Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 06:13 PM EDT

PDB ID	:	2MWQ
BMRB ID	:	25350
Title	:	Solution structure of PsbQ from spinacia oleracea
Authors	:	Rathner, P.; Mueller, N.; Wimmer, R.; Chandra, K.
Deposited on	:	2014-11-19

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:

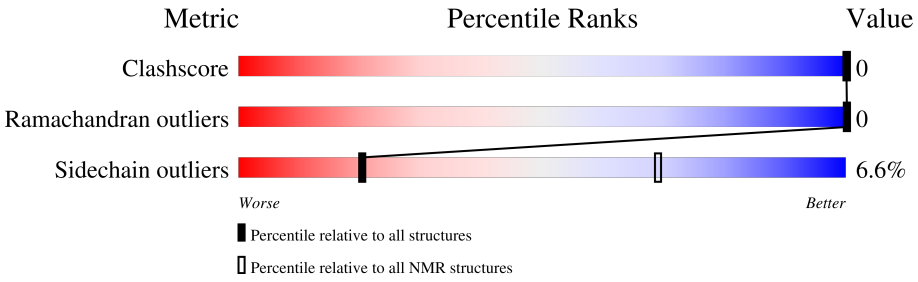
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 86%.

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	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	149	66% · 33%

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:45-A:95, A:101-A:149 (100)	0.63	7

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 and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2360 atoms, of which 1193 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	149	2360	738	1193	203	226	0

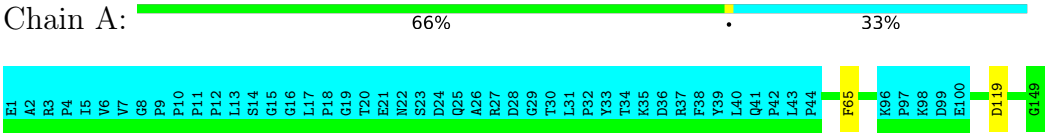
4 Residue-property plots (i)

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: Oxygen-evolving enhancer protein 3, chloroplastic

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

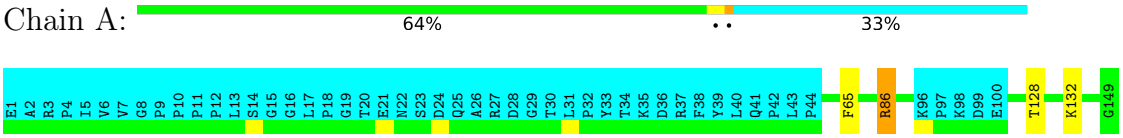
• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

Chain A:



4.2.3 Score per residue for model 3

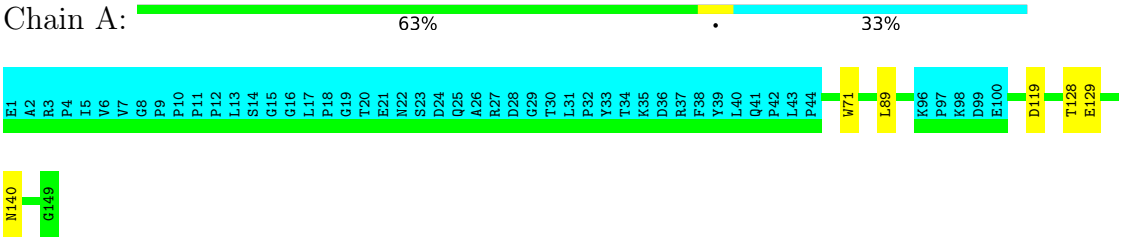
• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

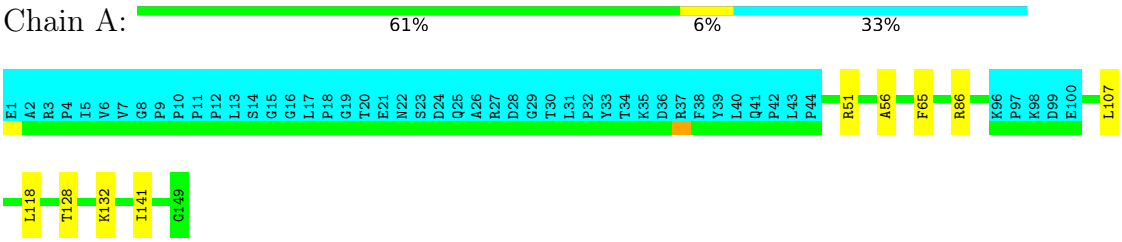
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

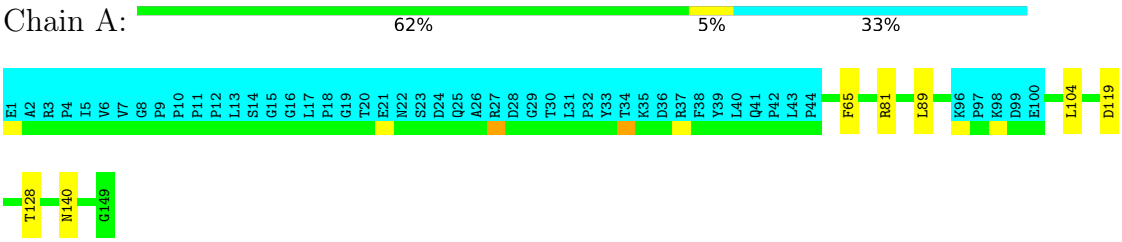
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

