc} wwPDB\text{-ShiftChecker} &:& v1.2\\ BMRB \ Restraints \ Analysis &:& v1.2 \end{array}$ 

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

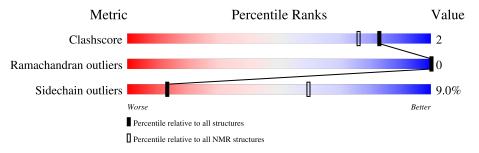
Validation Pipeline (wwPDB-VP) : 2.35.1

# 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 66%.

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
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries})$
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	A	20	95%	5%
1	В	20	100%	



# 2 Ensemble composition and analysis (i)

This entry contains 20 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 mod				
1	A:2-A:20, B:101-B:120 (39)	0.73	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 3 clusters and 1 single-model cluster was found.

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



# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 650 atoms, of which 324 are hydrogens and 0 are deuteriums.

 $\bullet$  Molecule 1 is a protein called BRICHOS domain-containing protein.

Mol	Chain	Residues	Atoms			Trace			
1	Λ	20	Total	С	Н	N	О	S	0
1	A	20	325	99	162	37	23	4	0
1	D	20	Total	С	Н	N	О	S	0
1	1 B	20	325	99	162	37	23	4	

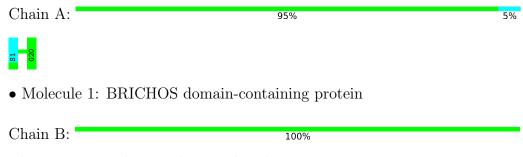


# 4 Residue-property plots (i)

#### 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: BRICHOS domain-containing protein



There are no outlier residues in this chain.

# 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: BRICHOS domain-containing protein

Chain A:

95%

Molecule 1: BRICHOS domain-containing protein

Chain B:

There are no outlier residues in this chain.



#### 5 Refinement protocol and experimental data overview (i)



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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: structures with the least restraint violations.

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

Software name	Classification	Version
CYANA	refinement	3.98.13
CYANA	structure calculation	3.98.13

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	399
Number of shifts mapped to atoms	399
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%



# 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	В	163	162	161	1±1
1	A	157	157	157	1±1
All	All	6400	6380	6360	30

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.

5 of 9 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	$\operatorname{Distance}(\mathring{\mathbf{A}})$	${f Models}$	
Atom-1	Atom-1 Atom-2 Clash(A)		Distance(A)	Worst	Total
1:A:4:VAL:HG22	1:B:108:VAL:HG13	0.81	1.52	14	2
1:A:4:VAL:HG13	1:B:108:VAL:HG22	0.61	1.71	14	1
1:A:8:VAL:HG13	1:B:104:VAL:HG22	0.57	1.76	20	3
1:A:6:ILE:HG22	1:A:17:ARG:O	0.55	2.02	4	5
1:B:106:ILE:HG22	1:B:117:ARG:O	0.54	2.03	2	4

## 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	Percer	ntiles
1	A	18/20 (90%)	17±0 (93±3%)	1±0 (7±3%)	0±0 (0±0%)	100	100
1	В	18/20 (90%)	17±1 (93±3%)	$1\pm1~(7\pm3\%)$	0±0 (0±0%)	100	100
All	All	$720/800 \; (90\%)$	670 (93%)	50 (7%)	0 (0%)	100	100

There are no Ramachandran outliers.

#### 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	Perce	entiles
1	A	17/18 (94%)	16±1 (92±6%)	1±1 (8±6%)	16	63
1	В	18/18 (100%)	16±1 (90±7%)	2±1 (10±7%)	11	56
All	All	700/720 (97%)	637 (91%)	63 (9%)	13	60

5 of 18 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	В	101	SER	9
1	A	7	ARG	8
1	В	107	ARG	7
1	В	105	CYS	5
1	A	16	ARG	4

#### 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 66% for the well-defined parts and 66% for the entire structure.

