Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2026 – 11:07 PM UTC

PDB ID	:	7L53 / pdb_00007l53
BMRB ID	:	30828
Title	:	Solution NMR structure of the monomeric form of the cyclic plant protein PDP-23 in CD3CN/H2O
Authors	:	Payne, C.D.; Rosengren, K.J.
Deposited on	:	2020-12-21

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 (i)) were used in the production of this report:

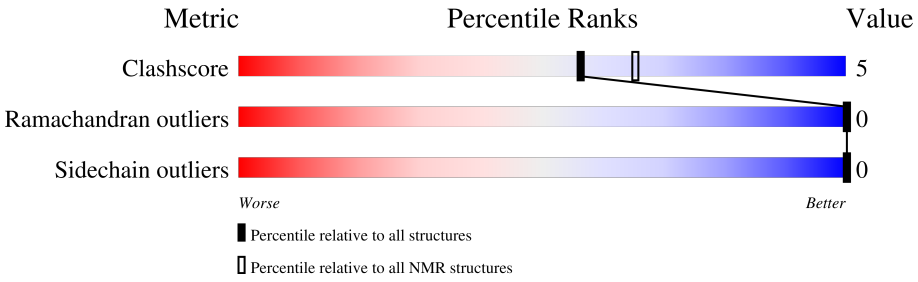
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 71%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	28	93% 7%

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:1-A:28 (28)	0.34	3

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 4 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 398 atoms, of which 179 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cyclic plant protein PDP-23.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	28	398	142	179	37	36	4	0

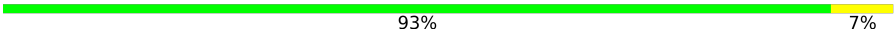
4 Residue-property plots

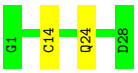
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Cyclic plant protein PDP-23

Chain A:





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: Cyclic plant protein PDP-23

Chain A:

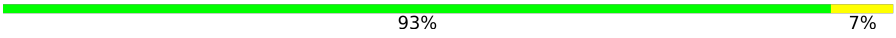


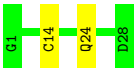


4.2.2 Score per residue for model 2

• Molecule 1: Cyclic plant protein PDP-23

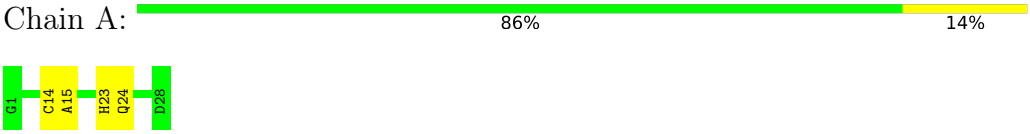
Chain A:





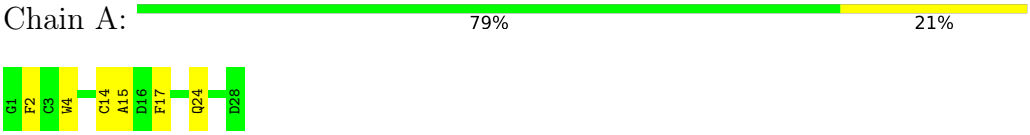
4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Cyclic plant protein PDP-23

Chain A: 

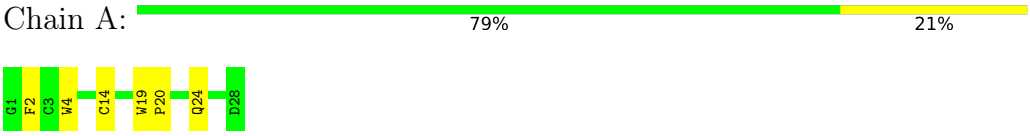
4.2.4 Score per residue for model 4

• Molecule 1: Cyclic plant protein PDP-23

Chain A: 

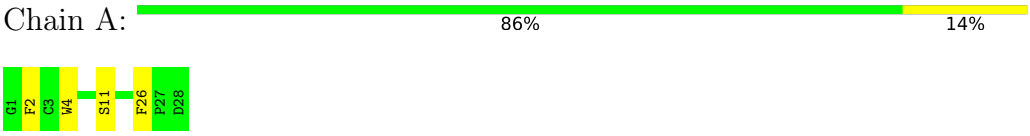
4.2.5 Score per residue for model 5

• Molecule 1: Cyclic plant protein PDP-23

Chain A: 

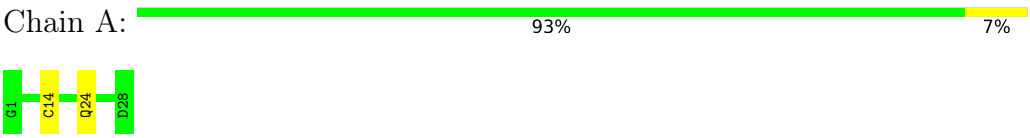
4.2.6 Score per residue for model 6

• Molecule 1: Cyclic plant protein PDP-23

Chain A: 

4.2.7 Score per residue for model 7

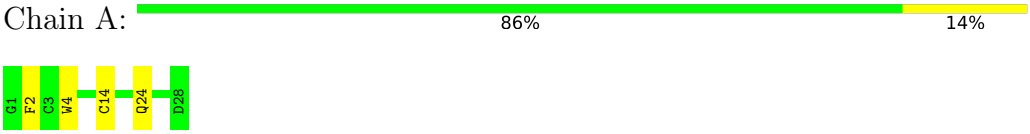
• Molecule 1: Cyclic plant protein PDP-23

Chain A: 

4.2.8 Score per residue for model 8

• Molecule 1: Cyclic plant protein PDP-23

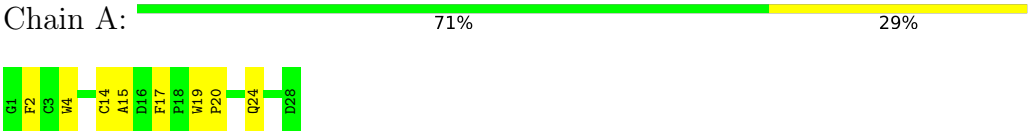
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Cyclic plant protein PDP-23

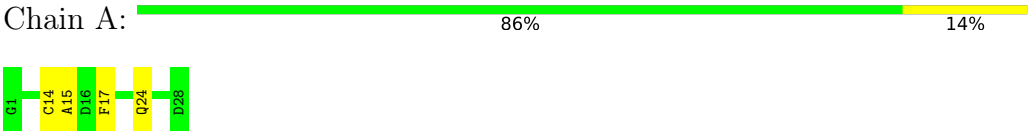
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Cyclic plant protein PDP-23

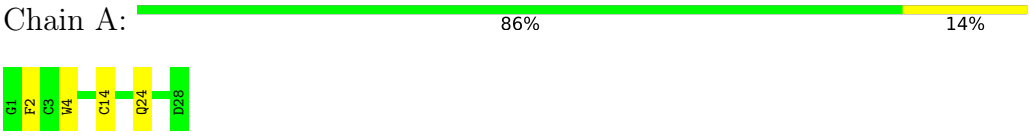
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Cyclic plant protein PDP-23

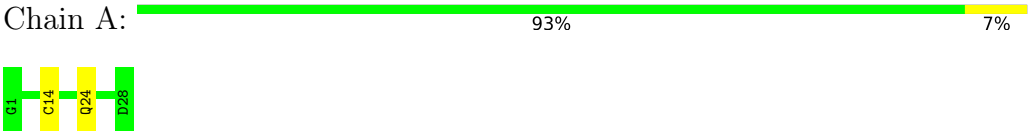
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Cyclic plant protein PDP-23

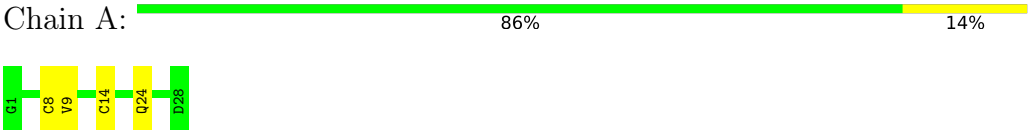
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Cyclic plant protein PDP-23