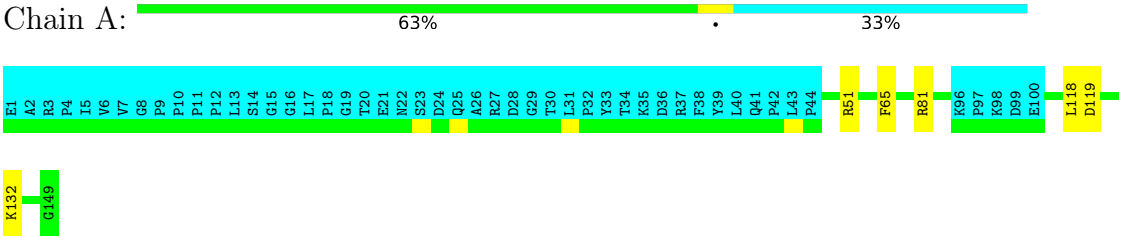
Chain A:



4.2.7 Score per residue for model 7 (medoid)

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

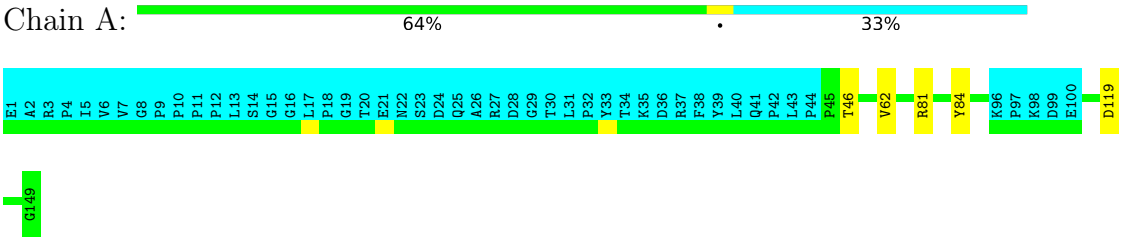
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

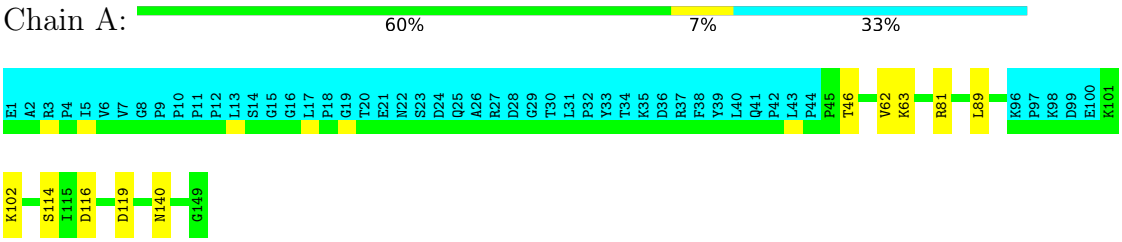
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

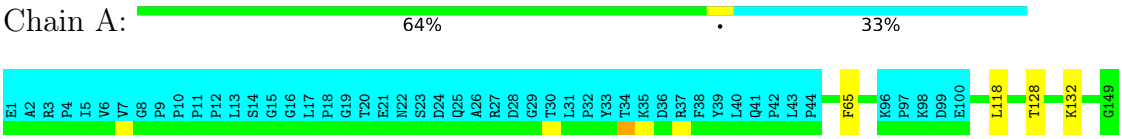
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

Chain A:



4.2.11 Score per residue for model 11

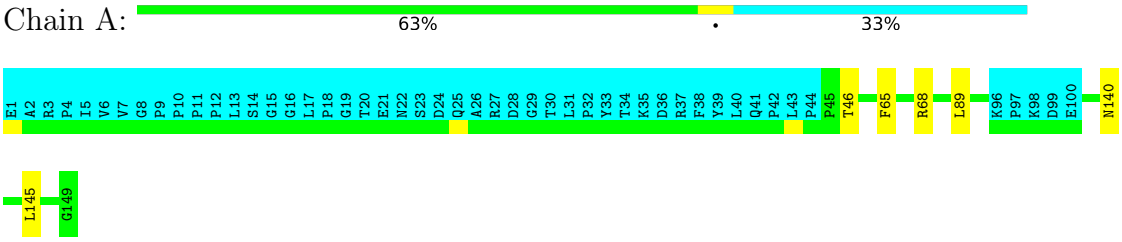
• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