### 7.1 Chemical shift list 1

File name: working cs.cif

Chemical shift list name: capitellacin\_dimer\_deposit\_2-HhmhTR5W.bmrb

#### 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	399
Number of shifts mapped to atoms	399
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

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

List ID	Chain	Dog	Trmo	Atom		a	
LISUID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	В	104	VAL	HG12	0.999	0.020	2
1	В	104	VAL	HG13	0.999	0.020	2
1	В	104	VAL	HG22	1.078	0.020	2
1	В	104	VAL	HG23	1.078	0.020	2
1	В	106	ILE	HG22	0.992	0.020	1
1	В	106	ILE	HG23	0.992	0.020	1
1	В	108	VAL	HG12	0.968	0.020	2
1	В	108	VAL	HG13	0.968	0.020	2
1	В	108	VAL	HG22	1.049	0.020	2
1	В	108	VAL	HG23	1.049	0.020	2
1	В	113	VAL	HG12	0.777	0.020	2
1	В	113	VAL	HG13	0.777	0.020	2
1	В	113	VAL	HG22	0.907	0.020	2
1	В	113	VAL	HG23	0.907	0.020	2



#### 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
$^{13}\mathrm{C}_{\alpha}$	12	_	None (insufficient data)
$^{13}C_{\beta}$	36	$-1.09 \pm 0.22$	Should be checked
<sup>13</sup> C′	0		None (insufficient data)
$^{15}N$	15	_	None (insufficient data)

#### 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 66%, i.e. 381 atoms were assigned a chemical shift out of a possible 574. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}{ m H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	106/195 (54%)	79/80 (99%)	12/78 (15%)	15/37 (41%)
Sidechain	247/337 (73%)	166/216 (77%)	76/89 (85%)	5/32 (16%)
Aromatic	28/42 (67%)	20/20 (100%)	7/20 (35%)	1/2 (50%)
Overall	381/574 (66%)	265/316 (84%)	95/187 (51%)	21/71 (30%)

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

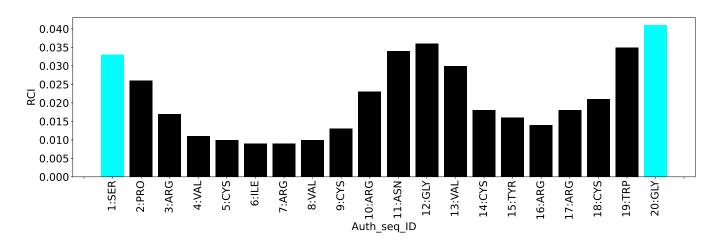
There are no statistically unusual chemical shifts.

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

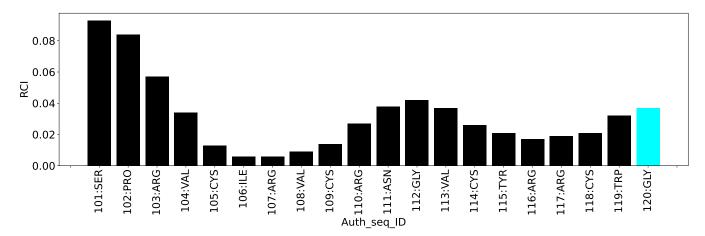
The image below reports random coil index values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted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

Random coil index (RCI) for chain A:





Random coil index (RCI) for chain B:





# 8 NMR restraints analysis (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	247
Intra-residue ( $ i-j =0$ )	38
Sequential ( i-j =1)	86
Medium range ( $ i-j >1$ and $ i-j <5$ )	20
Long range ( i-j ≥5)	49
Inter-chain	10
Hydrogen bond restraints	40
Disulfide bond restraints	4
Total dihedral-angle restraints	662
Number of unmapped restraints	0
Number of restraints per residue	22.7
Number of long range restraints per residue <sup>1</sup>	1.8

<sup>&</sup>lt;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)	12.1	0.2
0.2-0.5 (Medium)	44.1	0.5
>0.5 (Large)	131.6	3.82



## 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.

$\mathbf{Bins}\;(^{\circ})$	Average number of violations per model	$\mathbf{Max}$ (°)
1.0-10.0 (Small)	28.6	10.0
10.0-20.0 (Medium)	29.9	20.0
>20.0 (Large)	125.2	171.95