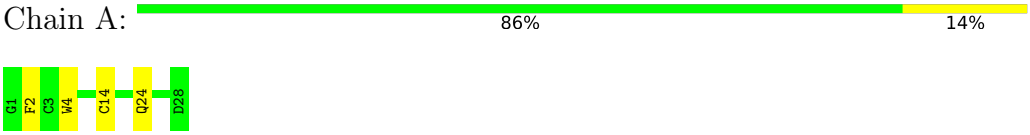
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Cyclic plant protein PDP-23

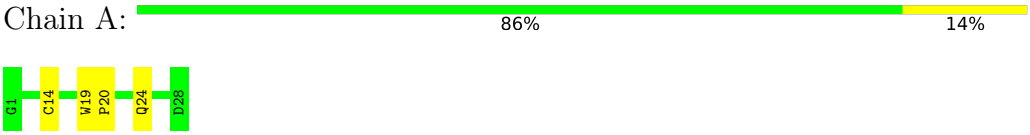
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Cyclic plant protein PDP-23

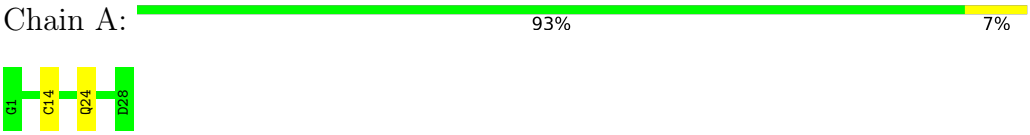
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Cyclic plant protein PDP-23

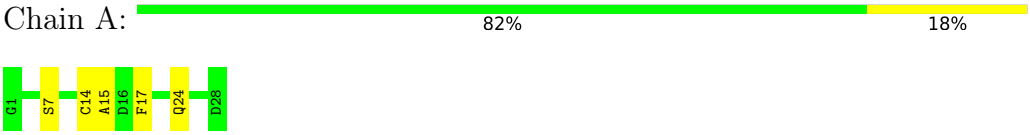
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Cyclic plant protein PDP-23

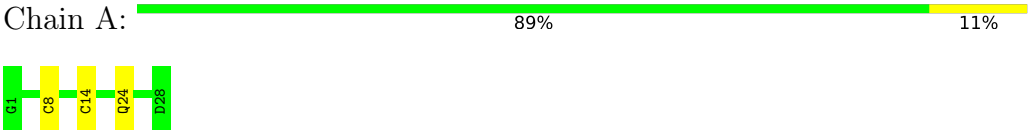
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Cyclic plant protein PDP-23

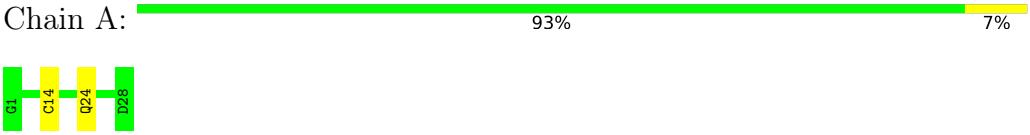
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Cyclic plant protein PDP-23

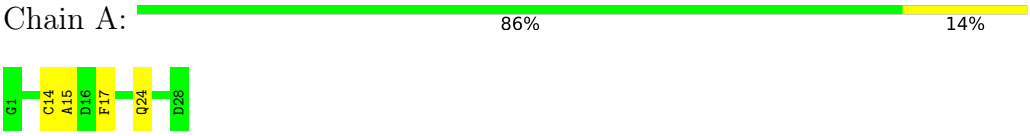
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Cyclic plant protein PDP-23

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with lowest energy.*

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

Software name	Classification	Version
CYANA	structure calculation	
CNS	structure calculation	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	241
Number of shifts mapped to atoms	241
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

6 Model quality

6.1 Standard geometry

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	1.11±0.05	0±1/232 (0.1± 0.2%)	1.05±0.02	0±0/319 (0.0± 0.0%)
All	All	1.11	4/4640 (0.1%)	1.05	0/6380 (0.0%)

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	8	CYS	C-N	-6.36	1.27	1.33	13	2
1	A	9	VAL	N-CA	-5.44	1.41	1.46	13	1
1	A	7	SER	C-N	-5.01	1.27	1.33	17	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	219	179	179	2±1
All	All	4380	3580	3580	39

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:PHE:CE2	1:A:4:TRP:HB2	0.51	2.41	1	3
1:A:15:ALA:HB3	1:A:17:PHE:CE2	0.50	2.41	9	3
1:A:14:CYS:HA	1:A:24:GLN:O	0.47	2.09	8	19
1:A:15:ALA:HB3	1:A:17:PHE:CE1	0.47	2.44	4	3
1:A:2:PHE:CE1	1:A:4:TRP:HB2	0.44	2.48	6	5
1:A:19:TRP:CG	1:A:20:PRO:HA	0.43	2.49	5	3
1:A:15:ALA:O	1:A:23:HIS:HA	0.42	2.14	3	1
1:A:11:SER:HA	1:A:26:PHE:O	0.41	2.16	6	1
1:A:15:ALA:HB3	1:A:17:PHE:CZ	0.40	2.51	4	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	26/28 (93%)	25±0 (98±2%)	1±0 (2±2%)	0±0 (0±0%)	100	100
All	All	520/560 (93%)	508 (98%)	12 (2%)	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	Percentiles	
1	A	24/24 (100%)	24±0 (100±0%)	0±0 (0±0%)	100	100
All	All	480/480 (100%)	480 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 71% for the well-defined parts and 71% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *PDP-23_Monomer_cs.str*

7.1.1 Bookkeeping

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

Total number of shifts	241
Number of shifts mapped to atoms	241
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

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 71%, i.e. 240 atoms were assigned a chemical shift out of a possible 339. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	90/135 (67%)	54/55 (98%)	16/56 (29%)	20/24 (83%)
Sidechain	118/129 (91%)	85/85 (100%)	33/43 (77%)	0/1 (0%)
Aromatic	32/75 (43%)	32/39 (82%)	0/31 (0%)	0/5 (0%)
Overall	240/339 (71%)	171/179 (96%)	49/130 (38%)	20/30 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 240 atoms were assigned a chemical shift out of a possible 339. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	90/135 (67%)	54/55 (98%)	16/56 (29%)	20/24 (83%)
Sidechain	118/129 (91%)	85/85 (100%)	33/43 (77%)	0/1 (0%)
Aromatic	32/75 (43%)	32/39 (82%)	0/31 (0%)	0/5 (0%)
Overall	240/339 (71%)	171/179 (96%)	49/130 (38%)	20/30 (67%)

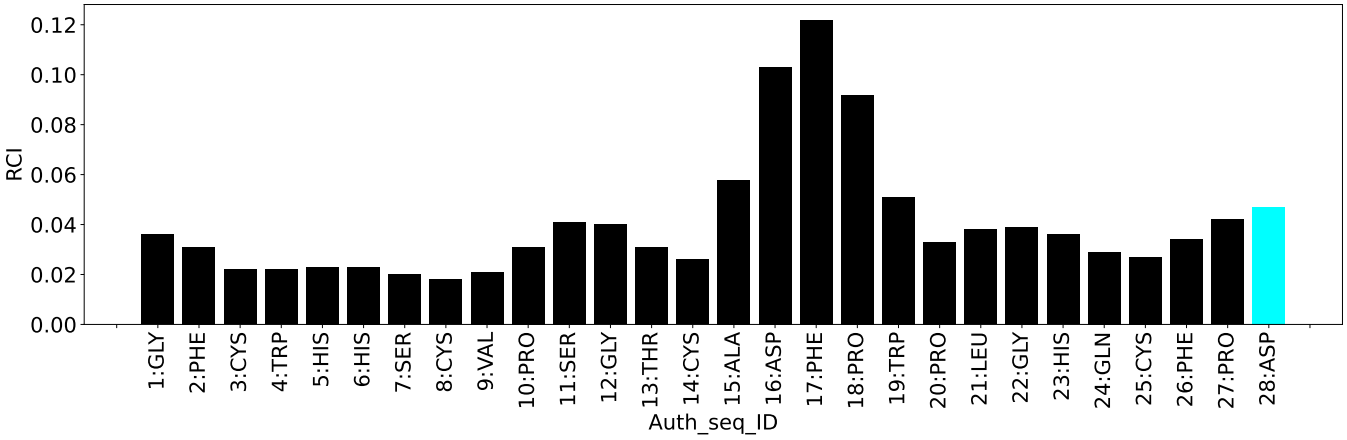
7.1.4 Statistically unusual chemical shifts (i)