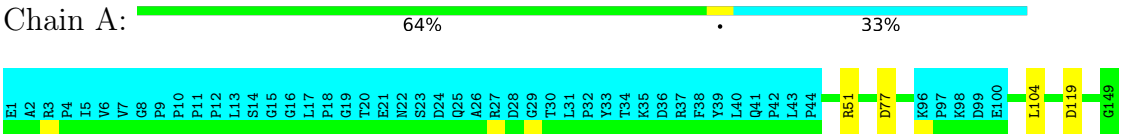
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

Chain A:



4.2.14 Score per residue for model 14

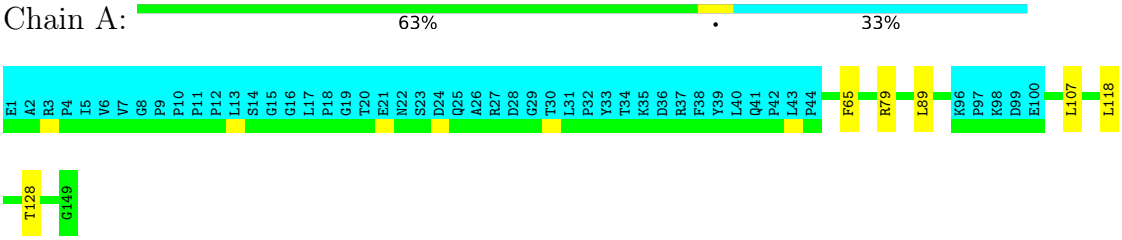
• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

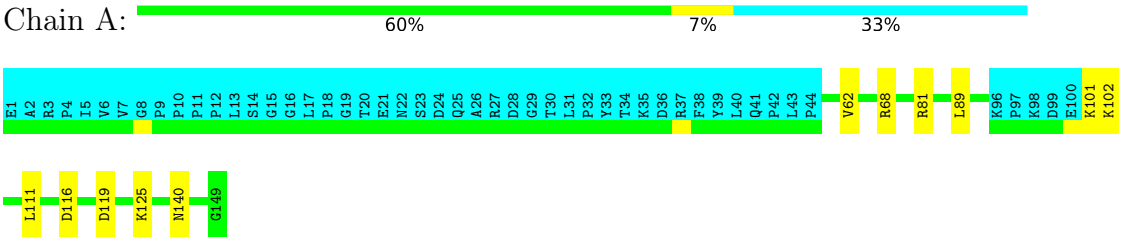
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

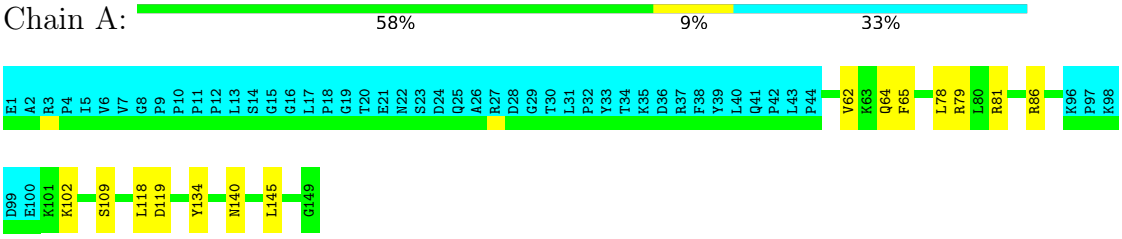
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

Chain A:



4.2.18 Score per residue for model 18

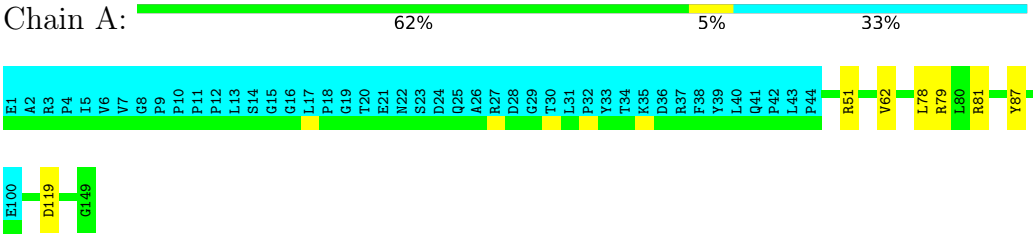
• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

Chain A:

4.2.19 Score per residue for model 19

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

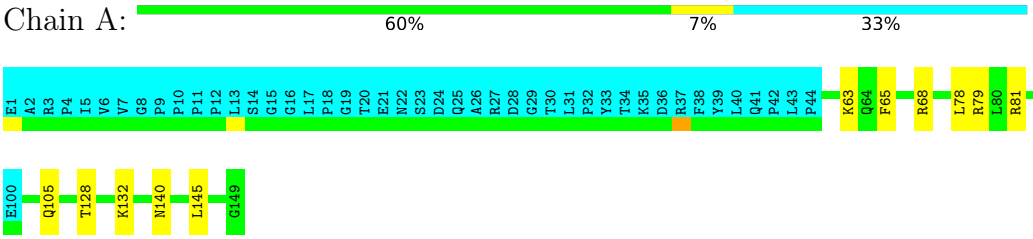
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Oxygen-evolving enhancer protein 3, chloroplastic

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	3.0
CYANA	geometry optimization	3.0
YASARA	geometry optimization	12.1.19
YASARA	refinement	12.1.19

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	1720
Number of shifts mapped to atoms	1720
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	0.61±0.01	0±0/803 (0.0± 0.0%)	0.67±0.02	1±1/1080 (0.1± 0.1%)
All	All	0.61	0/16060 (0.0%)	0.67	27/21600 (0.1%)

There are no bond-length outliers.