# 9 Distance violation analysis (i)

## 9.1 Summary of distance violations (i)

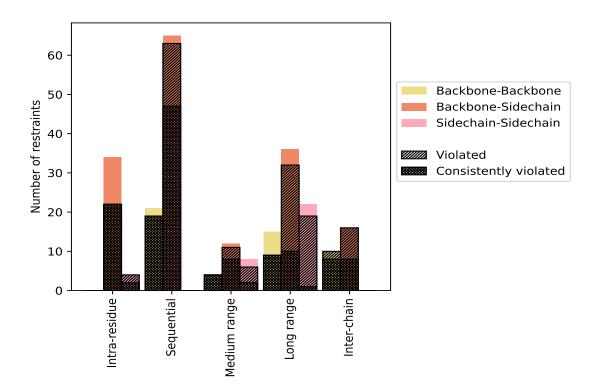
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Doctroints type	Count	<b>%</b> <sup>1</sup>	Vi	iolated	3	Consis	stently	$\overline{ ext{Violated}^4}$
Restraints type	Count	70	Count	$\%^2$	$\%^{1}$	Count	$\%^2$	$\%^1$
Intra-residue ( i-j =0)	38	15.4	26	68.4	10.5	24	63.2	9.7
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	34	13.8	22	64.7	8.9	22	64.7	8.9
Sidechain-Sidechain	4	1.6	4	100.0	1.6	2	50.0	0.8
Sequential ( i-j =1)	86	34.8	82	95.3	33.2	66	76.7	26.7
Backbone-Backbone	21	8.5	19	90.5	7.7	19	90.5	7.7
Backbone-Sidechain	65	26.3	63	96.9	25.5	47	72.3	19.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ( $ i-j >1 \&  i-j <5$ )	20	8.1	18	90.0	7.3	14	70.0	5.7
Backbone-Backbone	4	1.6	4	100.0	1.6	4	100.0	1.6
Backbone-Sidechain	8	3.2	8	100.0	3.2	8	100.0	3.2
Sidechain-Sidechain	8	3.2	6	75.0	2.4	2	25.0	0.8
Long range ( $ i-j  \ge 5$ )	49	19.8	39	79.6	15.8	14	28.6	5.7
Backbone-Backbone	15	6.1	9	60.0	3.6	9	60.0	3.6
Backbone-Sidechain	16	6.5	12	75.0	4.9	4	25.0	1.6
Sidechain-Sidechain	18	7.3	18	100.0	7.3	1	5.6	0.4
Inter-chain	10	4.0	10	100.0	4.0	8	80.0	3.2
Backbone-Backbone	10	4.0	10	100.0	4.0	8	80.0	3.2
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	40	16.2	39	97.5	15.8	14	35.0	5.7
Disulfide bond	4	1.6	1	25.0	0.4	0	0.0	0.0
Total	247	100.0	215	87.0	87.0	140	56.7	56.7
Backbone-Backbone	50	20.2	42	84.0	17.0	40	80.0	16.2
Backbone-Sidechain	163	66.0	144	88.3	58.3	95	58.3	38.5
Sidechain-Sidechain	34	13.8	29	85.3	11.7	5	14.7	2.0

 $<sup>^1</sup>$  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.

Madal ID		Nun	nber o	f viola	ations	;	M (8)	M (Å)	CD6 (%)	Madian (8)
Model ID	$IR^1$	$SQ^2$	$MR^3$	$LR^4$	$IC^5$	Total	Mean (Å)	Max (Å)	$\mathbf{SD}^6$ (Å)	Median (Å)
1	25	78	16	45	20	184	1.11	3.67	0.75	0.98
2	24	74	16	46	20	180	1.06	3.69	0.73	0.9
3	24	80	20	50	24	198	1.0	3.63	0.75	0.88
4	25	74	16	45	19	179	1.13	3.74	0.81	1.03
5	25	79	16	46	23	189	1.03	3.76	0.73	0.86
6	26	80	16	48	23	193	1.1	3.78	0.82	0.93
7	25	77	16	52	22	192	1.07	3.75	0.76	0.92
8	26	77	19	47	25	194	1.07	3.76	0.76	0.92
9	25	77	18	48	21	189	1.07	3.82	0.8	0.9
10	25	78	17	49	24	193	1.03	3.7	0.74	0.87
11	24	78	17	47	22	188	1.09	3.74	0.82	0.92