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	432
Intra-residue (|i-j|=0)	87
Sequential (|i-j|=1)	130
Medium range (|i-j|>1 and |i-j|<5)	74
Long range (|i-j|≥5)	115
Inter-chain	0
Hydrogen bond restraints	26
Disulfide bond restraints	0
Total dihedral-angle restraints	38
Number of unmapped restraints	0
Number of restraints per residue	16.8
Number of long range restraints per residue[1]	4.7

[1]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)	3.5	0.19
0.2-0.5 (Medium)	0.7	0.5
>0.5 (Large)	1.1	1.68

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)	1.3	1.76
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

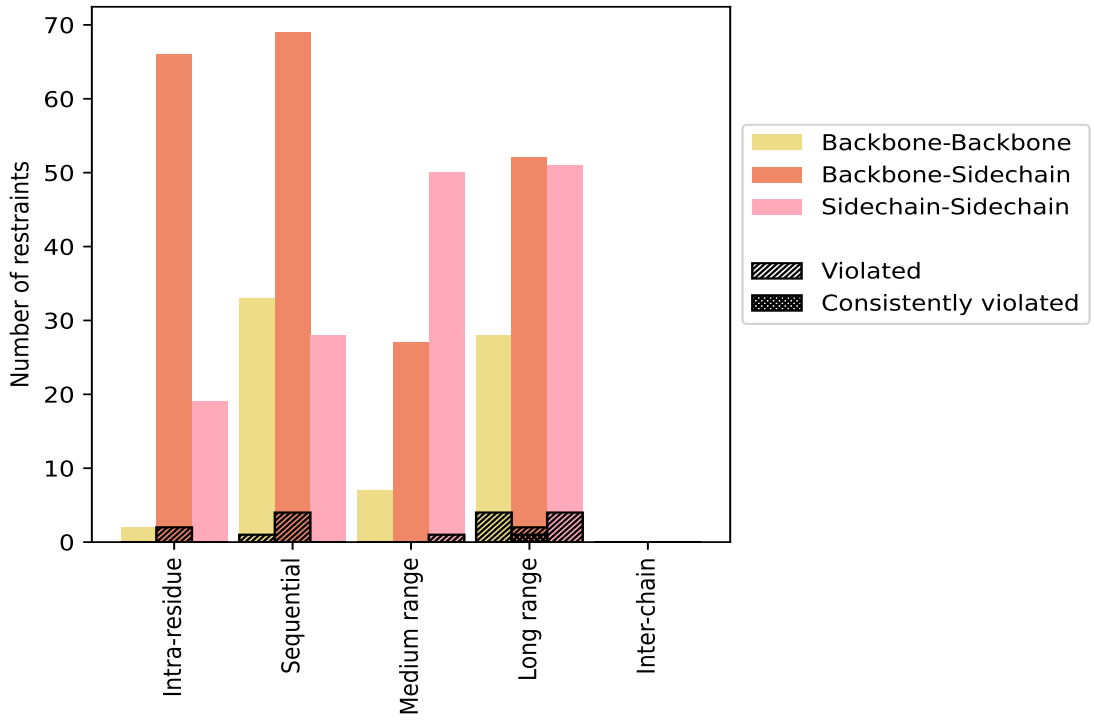
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	87	20.1	2	2.3	0.5	0	0.0	0.0
Backbone-Backbone	2	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	66	15.3	2	3.0	0.5	0	0.0	0.0
Sidechain-Sidechain	19	4.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	130	30.1	5	3.8	1.2	0	0.0	0.0
Backbone-Backbone	33	7.6	1	3.0	0.2	0	0.0	0.0
Backbone-Sidechain	69	16.0	4	5.8	0.9	0	0.0	0.0
Sidechain-Sidechain	28	6.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	74	17.1	1	1.4	0.2	0	0.0	0.0
Backbone-Backbone	7	1.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	17	3.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	50	11.6	1	2.0	0.2	0	0.0	0.0
Long range (|i-j|≥5)	115	26.6	9	7.8	2.1	0	0.0	0.0
Backbone-Backbone	28	6.5	4	14.3	0.9	0	0.0	0.0
Backbone-Sidechain	36	8.3	1	2.8	0.2	0	0.0	0.0
Sidechain-Sidechain	51	11.8	4	7.8	0.9	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	26	6.0	1	3.8	0.2	1	3.8	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	432	100.0	18	4.2	4.2	1	0.2	0.2
Backbone-Backbone	70	16.2	5	7.1	1.2	0	0.0	0.0
Backbone-Sidechain	214	49.5	8	3.7	1.9	1	0.5	0.2
Sidechain-Sidechain	148	34.3	5	3.4	1.2	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



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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	3	0	4	0	7	0.18	0.49	0.13	0.11
2	1	2	0	2	0	5	0.16	0.3	0.07	0.13
3	1	1	0	6	0	8	0.46	1.56	0.52	0.15
4	0	3	0	2	0	5	0.21	0.53	0.16	0.13
5	0	2	1	2	0	5	0.23	0.65	0.21	0.13
6	1	3	0	1	0	5	0.2	0.54	0.17	0.12
7	0	0	0	5	0	5	0.76	1.57	0.62	0.57
8	0	3	0	2	0	5	0.19	0.45	0.13	0.13
9	0	3	0	5	0	8	0.49	1.45	0.54	0.16
10	0	3	0	5	0	8	0.48	1.56	0.53	0.16