All unique angle 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	81	ARG	NE-CZ-NH1	6.60	123.60	120.30	6	9
1	A	79	ARG	NE-CZ-NH1	6.53	123.56	120.30	14	9
1	A	68	ARG	NE-CZ-NH1	6.24	123.42	120.30	20	2
1	A	51	ARG	NE-CZ-NH1	5.74	123.17	120.30	19	4
1	A	86	ARG	NE-CZ-NH1	5.51	123.05	120.30	2	3

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	792	820	820	0±0
All	All	15840	16400	16400	1

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ALA:HB1	1:A:141:ILE:HG23	0.48	1.86	5	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	99/149 (66%)	98±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
All	All	1980/2980 (66%)	1965 (99%)	15 (1%)	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	87/129 (67%)	81±2 (93±3%)	6±2 (7±3%)	20	69
All	All	1740/2580 (67%)	1626 (93%)	114 (7%)	20	69

All 34 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	65	PHE	11
1	A	119	ASP	11
1	A	128	THR	9
1	A	89	LEU	8
1	A	140	ASN	8
1	A	118	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	62	VAL	6
1	A	145	LEU	5
1	A	132	LYS	5
1	A	78	LEU	4
1	A	46	THR	4
1	A	104	LEU	3
1	A	86	ARG	3
1	A	102	LYS	3
1	A	75	GLN	2
1	A	77	ASP	2
1	A	114	SER	2
1	A	107	LEU	2
1	A	63	LYS	2
1	A	116	ASP	2
1	A	68	ARG	2
1	A	105	GLN	2
1	A	71	TRP	1
1	A	129	GLU	1
1	A	84	TYR	1
1	A	51	ARG	1
1	A	53	LYS	1
1	A	101	LYS	1
1	A	111	LEU	1
1	A	125	LYS	1
1	A	64	GLN	1
1	A	109	SER	1
1	A	134	TYR	1
1	A	87	TYR	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

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 86% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1720
Number of shifts mapped to atoms	1720
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- Chemical shift has been reported more than once. All 7 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	104	LEU	HD11	0.848	0.000	.
1	A	13	LEU	HD11	0.877	0.000	.
1	A	13	LEU	HD12	0.877	0.000	.
1	A	13	LEU	HD13	0.877	0.000	.
1	A	107	LEU	HD11	0.875	0.000	.
1	A	107	LEU	HD12	0.875	0.000	.
1	A	107	LEU	HD13	0.875	0.000	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	148	-0.47 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	140	0.47 ± 0.09	None needed (< 0.5 ppm)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C'$	145	-0.34 ± 0.11	None needed (< 0.5 ppm)
^{15}N	143	0.20 ± 0.23	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 1197 atoms were assigned a chemical shift out of a possible 1393. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	488/496 (98%)	196/199 (98%)	197/200 (98%)	95/97 (98%)
Sidechain	660/822 (80%)	438/533 (82%)	218/253 (86%)	4/36 (11%)
Aromatic	49/75 (65%)	25/36 (69%)	24/37 (65%)	0/2 (0%)
Overall	1197/1393 (86%)	659/768 (86%)	439/490 (90%)	99/135 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1701 atoms were assigned a chemical shift out of a possible 2037. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	706/726 (97%)	282/292 (97%)	293/298 (98%)	131/136 (96%)
Sidechain	932/1208 (77%)	613/782 (78%)	314/375 (84%)	5/51 (10%)
Aromatic	63/103 (61%)	32/49 (65%)	31/52 (60%)	0/2 (0%)
Overall	1701/2037 (84%)	927/1123 (83%)	638/725 (88%)	136/189 (72%)