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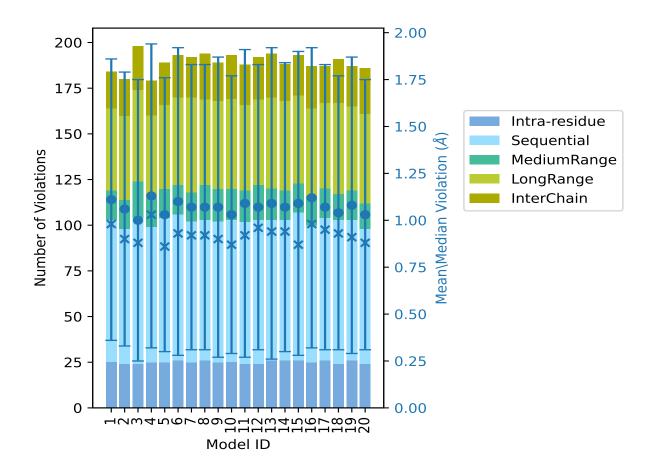


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Model ID		Nun	nber o	f viola	ations	3	Mean (Å)	Max (Å)	$SD^6$ (Å)	Median (Å)
Model 1D	$IR^1$	$SQ^2$	$ m MR^3$	$LR^4$	$IC^5$	Total	Mean (A)	Max (A)	$SD^*(A)$	Median (A)
12	24	79	19	47	23	192	1.07	3.81	0.76	0.96
13	26	77	17	50	24	194	1.09	3.79	0.83	0.94
14	26	77	16	49	20	188	1.07	3.79	0.77	0.94
15	26	81	16	48	22	193	1.09	3.77	0.81	0.87
16	25	75	16	48	23	187	1.12	3.81	0.8	0.98
17	26	78	16	47	20	187	1.07	3.67	0.76	0.95
18	24	79	14	50	24	191	1.04	3.8	0.73	0.93
19	26	77	16	46	22	187	1.08	3.64	0.79	0.91
20	24	74	14	49	25	186	1.03	3.8	0.72	0.88

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

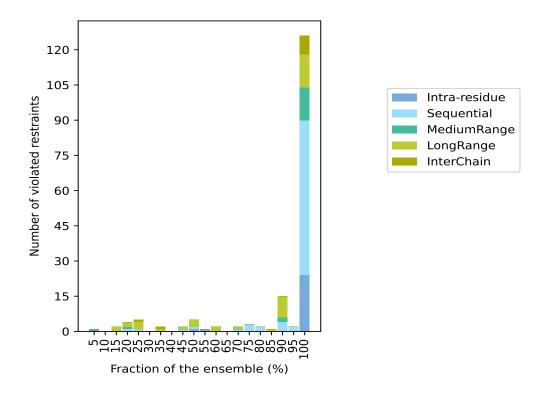
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 28(IR:12, SQ:4, MR:2, LR:10, IC:0) restraints are not violated in the ensemble.

Nu	$\overline{\mathbf{mber}}$	of vio	lated	restra	aints	Fraction	n of the ensemble
$IR^1$	$SQ^2$	$MR^3$	$LR^4$	$IC^5$	Total	Count <sup>6</sup>	%
0	0	1	0	0	1	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	2	0	2	3	15.0
0	1	1	2	0	4	4	20.0
0	1	0	3	1	5	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	1	1	2	7	35.0
0	0	0	0	0	0	8	40.0
0	1	0	1	0	2	9	45.0
1	1	0	3	0	5	10	50.0
1	0	0	0	0	1	11	55.0
0	0	0	2	0	2	12	60.0
0	0	0	0	0	0	13	65.0
0	1	0	1	0	2	14	70.0
0	3	0	0	0	3	15	75.0
0	2	0	0	0	2	16	80.0
0	0	0	1	0	1	17	85.0
0	4	2	9	0	15	18	90.0
0	2	0	0	0	2	19	95.0
24	66	14	14	8	126	20	100.0

 $<sup>^1</sup>$ 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)