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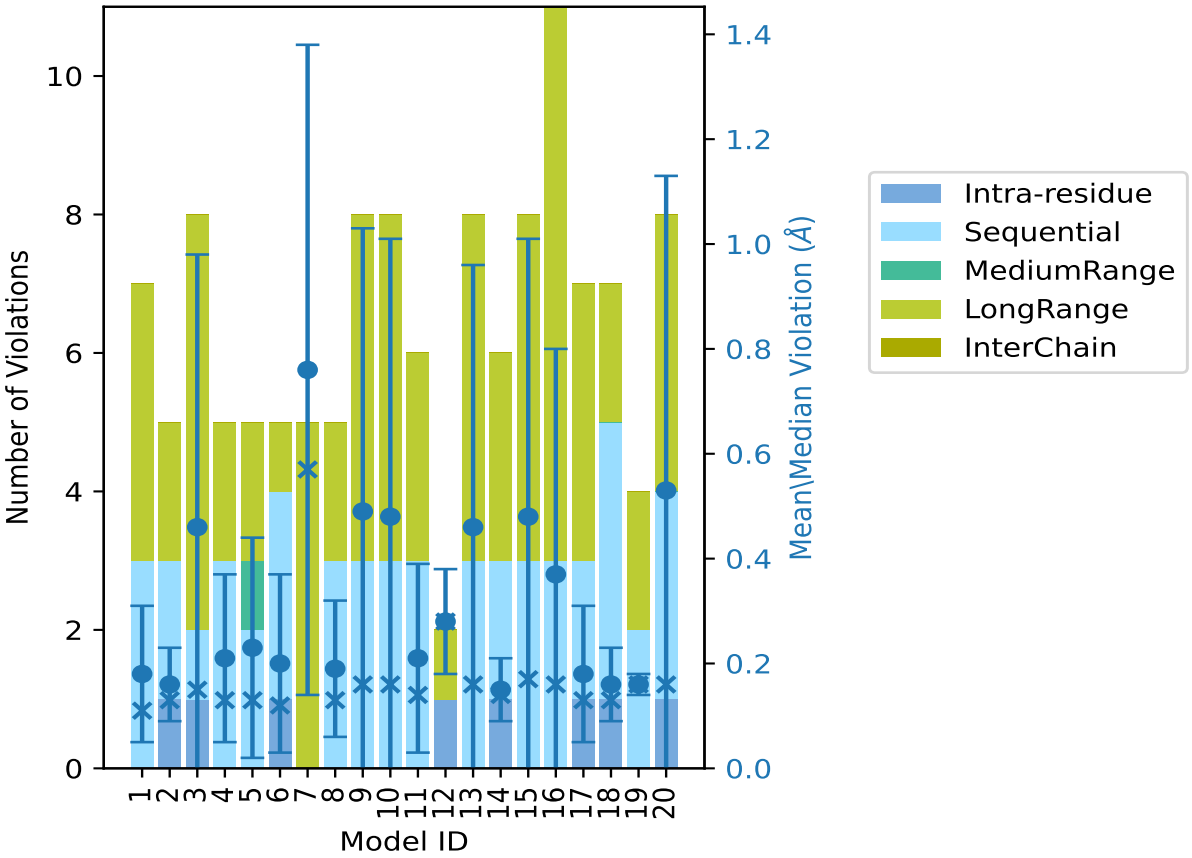
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	3	0	3	0	6	0.21	0.61	0.18	0.14
12	1	0	0	1	0	2	0.28	0.38	0.1	0.28
13	0	3	0	5	0	8	0.46	1.47	0.5	0.16
14	1	2	0	3	0	6	0.15	0.25	0.06	0.14
15	0	3	0	5	0	8	0.48	1.57	0.53	0.17
16	0	3	0	8	0	11	0.37	1.45	0.43	0.16
17	1	2	0	4	0	7	0.18	0.5	0.13	0.13
18	1	4	0	2	0	7	0.16	0.32	0.07	0.13
19	0	2	0	2	0	4	0.16	0.18	0.02	0.16
20	1	3	0	4	0	8	0.53	1.68	0.6	0.16

[1]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



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

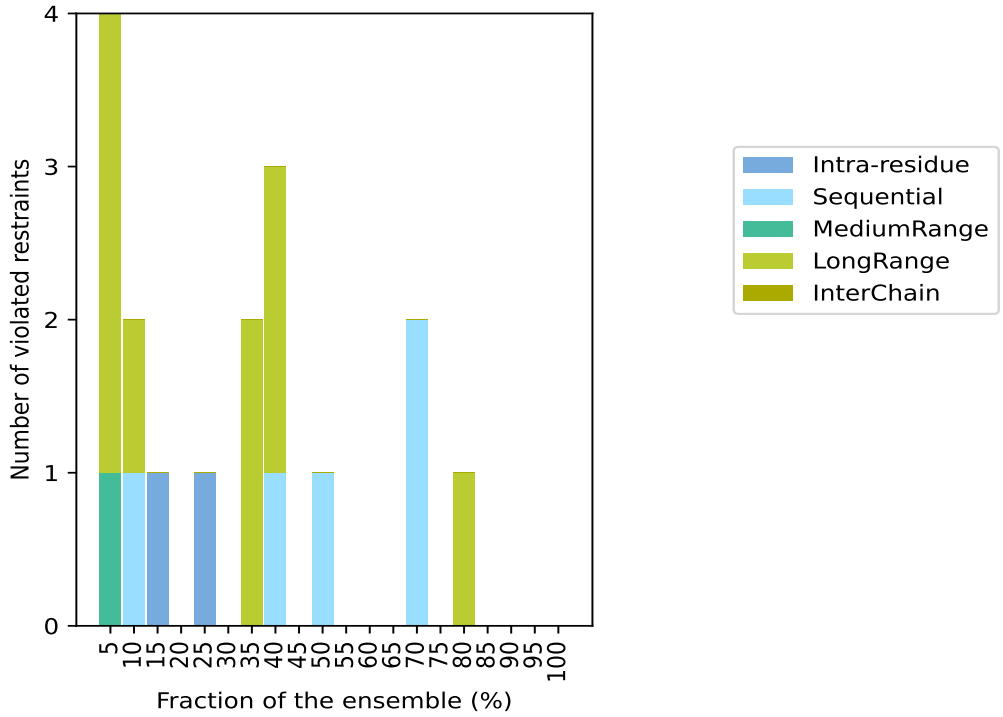
9.3 Distance violation statistics for the ensemble (i)

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, 389(IR:85, SQ:125, MR:73, LR:106, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	1	3	0	4	1	5.0
0	1	0	1	0	2	2	10.0
1	0	0	0	0	1	3	15.0
0	0	0	0	0	0	4	20.0
1	0	0	0	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	2	0	2	7	35.0
0	1	0	2	0	3	8	40.0
0	0	0	0	0	0	9	45.0
0	1	0	0	0	1	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	2	0	0	0	2	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	1	0	1	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

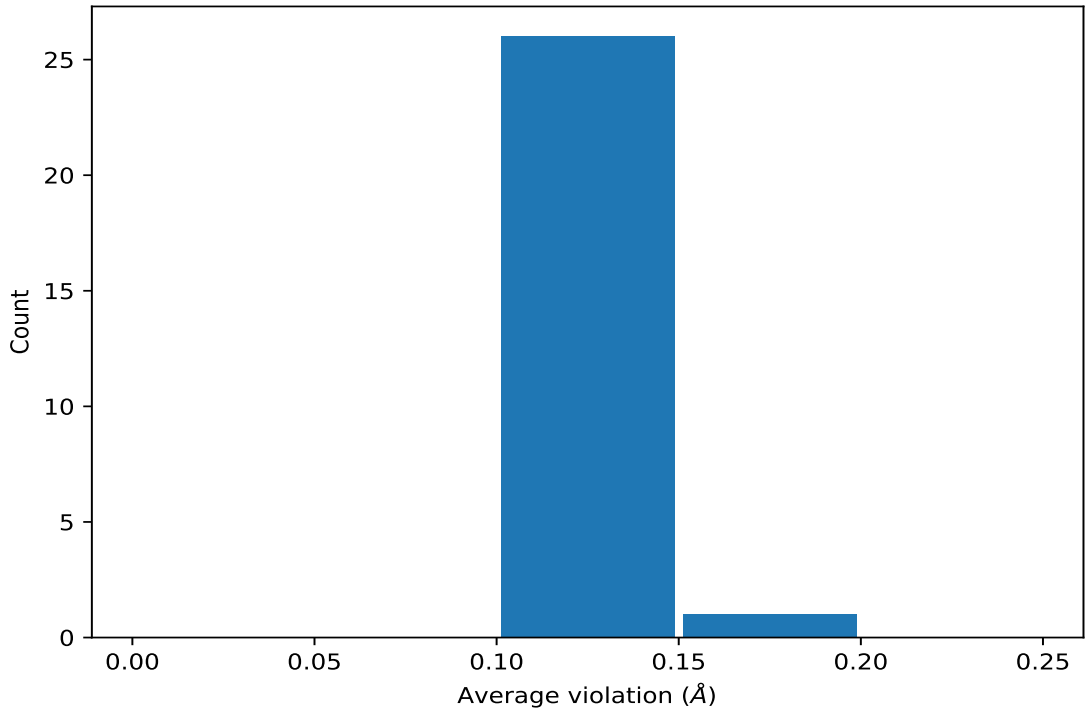
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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 theviolation 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)
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	16	0.15	0.02	0.15
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	16	0.15	0.02	0.15
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	16	0.15	0.02	0.15
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	16	0.15	0.02	0.15
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	16	0.15	0.02	0.15
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	16	0.15	0.02	0.15
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	14	0.15	0.03	0.16
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	14	0.12	0.02	0.11
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	10	0.12	0.01	0.12
(2,197)	1:8:A:CYS:HB2	1:9:A:VAL:H	8	0.15	0.02	0.16
(2,197)	1:8:A:CYS:HB3	1:9:A:VAL:H	8	0.15	0.02	0.16
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD1	7	0.11	0.01	0.1
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD2	7	0.11	0.01	0.1
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD1	7	0.11	0.01	0.1
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD2	7	0.11	0.01	0.1
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD1	7	0.11	0.01	0.1