7.1.4 Statistically unusual chemical shifts

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

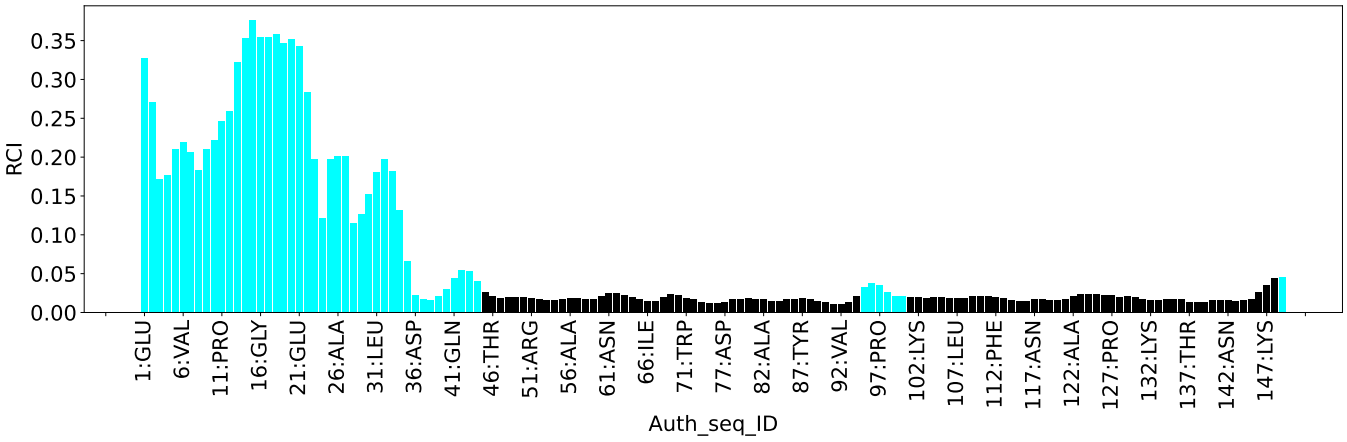
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	120	HIS	CE1	120.31	126.08 – 149.12	-7.5
1	A	39	TYR	CD2	123.46	125.28 – 140.14	-6.2
1	A	65	PHE	CZ	120.02	121.82 – 136.66	-6.2

7.1.5 Random Coil Index (RCI) plots

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	1283
Intra-residue (|i-j|=0)	566
Sequential (|i-j|=1)	404
Medium range (|i-j|>1 and |i-j|<5)	122
Long range (|i-j|≥5)	191
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	190
Number of unmapped restraints	0
Number of restraints per residue	9.9
Number of long range restraints per residue[1]	1.3

[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.There are no distance violations

8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.3	5.0

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Bins (°)	Average number of violations per model	Max (°)
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

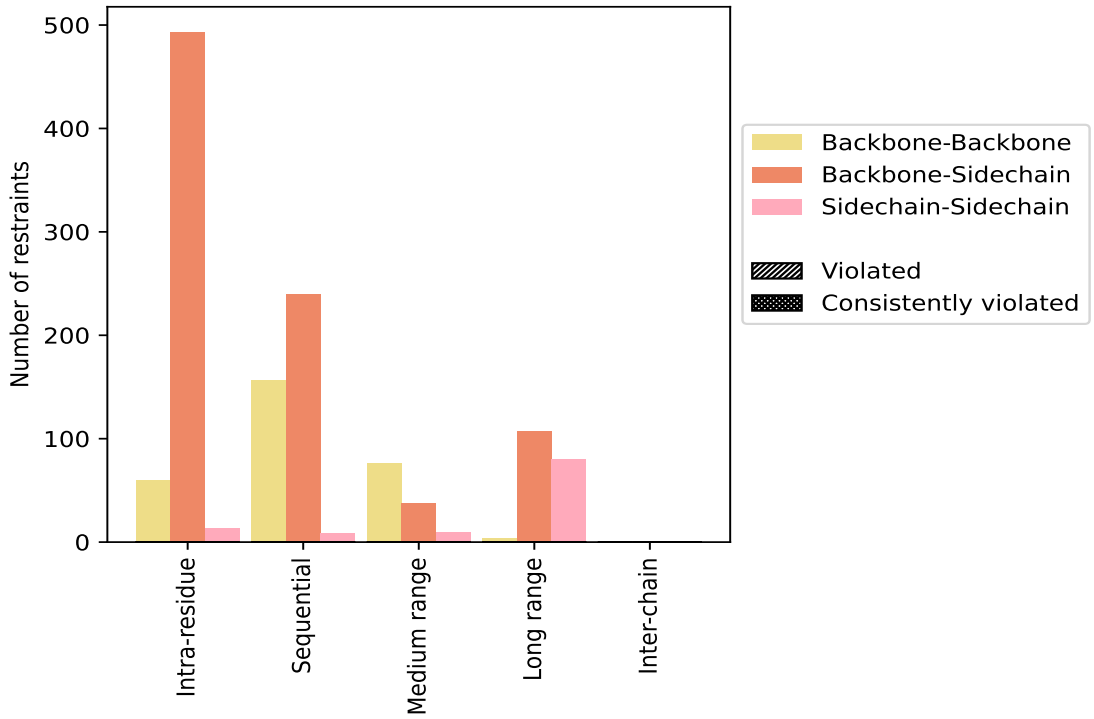
9.1 Summary of distance violations (i)

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)	566	44.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	60	4.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	493	38.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	13	1.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	404	31.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	156	12.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	240	18.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	8	0.6	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	122	9.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	76	5.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	37	2.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	9	0.7	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	191	14.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	4	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	107	8.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	80	6.2	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	0	0.0	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	1283	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	296	23.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	877	68.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	110	8.6	0	0.0	0.0	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