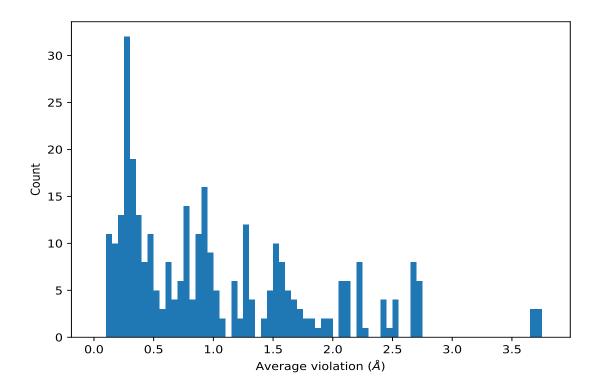


## 9.4 Most violated distance restraints in the ensemble (i)

## 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 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	$\mathbf{Models}^1$	Mean (Å)	$SD^1$ (Å)	Median (Å)
(4,145)	1:108:B:VAL:HG11	1:109:B:CYS:H	20	3.72	0.07	3.71
(4,145)	1:108:B:VAL:HG12	1:109:B:CYS:H	20	3.72	0.07	3.71
(4,145)	1:108:B:VAL:HG13	1:109:B:CYS:H	20	3.72	0.07	3.71
(4,144)	1:8:A:VAL:HG11	1:9:A:CYS:H	20	3.68	0.08	3.7
(4,144)	1:8:A:VAL:HG12	1:9:A:CYS:H	20	3.68	0.08	3.7
(4,144)	1:8:A:VAL:HG13	1:9:A:CYS:H	20	3.68	0.08	3.7
(4,122)	1:104:B:VAL:H	1:104:B:VAL:HG21	20	2.7	0.07	2.7
(4,122)	1:104:B:VAL:H	1:104:B:VAL:HG22	20	2.7	0.07	2.7
(4,122)	1:104:B:VAL:H	1:104:B:VAL:HG23	20	2.7	0.07	2.7
(4,121)	1:4:A:VAL:H	1:4:A:VAL:HG21	20	2.7	0.07	2.7
(4,121)	1:4:A:VAL:H	1:4:A:VAL:HG22	20	2.7	0.07	2.7
(4,121)	1:4:A:VAL:H	1:4:A:VAL:HG23	20	2.7	0.07	2.7
(4,78)	1:113:B:VAL:H	1:113:B:VAL:HG21	20	2.66	0.08	2.66
(4,78)	1:113:B:VAL:H	1:113:B:VAL:HG22	20	2.66	0.08	2.66
(4,78)	1:113:B:VAL:H	1:113:B:VAL:HG23	20	2.66	0.08	2.66
(4,50)	1:106:B:ILE:HG12	1:107:B:ARG:H	20	2.66	0.71	2.98

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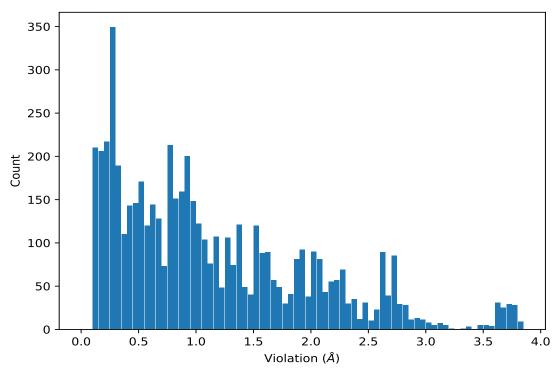
Key	Atom-1	Atom-2	$\mathbf{Models}^1$	Mean (Å)	${ m SD}^1$ (Å)	Median (Å)
(4,77)	1:13:A:VAL:H	1:13:A:VAL:HG21	20	2.65	0.07	2.64
(4,77)	1:13:A:VAL:H	1:13:A:VAL:HG22	20	2.65	0.07	2.64
(4,77)	1:13:A:VAL:H	1:13:A:VAL:HG23	20	2.65	0.07	2.64
(4,49)	1:6:A:ILE:HG12	1:7:A:ARG:H	20	2.65	0.7	2.85
(4,99)	1:3:A:ARG:HB3	1:4:A:VAL:H	20	2.51	0.41	2.58
(4,100)	1:103:B:ARG:HB3	1:104:B:VAL:H	20	2.47	0.41	2.52