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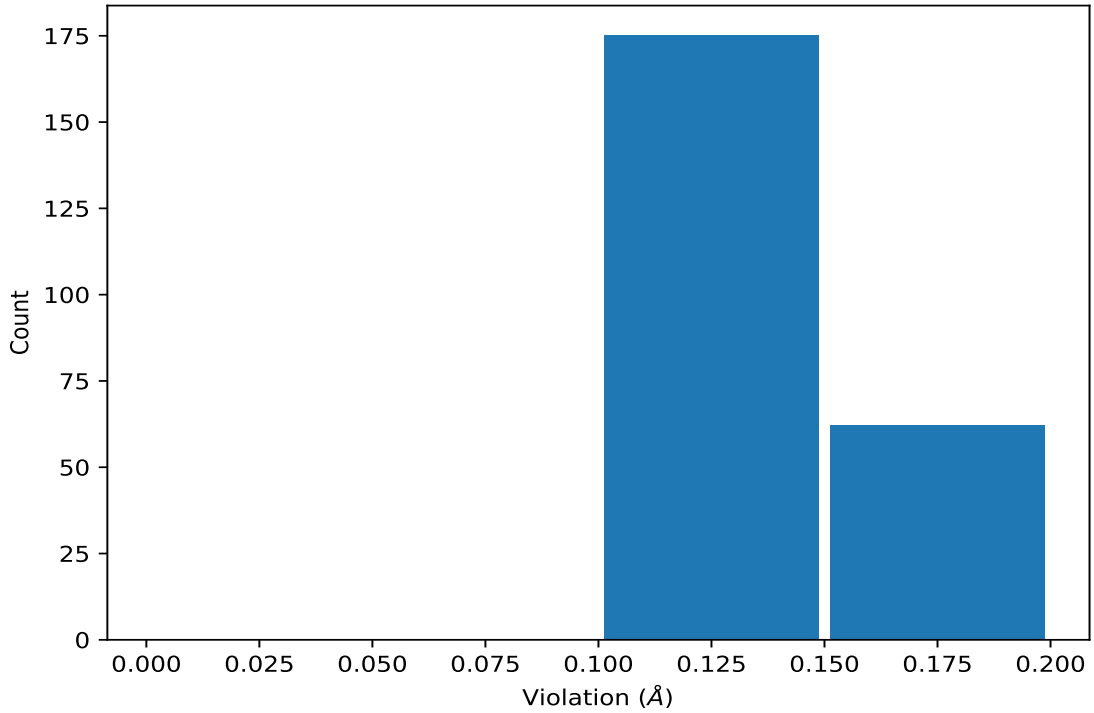
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD2	7	0.11	0.01	0.1
(2,306)	1:9:A:VAL:HG21	1:14:A:CYS:H	7	0.1	0.0	0.1
(2,306)	1:9:A:VAL:HG22	1:14:A:CYS:H	7	0.1	0.0	0.1
(2,306)	1:9:A:VAL:HG23	1:14:A:CYS:H	7	0.1	0.0	0.1
(2,228)	1:5:A:HIS:H	1:5:A:HIS:HD2	5	0.11	0.01	0.11
(2,42)	1:16:A:ASP:H	1:16:A:ASP:HB2	3	0.16	0.02	0.17
(2,338)	1:4:A:TRP:HZ3	1:9:A:VAL:HG21	2	0.13	0.0	0.13
(2,338)	1:4:A:TRP:HZ3	1:9:A:VAL:HG22	2	0.13	0.0	0.13
(2,338)	1:4:A:TRP:HZ3	1:9:A:VAL:HG23	2	0.13	0.0	0.13
(2,253)	1:7:A:SER:HA	1:8:A:CYS:HB2	2	0.11	0.0	0.11
(2,253)	1:7:A:SER:HA	1:8:A:CYS:HB3	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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)
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	15	0.19
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	16	0.19
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	16	0.19
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	16	0.19
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	16	0.19
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	16	0.19
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	16	0.19
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	14	0.18
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	19	0.18
(2,197)	1:8:A:CYS:HB2	1:9:A:VAL:H	18	0.18
(2,197)	1:8:A:CYS:HB3	1:9:A:VAL:H	18	0.18
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	1	0.18
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	1	0.18
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	1	0.18
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	1	0.18
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	1	0.18
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	1	0.18
(2,42)	1:16:A:ASP:H	1:16:A:ASP:HB2	14	0.18
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	1	0.17
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	5	0.17
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	8	0.17
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	11	0.17
(2,197)	1:8:A:CYS:HB2	1:9:A:VAL:H	13	0.17
(2,197)	1:8:A:CYS:HB3	1:9:A:VAL:H	13	0.17
(2,197)	1:8:A:CYS:HB2	1:9:A:VAL:H	19	0.17
(2,197)	1:8:A:CYS:HB3	1:9:A:VAL:H	19	0.17
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	3	0.17
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	3	0.17
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	3	0.17
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	3	0.17
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	3	0.17
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	3	0.17
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	9	0.17
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	9	0.17
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	9	0.17
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	9	0.17
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	9	0.17
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	10	0.17
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	10	0.17
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	10	0.17
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	10	0.17
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	10	0.17
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	10	0.17
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	20	0.17
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	20	0.17
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	20	0.17
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	20	0.17
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	20	0.17
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	20	0.17
(2,42)	1:16:A:ASP:H	1:16:A:ASP:HB2	12	0.17
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	4	0.16
(2,197)	1:8:A:CYS:HB2	1:9:A:VAL:H	10	0.16
(2,197)	1:8:A:CYS:HB3	1:9:A:VAL:H	10	0.16
(2,197)	1:8:A:CYS:HB2	1:9:A:VAL:H	16	0.16
(2,197)	1:8:A:CYS:HB3	1:9:A:VAL:H	16	0.16
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	2	0.16
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	2	0.16
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	2	0.16
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	2	0.16
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	2	0.16
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	2	0.16
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	7	0.15
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	7	0.15
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	7	0.15
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	7	0.15
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	7	0.15
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	7	0.15
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	13	0.15
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	13	0.15
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	13	0.15
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	13	0.15
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	13	0.15
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	13	0.15
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	17	0.15
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	17	0.15
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	17	0.15
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	17	0.15
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	17	0.15
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	15	0.15
(2,197)	1:8:A:CYS:HB2	1:9:A:VAL:H	9	0.14
(2,197)	1:8:A:CYS:HB3	1:9:A:VAL:H	9	0.14
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	11	0.14
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	11	0.14
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	11	0.14
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	11	0.14
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	11	0.14
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	11	0.14
(2,42)	1:16:A:ASP:H	1:16:A:ASP:HB2	20	0.14
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	11	0.14
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	16	0.14
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	18	0.14
(2,338)	1:4:A:TRP:HZ3	1:9:A:VAL:HG21	5	0.13
(2,338)	1:4:A:TRP:HZ3	1:9:A:VAL:HG22	5	0.13
(2,338)	1:4:A:TRP:HZ3	1:9:A:VAL:HG23	5	0.13
(2,338)	1:4:A:TRP:HZ3	1:9:A:VAL:HG21	15	0.13
(2,338)	1:4:A:TRP:HZ3	1:9:A:VAL:HG22	15	0.13
(2,338)	1:4:A:TRP:HZ3	1:9:A:VAL:HG23	15	0.13
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	13	0.13
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	8	0.13
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	18	0.13
(2,197)	1:8:A:CYS:HB2	1:9:A:VAL:H	2	0.13
(2,197)	1:8:A:CYS:HB3	1:9:A:VAL:H	2	0.13
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD1	17	0.13
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD2	17	0.13
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD1	17	0.13
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD2	17	0.13
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD1	17	0.13