No violations found

9.3 Distance violation statistics for the ensemble

No violations found

9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

No violations found

10 Dihedral-angle violation analysis

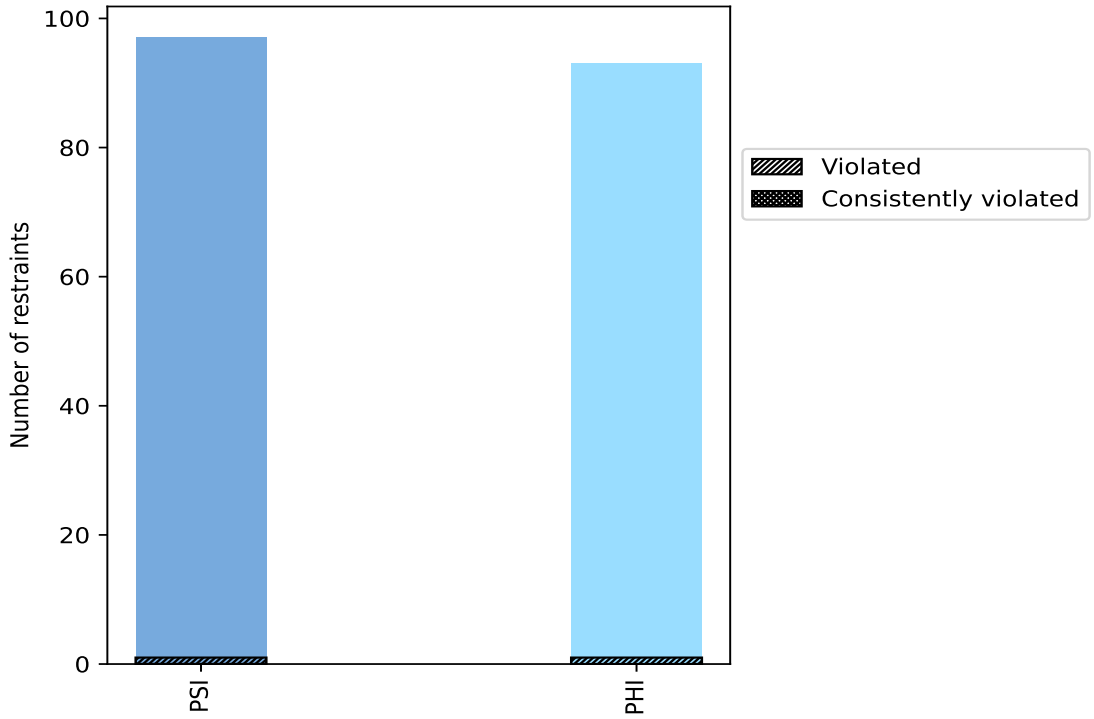
10.1 Summary of dihedral-angle violations

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	97	51.1	1	1.0	0.5	0	0.0	0.0
PHI	93	48.9	1	1.1	0.5	0	0.0	0.0
Total	190	100.0	2	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



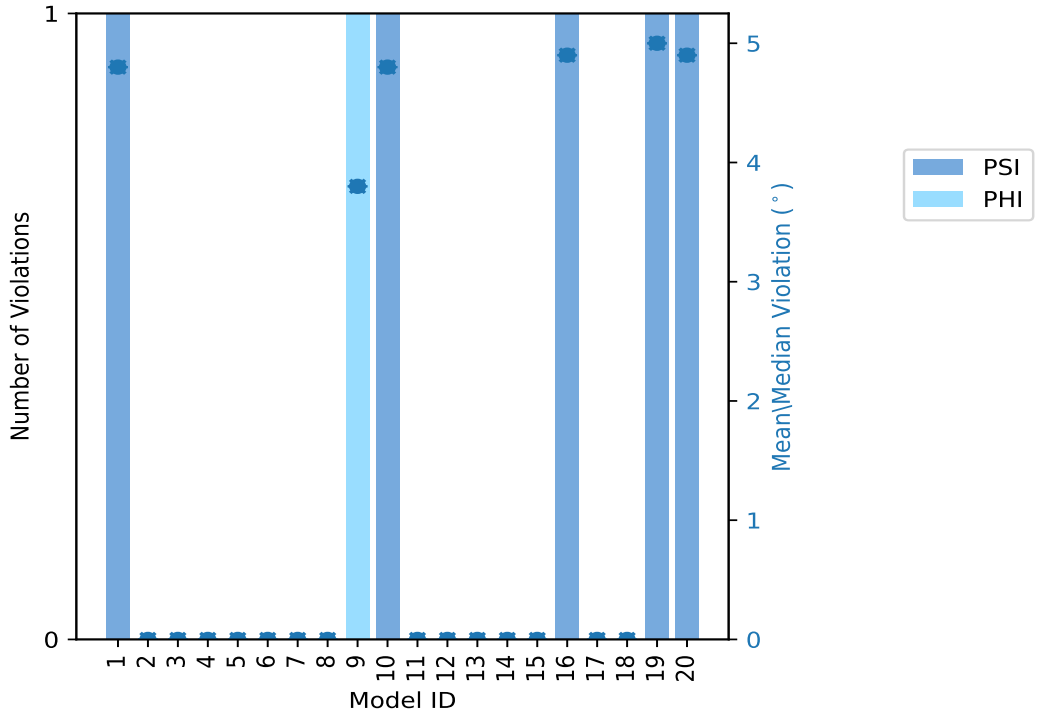
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	1	0	1	4.8	4.8	0.0	4.8
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	0	0	0.0	0.0	0.0	0.0
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	1	1	3.8	3.8	0.0	3.8
10	1	0	1	4.8	4.8	0.0	4.8
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	1	0	1	4.9	4.9	0.0	4.9
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	1	0	1	5.0	5.0	0.0	5.0
20	1	0	1	4.9	4.9	0.0	4.9