<sup>&</sup>lt;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)
(4,145)	1:108:B:VAL:HG11	1:109:B:CYS:H	9	3.82
(4,145)	1:108:B:VAL:HG12	1:109:B:CYS:H	9	3.82
(4,145)	1:108:B:VAL:HG13	1:109:B:CYS:H	9	3.82
(4,145)	1:108:B:VAL:HG11	1:109:B:CYS:H	12	3.81
(4,145)	1:108:B:VAL:HG12	1:109:B:CYS:H	12	3.81
(4,145)	1:108:B:VAL:HG13	1:109:B:CYS:H	12	3.81
(4,145)	1:108:B:VAL:HG11	1:109:B:CYS:H	16	3.81
(4,145)	1:108:B:VAL:HG12	1:109:B:CYS:H	16	3.81
(4,145)	1:108:B:VAL:HG13	1:109:B:CYS:H	16	3.81
(4,145)	1:108:B:VAL:HG11	1:109:B:CYS:H	20	3.8
(4,145)	1:108:B:VAL:HG12	1:109:B:CYS:H	20	3.8
(4,145)	1:108:B:VAL:HG13	1:109:B:CYS:H	20	3.8
(4,144)	1:8:A:VAL:HG11	1:9:A:CYS:H	18	3.8
(4,144)	1:8:A:VAL:HG12	1:9:A:CYS:H	18	3.8
(4,144)	1:8:A:VAL:HG13	1:9:A:CYS:H	18	3.8
(4,145)	1:108:B:VAL:HG11	1:109:B:CYS:H	14	3.79
(4,145)	1:108:B:VAL:HG12	1:109:B:CYS:H	14	3.79
(4,145)	1:108:B:VAL:HG13	1:109:B:CYS:H	14	3.79
(4,83)	1:16:A:ARG:H	1:16:A:ARG:HG2	13	3.79
(4,144)	1:8:A:VAL:HG11	1:9:A:CYS:H	6	3.78
(4,144)	1:8:A:VAL:HG12	1:9:A:CYS:H	6	3.78
(4,144)	1:8:A:VAL:HG13	1:9:A:CYS:H	6	3.78
(4,144)	1:8:A:VAL:HG11	1:9:A:CYS:H	16	3.78
(4,144)	1:8:A:VAL:HG12	1:9:A:CYS:H	16	3.78
(4,144)	1:8:A:VAL:HG13	1:9:A:CYS:H	16	3.78
(4,145)	1:108:B:VAL:HG11	1:109:B:CYS:H	15	3.77



## 10 Dihedral-angle violation analysis (i)

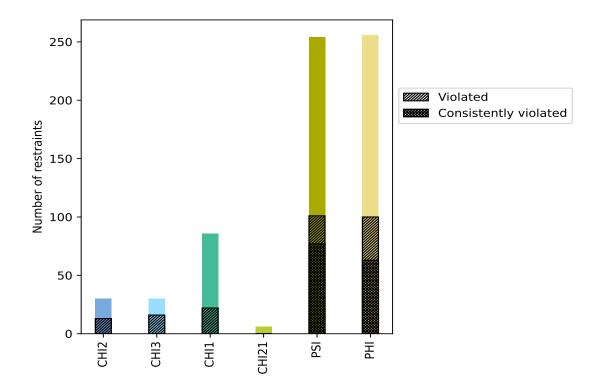
## 10.1 Summary of dihedral-angle violations (i)

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 tree	Count	$\%^{1}$	Vie	olated	3	Consistently Violated <sup>4</sup>		
Angle type	Count	70	Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
CHI2	30	4.5	13	43.3	2.0	0	0.0	0.0
CHI3	30	4.5	16	53.3	2.4	0	0.0	0.0
CHI1	86	13.0	22	25.6	3.3	0	0.0	0.0
CHI21	6	0.9	0	0.0	0.0	0	0.0	0.0
PSI	254	38.4	101	39.8	15.3	77	30.3	11.6
PHI	256	38.7	100	39.1	15.1	63	24.6	9.5
Total	662	100.0	252	38.1	38.1	140	21.1	21.1

 $<sup>^1</sup>$  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

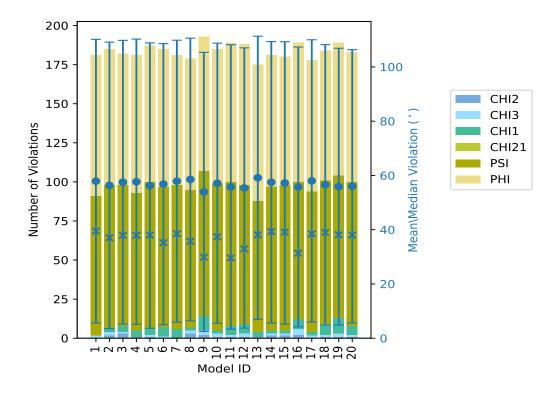
## 10.2 Dihedral-angle violation statistics for each model (i)