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD2	17	0.13
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	4	0.13
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	4	0.13
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	4	0.13
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	4	0.13
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	4	0.13
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	4	0.13
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	19	0.13
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	19	0.13
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	19	0.13
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	19	0.13
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	19	0.13
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	6	0.12
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	16	0.12
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	4	0.12
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	6	0.12
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	9	0.12
(2,228)	1:5:A:HIS:H	1:5:A:HIS:HD2	17	0.12
(2,197)	1:8:A:CYS:HB2	1:9:A:VAL:H	3	0.12
(2,197)	1:8:A:CYS:HB3	1:9:A:VAL:H	3	0.12
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD1	3	0.12
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD2	3	0.12
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD1	3	0.12
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD2	3	0.12
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD1	3	0.12
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD2	3	0.12
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	8	0.12
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	8	0.12
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	8	0.12
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	8	0.12
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	8	0.12
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	8	0.12
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	18	0.12
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	18	0.12
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	18	0.12
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	18	0.12
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	18	0.12
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	18	0.12
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	2	0.12
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	20	0.11
(2,306)	1:9:A:VAL:HG21	1:14:A:CYS:H	16	0.11
(2,306)	1:9:A:VAL:HG22	1:14:A:CYS:H	16	0.11
(2,306)	1:9:A:VAL:HG23	1:14:A:CYS:H	16	0.11
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	11	0.11
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	13	0.11
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	15	0.11
(2,253)	1:7:A:SER:HA	1:8:A:CYS:HB2	17	0.11
(2,253)	1:7:A:SER:HA	1:8:A:CYS:HB3	17	0.11
(2,228)	1:5:A:HIS:H	1:5:A:HIS:HD2	2	0.11
(2,228)	1:5:A:HIS:H	1:5:A:HIS:HD2	18	0.11
(2,186)	1:17:A:PHE:HB3	1:21:A:LEU:HD21	5	0.11
(2,186)	1:17:A:PHE:HB3	1:21:A:LEU:HD22	5	0.11
(2,186)	1:17:A:PHE:HB3	1:21:A:LEU:HD23	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD1	1	0.11
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD2	1	0.11
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD1	1	0.11
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD2	1	0.11
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD1	1	0.11
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD2	1	0.11
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	4	0.11
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	6	0.11
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	9	0.11
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	10	0.11
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	14	0.11
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	17	0.11
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	20	0.11
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	10	0.1
(2,328)	1:4:A:TRP:HZ2	1:5:A:HIS:H	18	0.1
(2,306)	1:9:A:VAL:HG21	1:14:A:CYS:H	1	0.1
(2,306)	1:9:A:VAL:HG22	1:14:A:CYS:H	1	0.1
(2,306)	1:9:A:VAL:HG23	1:14:A:CYS:H	1	0.1
(2,306)	1:9:A:VAL:HG21	1:14:A:CYS:H	3	0.1
(2,306)	1:9:A:VAL:HG22	1:14:A:CYS:H	3	0.1
(2,306)	1:9:A:VAL:HG23	1:14:A:CYS:H	3	0.1
(2,306)	1:9:A:VAL:HG21	1:14:A:CYS:H	10	0.1
(2,306)	1:9:A:VAL:HG22	1:14:A:CYS:H	10	0.1
(2,306)	1:9:A:VAL:HG23	1:14:A:CYS:H	10	0.1
(2,306)	1:9:A:VAL:HG21	1:14:A:CYS:H	11	0.1
(2,306)	1:9:A:VAL:HG22	1:14:A:CYS:H	11	0.1
(2,306)	1:9:A:VAL:HG23	1:14:A:CYS:H	11	0.1
(2,306)	1:9:A:VAL:HG21	1:14:A:CYS:H	13	0.1
(2,306)	1:9:A:VAL:HG22	1:14:A:CYS:H	13	0.1
(2,306)	1:9:A:VAL:HG23	1:14:A:CYS:H	13	0.1
(2,306)	1:9:A:VAL:HG21	1:14:A:CYS:H	14	0.1
(2,306)	1:9:A:VAL:HG22	1:14:A:CYS:H	14	0.1
(2,306)	1:9:A:VAL:HG23	1:14:A:CYS:H	14	0.1
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	1	0.1
(2,296)	1:3:A:CYS:H	1:4:A:TRP:H	20	0.1
(2,274)	1:13:A:THR:HG21	1:26:A:PHE:HZ	16	0.1
(2,274)	1:13:A:THR:HG22	1:26:A:PHE:HZ	16	0.1
(2,274)	1:13:A:THR:HG23	1:26:A:PHE:HZ	16	0.1
(2,253)	1:7:A:SER:HA	1:8:A:CYS:HB2	1	0.1
(2,253)	1:7:A:SER:HA	1:8:A:CYS:HB3	1	0.1
(2,228)	1:5:A:HIS:H	1:5:A:HIS:HD2	3	0.1
(2,228)	1:5:A:HIS:H	1:5:A:HIS:HD2	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD1	7	0.1
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD2	7	0.1
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD1	7	0.1
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD2	7	0.1
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD1	7	0.1
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD2	7	0.1
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD1	9	0.1
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD2	9	0.1
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD1	9	0.1
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD2	9	0.1
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD1	9	0.1
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD2	9	0.1
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD1	15	0.1
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD2	15	0.1
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD1	15	0.1
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD2	15	0.1
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD1	15	0.1
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD2	15	0.1
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD1	16	0.1
(2,130)	1:9:A:VAL:HG11	1:26:A:PHE:HD2	16	0.1
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD1	16	0.1
(2,130)	1:9:A:VAL:HG12	1:26:A:PHE:HD2	16	0.1
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD1	16	0.1
(2,130)	1:9:A:VAL:HG13	1:26:A:PHE:HD2	16	0.1
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD1	14	0.1
(2,129)	1:9:A:VAL:HG21	1:17:A:PHE:HD2	14	0.1
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD1	14	0.1
(2,129)	1:9:A:VAL:HG22	1:17:A:PHE:HD2	14	0.1
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD1	14	0.1
(2,129)	1:9:A:VAL:HG23	1:17:A:PHE:HD2	14	0.1
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	5	0.1
(2,34)	1:13:A:THR:HB	1:14:A:CYS:H	8	0.1