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	1	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
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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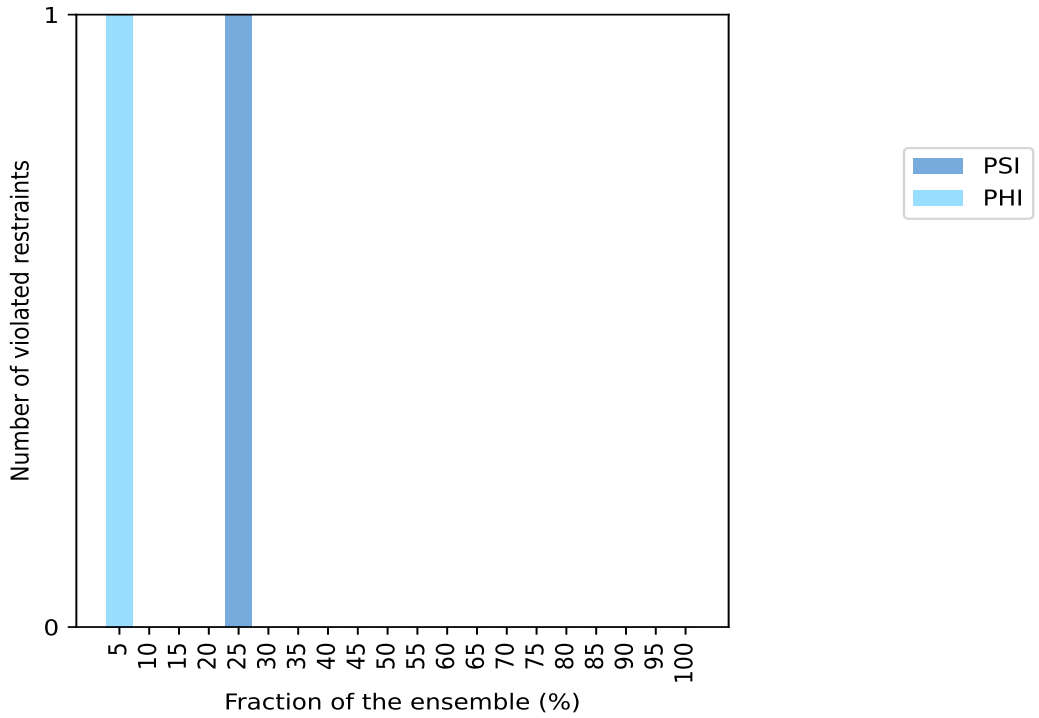
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