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		N	lumber	of viola	ations	3		Mean (°)	Max (°)	SD (°)	Media
Model 1D	CHI2	CHI3	CHI1	CHI21	PSI	PHI	Total	Mean ()	Max ()	$\mathbf{SD}$ (°)	Media
1	0	2	0	0	89	90	181	57.9	171.8	52.28	39.4
2	2	2	2	0	92	87	185	56.36	171.72	52.79	37.0
3	3	1	4	0	90	84	182	57.52	171.61	52.28	37.9
4	1	0	4	0	88	88	181	57.69	171.51	52.58	37.9
5	1	1	4	0	94	87	187	56.26	171.27	52.61	38.0
6	0	1	6	0	90	88	185	56.79	169.03	51.8	35.2
7	0	0	6	0	92	83	181	57.9	171.89	51.96	38.
8	3	2	2	0	88	84	179	58.52	170.87	52.09	35.7
9	2	3	9	0	93	86	193	53.94	171.55	51.44	29.8
10	1	2	2	0	94	86	185	57.13	170.47	51.64	37.4
11	1	1	6	0	92	89	189	55.77	171.95	52.42	29.5
12	1	2	6	0	89	90	188	55.38	168.96	51.66	32.9
13	1	0	3	0	84	87	175	59.15	171.33	52.19	38.1
14	2	1	2	0	92	84	181	57.5	168.26	51.86	39.3
15	2	1	2	0	93	82	180	57.24	171.89	52.06	39.1
16	2	4	6	0	88	89	189	55.77	169.29	51.58	31.3
17	0	2	2	0	90	84	178	58.01	171.71	52.01	38.4
18	1	1	7	0	92	83	184	56.56	170.62	51.68	39.0
19	1	2	10	0	91	85	189	55.88	170.91	51.01	38.1
20	1	1	6	0	92	83	183	56.0	168.65	50.37	38.0



#### 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.

	Numb	oer of v	Fractio	n of the ensemble				
CHI2	CHI3	CHI1	CHI21	PSI	PHI	Total	Count <sup>1</sup>	%
5	9	4	0	1	4	23	1	5.0
6	3	5	0	4	4	22	2	10.0
1	2	1	0	0	0	4	3	15.0
0	2	4	0	0	0	6	4	20.0
1	0	1	0	0	1	3	5	25.0
0	0	2	0	0	1	3	6	30.0
0	0	3	0	2	1	6	7	35.0
0	0	1	0	2	1	4	8	40.0
0	0	0	0	1	0	1	9	45.0
0	0	1	0	1	0	2	10	50.0
0	0	0	0	0	4	4	11	55.0

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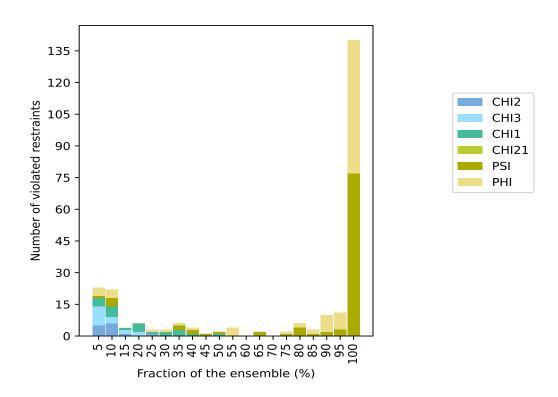


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	Numl	oer of v	Fraction of the ensemble					
CHI2	CHI3	CHI1	CHI21	PSI	PHI	Total	Count <sup>1</sup>	%
0	0	0	0	0	0	0	12	60.0
0	0	0	0	2	0	2	13	65.0
0	0	0	0	0	0	0	14	70.0
0	0	0	0	1	1	2	15	75.0
0	0	0	0	4	2	6	16	80.0
0	0	0	0	1	2	3	17	85.0
0	0	0	0	2	8	10	18	90.0
0	0	0	0	3	8	11	19	95.0
0	0	0	0	77	63	140	20	100.0

<sup>&</sup>lt;sup>1</sup> Number of models with violations

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



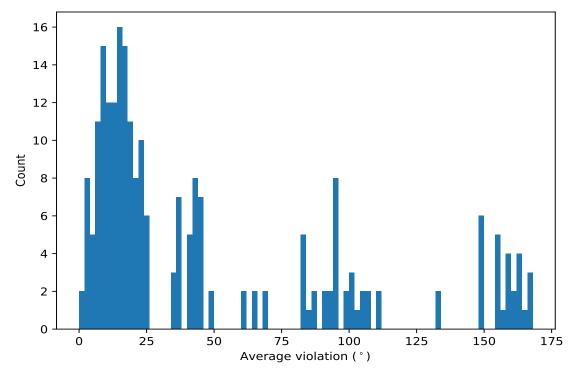
## 10.4 Most violated dihedral-angle restraints in the ensemble (i)