10 Dihedral-angle violation analysis

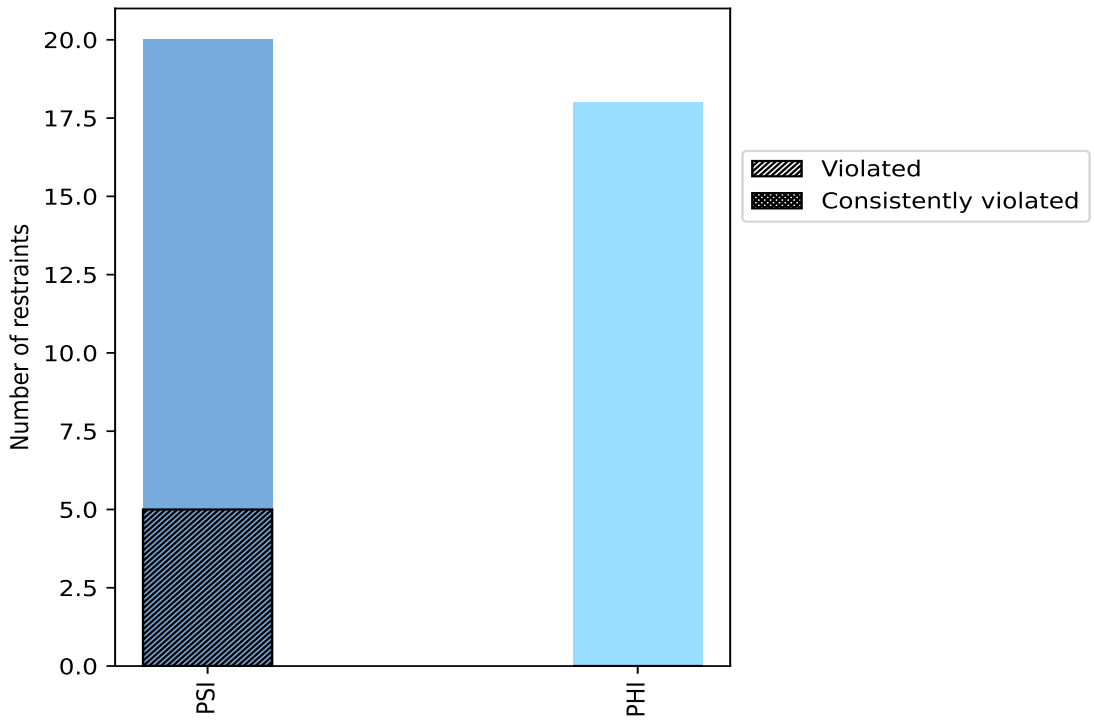
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	20	52.6	5	25.0	13.2	0	0.0	0.0
PHI	18	47.4	0	0.0	0.0	0	0.0	0.0
Total	38	100.0	5	13.2	13.2	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



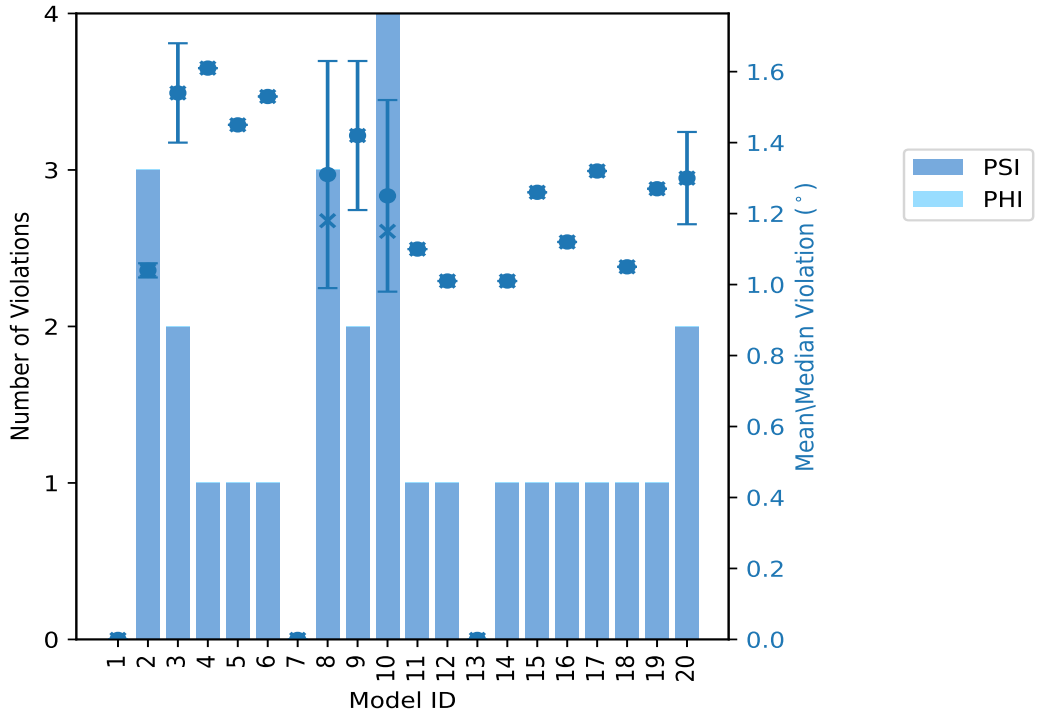
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	0	0	0	0.0	0.0	0.0	0.0
2	3	0	3	1.04	1.06	0.02	1.04
3	2	0	2	1.54	1.68	0.14	1.54
4	1	0	1	1.61	1.61	0.0	1.61
5	1	0	1	1.45	1.45	0.0	1.45
6	1	0	1	1.53	1.53	0.0	1.53
7	0	0	0	0.0	0.0	0.0	0.0
8	3	0	3	1.31	1.76	0.32	1.18
9	2	0	2	1.42	1.64	0.21	1.42
10	4	0	4	1.25	1.68	0.27	1.15
11	1	0	1	1.1	1.1	0.0	1.1
12	1	0	1	1.01	1.01	0.0	1.01
13	0	0	0	0.0	0.0	0.0	0.0
14	1	0	1	1.01	1.01	0.0	1.01
15	1	0	1	1.26	1.26	0.0	1.26
16	1	0	1	1.12	1.12	0.0	1.12
17	1	0	1	1.32	1.32	0.0	1.32
18	1	0	1	1.05	1.05	0.0	1.05
19	1	0	1	1.27	1.27	0.0	1.27
20	2	0	2	1.3	1.43	0.13	1.3

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	0	1	1	5.0
0	0	0	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
1	0	1	5	25.0
1	0	1	6	30.0
1	0	1	7	35.0
1	0	1	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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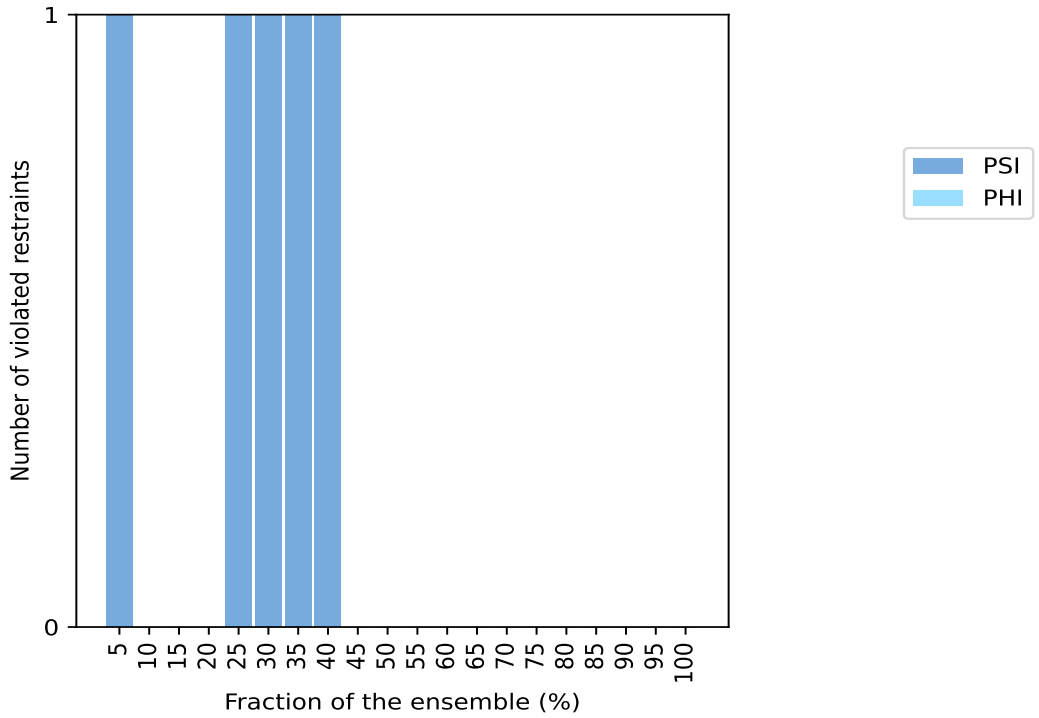
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