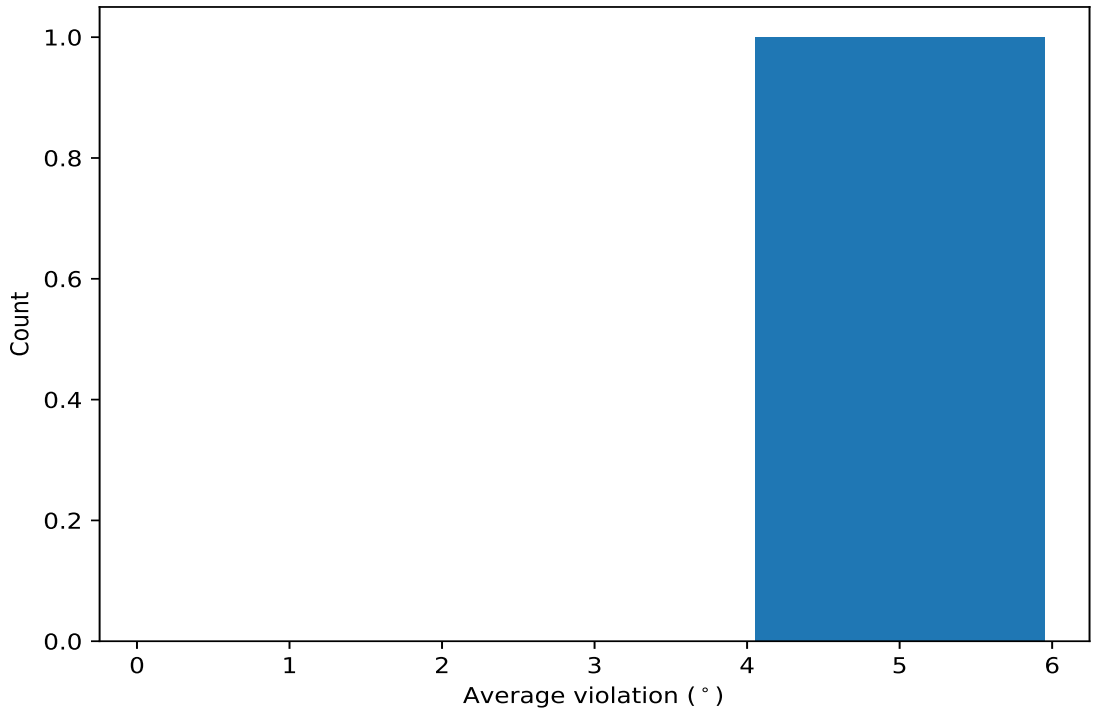


10.4 Most violated dihedral-angle restraints in the ensemble

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

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.

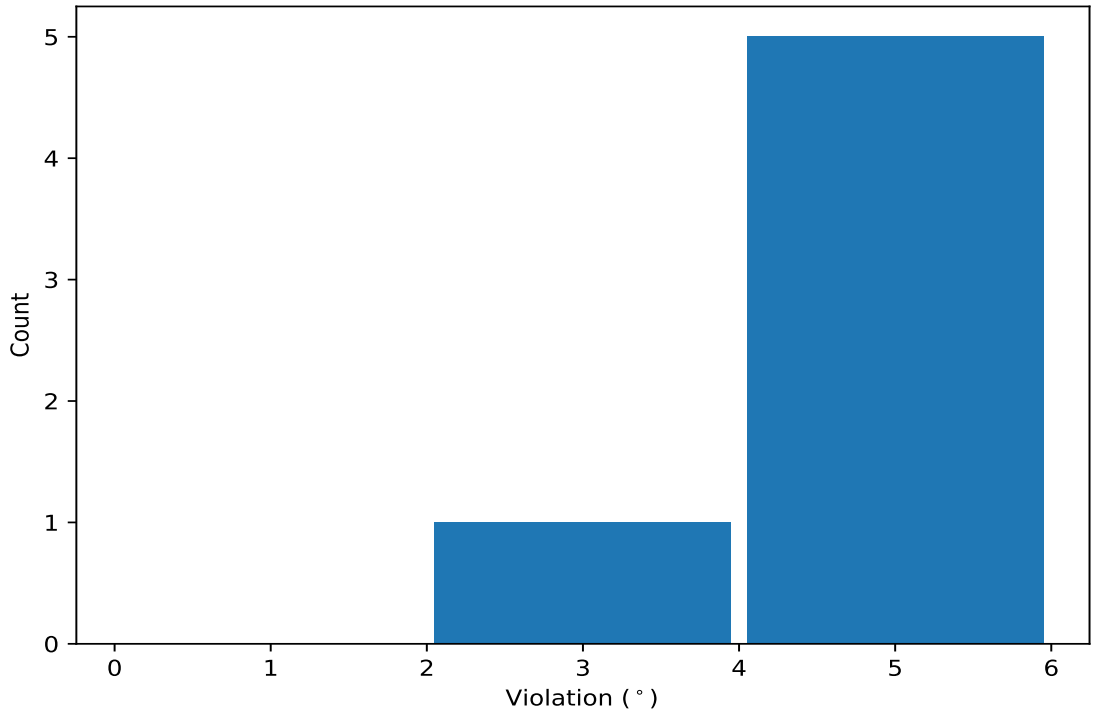
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,44)	1:A:61:ASN:N	1:A:61:ASN:CA	1:A:61:ASN:C	1:A:62:VAL:N	5	4.88	0.07	4.9

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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

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 (°)
(1,44)	1:A:61:ASN:N	1:A:61:ASN:CA	1:A:61:ASN:C	1:A:62:VAL:N	19	5.0
(1,44)	1:A:61:ASN:N	1:A:61:ASN:CA	1:A:61:ASN:C	1:A:62:VAL:N	16	4.9
(1,44)	1:A:61:ASN:N	1:A:61:ASN:CA	1:A:61:ASN:C	1:A:62:VAL:N	20	4.9
(1,44)	1:A:61:ASN:N	1:A:61:ASN:CA	1:A:61:ASN:C	1:A:62:VAL:N	1	4.8
(1,44)	1:A:61:ASN:N	1:A:61:ASN:CA	1:A:61:ASN:C	1:A:62:VAL:N	10	4.8
(1,9)	1:A:40:LEU:C	1:A:41:GLN:N	1:A:41:GLN:CA	1:A:41:GLN:C	9	3.8