#### 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	$\mathbf{Models}^1$	Mean	$\mathbf{S}\mathbf{D}^2$	Median
(1,471)	1:106:B:ILE:C	1:107:B:ARG:N	1:107:B:ARG:CA	1:107:B:ARG:C	20	167.12	5.47	168.76
(1,247)	1:6:A:ILE:C	1:7:A:ARG:N	1:7:A:ARG:CA	1:7:A:ARG:C	20	166.31	5.77	168.78
(1,611)	1:117:B:ARG:C	1:118:B:CYS:N	1:118:B:CYS:CA	1:118:B:CYS:C	20	166.18	4.99	168.59
(1,387)	1:17:A:ARG:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	20	165.27	6.25	168.16
(1,583)	1:115:B:TYR:C	1:116:B:ARG:N	1:116:B:ARG:CA	1:116:B:ARG:C	20	163.01	12.45	168.22
(1,359)	1:15:A:TYR:C	1:16:A:ARG:N	1:16:A:ARG:CA	1:16:A:ARG:C	20	162.81	10.21	167.1
(1,555)	1:113:B:VAL:C	1:114:B:CYS:N	1:114:B:CYS:CA	1:114:B:CYS:C	20	162.77	4.27	163.55
(1,331)	1:13:A:VAL:C	1:14:A:CYS:N	1:14:A:CYS:CA	1:14:A:CYS:C	20	162.67	4.96	164.0
(1,625)	1:118:B:CYS:C	1:119:B:TRP:N	1:119:B:TRP:CA	1:119:B:TRP:C	20	161.03	8.42	164.29
(1,401)	1:18:A:CYS:C	1:19:A:TRP:N	1:19:A:TRP:CA	1:19:A:TRP:C	20	160.84	8.82	164.39

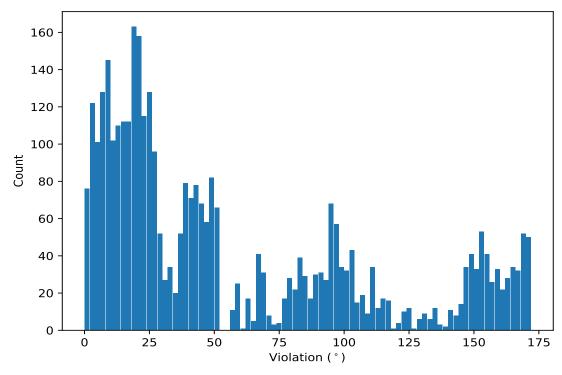
 $<sup>^1</sup>$  Number of violated models,  $^2\mathrm{Standard}$  deviation, All angle values are in degree (°)



## 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 (°)
(1,611)	1:117:B:ARG:C	1:118:B:CYS:N	1:118:B:CYS:CA	1:118:B:CYS:C	11	171.95
(1,471)	1:106:B:ILE:C	1:107:B:ARG:N	1:107:B:ARG:CA	1:107:B:ARG:C	15	171.89
(1,457)	1:105:B:CYS:C	1:106:B:ILE:N	1:106:B:ILE:CA	1:106:B:ILE:C	7	171.89
(1,583)	1:115:B:TYR:C	1:116:B:ARG:N	1:116:B:ARG:CA	1:116:B:ARG:C	1	171.8
(1,359)	1:15:A:TYR:C	1:16:A:ARG:N	1:16:A:ARG:CA	1:16:A:ARG:C	11	171.77
(1,611)	1:117:B:ARG:C	1:118:B:CYS:N	1:118:B:CYS:CA	1:118:B:CYS:C	2	171.72
(1,219)	1:4:A:VAL:C	1:5:A:CYS:N	1:5:A:CYS:CA	1:5:A:CYS:C	17	171.71
(1,611)	1:117:B:ARG:C	1:118:B:CYS:N	1:118:B:CYS:CA	1:118:B:CYS:C	3	171.61
(1,387)	1:17:A:ARG:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	2	171.61
(1,401)	1:18:A:CYS:C	1:19:A:TRP:N	1:19:A:TRP:CA	1:19:A:TRP:C	11	171.57