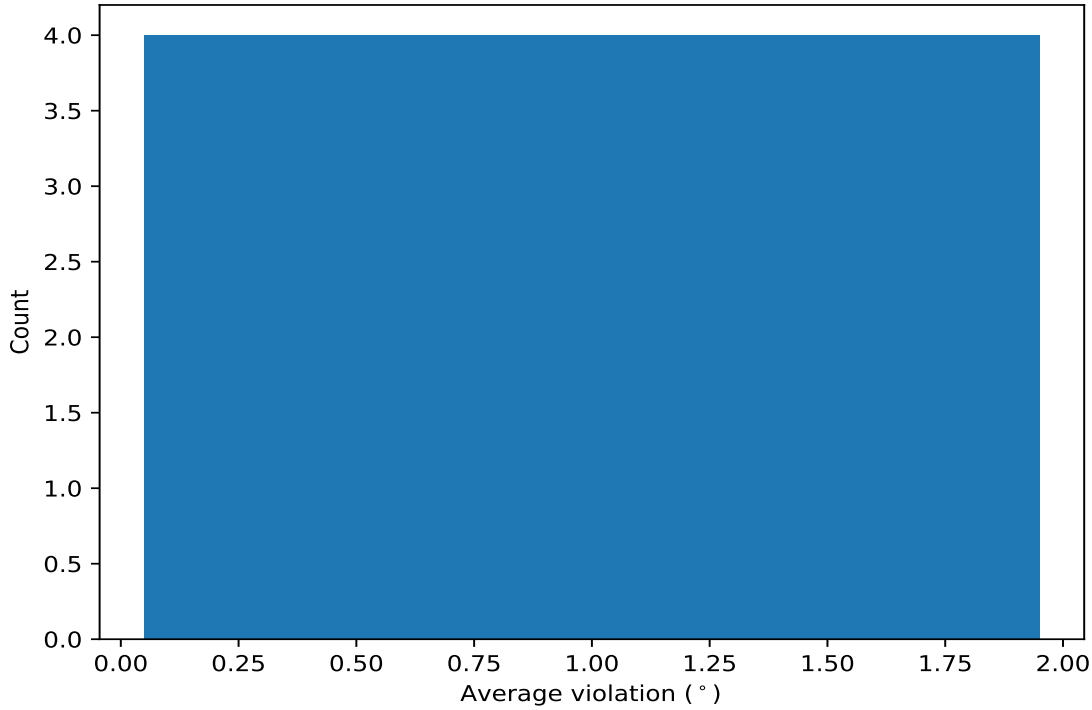


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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.

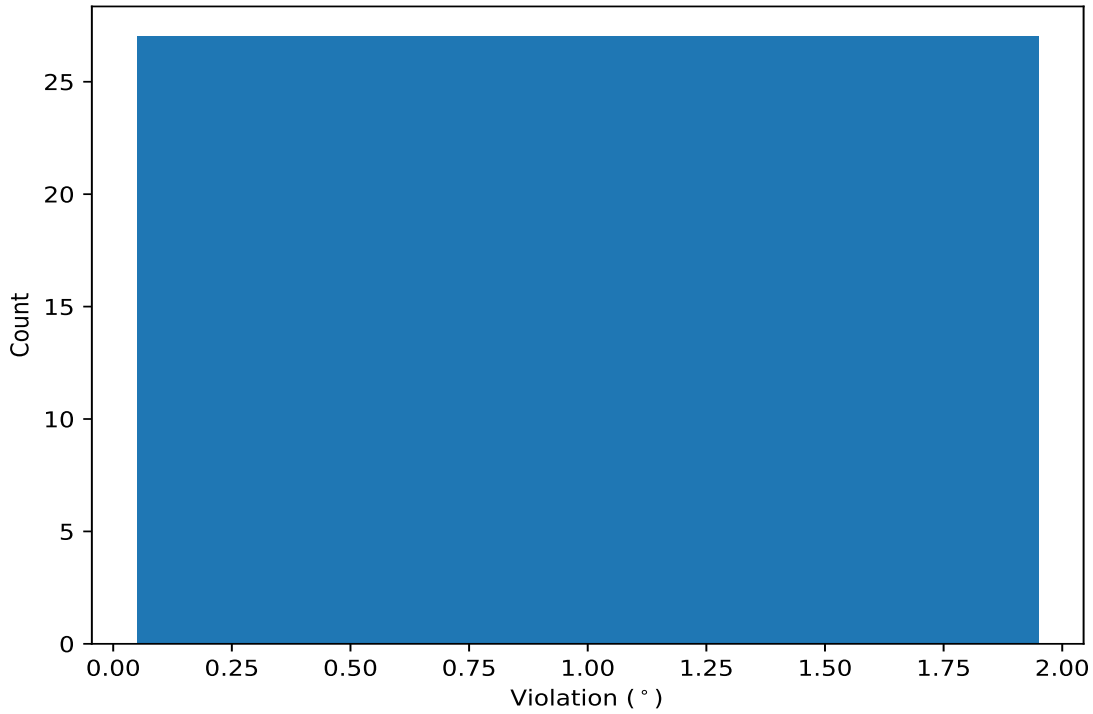
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,30)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLY:N	8	1.28	0.27	1.21
(1,20)	1:14:A:CYS:N	1:14:A:CYS:CA	1:14:A:CYS:C	1:15:A:ALA:N	7	1.3	0.25	1.21
(1,27)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:TRP:N	6	1.24	0.23	1.18
(1,14)	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	1:11:A:SER:N	5	1.25	0.2	1.12

[1] Number of violated models, [2]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 lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLY:N	8	1.76
(1,20)	1:14:A:CYS:N	1:14:A:CYS:CA	1:14:A:CYS:C	1:15:A:ALA:N	3	1.68
(1,20)	1:14:A:CYS:N	1:14:A:CYS:CA	1:14:A:CYS:C	1:15:A:ALA:N	10	1.68
(1,30)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLY:N	9	1.64
(1,27)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:TRP:N	4	1.61
(1,14)	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	1:11:A:SER:N	6	1.53
(1,14)	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	1:11:A:SER:N	5	1.45
(1,27)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:TRP:N	20	1.43
(1,30)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLY:N	3	1.4
(1,27)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:TRP:N	17	1.32
(1,20)	1:14:A:CYS:N	1:14:A:CYS:CA	1:14:A:CYS:C	1:15:A:ALA:N	19	1.27
(1,4)	1:3:A:CYS:N	1:3:A:CYS:CA	1:3:A:CYS:C	1:4:A:TRP:N	10	1.27
(1,30)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLY:N	15	1.26
(1,20)	1:14:A:CYS:N	1:14:A:CYS:CA	1:14:A:CYS:C	1:15:A:ALA:N	9	1.21
(1,20)	1:14:A:CYS:N	1:14:A:CYS:CA	1:14:A:CYS:C	1:15:A:ALA:N	8	1.18
(1,30)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLY:N	20	1.17
(1,14)	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	1:11:A:SER:N	16	1.12
(1,14)	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	1:11:A:SER:N	11	1.1
(1,20)	1:14:A:CYS:N	1:14:A:CYS:CA	1:14:A:CYS:C	1:15:A:ALA:N	2	1.06
(1,14)	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	1:11:A:SER:N	18	1.05
(1,27)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:TRP:N	2	1.04

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,27)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:TRP:N	10	1.03
(1,30)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLY:N	2	1.02
(1,30)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLY:N	10	1.02
(1,30)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLY:N	12	1.01
(1,20)	1:14:A:CYS:N	1:14:A:CYS:CA	1:14:A:CYS:C	1:15:A:ALA:N	14	1.01
(1,27)	1:18:A:PRO:N	1:18:A:PRO:CA	1:18:A:PRO:C	1:19:A:TRP:N	8	1.0