



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:20 AM UTC

PDB ID : 8S8O / pdb_00008s8o
BMRB ID : 34908
Title : Solution Structure of cAMP-dependent Protein Kinase RII-alpha Subunit Dimerization and Docking Domain Complex with Microtubule Associated Protein 2c (84-111)
Authors : Bartosik, V.; Lanikova, A.; Janackova, Z.; Padrta, P.; Zidek, L.
Deposited on : 2024-03-06

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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 ⓘ 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 ⓘ](#)) 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

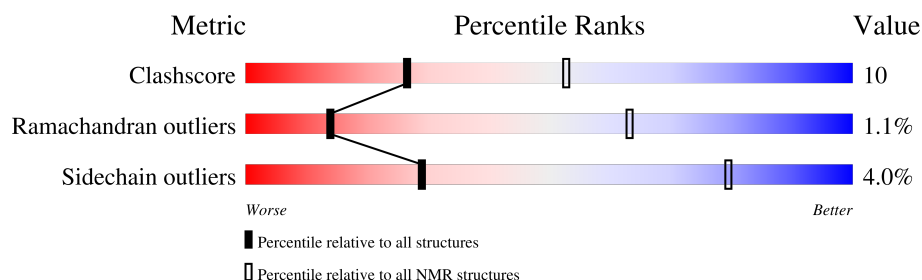
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 67%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	52	
1	B	52	
2	C	28	

2 Ensemble composition and analysis

This entry contains 20 models. Model 20 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:7-A:48, B:10-B:46, C:86-C:109 (103)	0.88	20

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. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2050 atoms, of which 1028 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called cAMP-dependent protein kinase type II-alpha regulatory sub-unit.

Mol	Chain	Residues	Atoms						Trace
1	A	52	Total	C	H	N	O	S	0
			814	259	408	70	75	2	
1	B	52	Total	C	H	N	O	S	0
			812	259	406	70	75	2	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P13861
A	2	ALA	-	expression tag	UNP P13861
A	3	MET	-	expression tag	UNP P13861
A	4	GLY	-	expression tag	UNP P13861
B	1	GLY	-	expression tag	UNP P13861
B	2	ALA	-	expression tag	UNP P13861
B	3	MET	-	expression tag	UNP P13861
B	4	GLY	-	expression tag	UNP P13861

- Molecule 2 is a protein called Isoform 3 of Microtubule-associated protein 2.

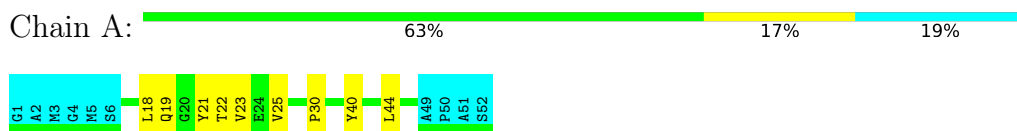
Mol	Chain	Residues	Atoms					Trace
2	C	28	Total	C	H	N	O	0
			424	128	214	37	45	

4 Residue-property plots [i](#)

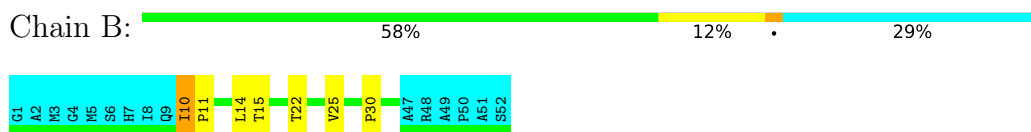
4.1 Average score per residue in the NMR ensemble

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: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



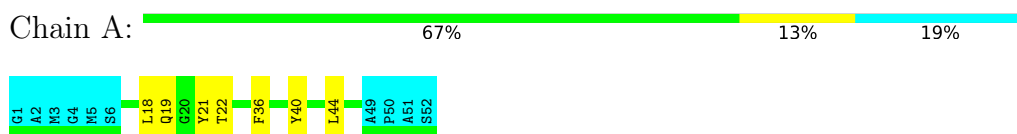
- Molecule 2: Isoform 3 of Microtubule-associated protein 2



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

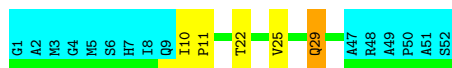
The representative model is number 20. Colouring as in section 4.1 above.

- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



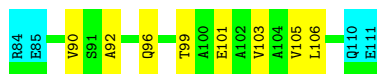
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain B:  62% 8% 29%



- Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C:  57% 29% 14%



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CNS	structure calculation	1.21
SCULPTOR	structure calculation	3.1
CNS	refinement	1.21
SCULPTOR	refinement	3.1

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1430
Number of shifts mapped to atoms	1243
Number of unparsed shifts	0
Number of shifts with mapping errors	187
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	67%

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	1.19±0.07	1±1/357 (0.2± 0.3%)	1.17±0.05	0±1/488 (0.1± 0.2%)
1	B	1.11±0.05	1±1/313 (0.4± 0.4%)	1.14±0.06	1±1/429 (0.3± 0.3%)
2	C	1.21±0.07	0±0/172 (0.0± 0.0%)	1.00±0.05	0±0/235 (0.0± 0.0%)
All	All	1.17	43/16840 (0.3%)	1.13	33/23040 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.1±0.4
1	A	0.0±0.0	0.1±0.4
All	All	0	6

5 of 17 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	11	PRO	CA-C	7.35	1.58	1.52	16	2
1	B	30	PRO	CA-C	7.24	1.58	1.52	2	8
1	A	7	HIS	C-N	-7.06	1.26	1.33	11	3
1	B	10	ILE	N-CA	-6.69	1.41	1.46	11	6
1	A	10	ILE	N-CA	-6.68	1.41	1.46	17	4

5 of 12 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(°)	Ideal(°)	Models	
								Worst	Total
1	B	34	VAL	N-CA-C	6.75	116.90	110.42	14	1
1	B	10	ILE	CA-C-N	6.69	127.27	120.38	18	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	10	ILE	C-N-CA	6.69	127.27	120.38	18	5
1	A	29	GLN	CA-C-N	6.36	124.31	119.66	13	2
1	A	29	GLN	C-N-CA	6.36	124.31	119.66	13	2

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	45	ARG	Sidechain	2
1	B	45	ARG	Sidechain	2
1	A	43	ARG	Sidechain	1
1	B	43	ARG	Sidechain	1

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	348	350	350	9±2
1	B	305	306	306	5±3
2	C	172	181	181	4±2
All	All	16500	16740	16740	332

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 10.

5 of 105 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:103:VAL:O	2:C:106:LEU:HG	0.65	1.91	13	14
2:C:97:VAL:O	2:C:101:GLU:HG3	0.63	1.94	14	2
1:A:14:LEU:HG	1:B:33:LEU:HD22	0.62	1.72	3	2
1:A:36:PHE:O	1:A:40:TYR:HB2	0.61	1.95	12	2
1:A:22:THR:HB	1:A:40:TYR:CE1	0.60	2.31	10	8

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	42/52 (81%)	40±1 (95±2%)	2±1 (5±2%)	0±0 (0±1%)	31	76
1	B	37/52 (71%)	34±1 (93±3%)	2±1 (4±3%)	1±0 (3±1%)	6	42
2	C	24/28 (86%)	24±0 (99±2%)	0±0 (1±2%)	0±0 (0±1%)	44	80
All	All	2060/2640 (78%)	1959 (95%)	78 (4%)	23 (1%)	14	63

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	11	PRO	17
1	A	11	PRO	2
1	B	12	PRO	2
1	A	31	PRO	1
2	C	108	GLY	1

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	38/43 (88%)	37±1 (97±3%)	1±1 (2±3%)	42	88
1	B	34/43 (79%)	32±1 (94±3%)	2±1 (6±3%)	18	68
2	C	18/22 (82%)	17±1 (97±4%)	1±1 (3±4%)	36	85
All	All	1800/2160 (83%)	1728 (96%)	72 (4%)	29	79

5 of 22 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	B	10	ILE	19
1	B	14	LEU	8
1	B	15	THR	5
2	C	106	LEU	5
1	A	19	GLN	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 67% for the well-defined parts and 69% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	1430
Number of shifts mapped to atoms	1243
Number of unparsed shifts	0
Number of shifts with mapping errors	187
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 187) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	PRO	H	8.189	0.004	1
1	A	13	GLY	CB	30.383	0.000	1
1	A	20	GLY	HG21	1.19	0.000	1
1	A	20	GLY	HG22	1.19	0.000	1
1	A	20	GLY	HG23	1.19	0.000	1
1	A	20	GLY	CB	69.746	0.026	1
1	A	30	PRO	H	8.494	0.002	1
1	A	38	VAL	HA2	3.98	0.000	2
1	A	38	VAL	HA3	3.98	0.000	2
1	A	47	ALA	HA2	3.846	0.000	2
1	A	47	ALA	HA3	3.846	0.000	2
1	A	50	PRO	H	8.043	0.004	1
1	A	51	ALA	HD2	3.163	0.000	2
1	A	51	ALA	HD3	3.163	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	52	GLU	H	8.515	0.004	1
1	A	52	GLY	H	8.372	0.003	1
1	A	52	ALA	H	8.005	0.003	1
1	A	52	PHE	H	8.199	0.003	1
1	A	52	HIS	H	8.445	0.006	1
1	A	52	GLN	H	8.475	0.007	1
1	A	52	THR	H	7.982	0.006	1
1	A	52	TYR	H	8.256	0.004	1
1	A	52	ASP	H	8.313	0.004	1
1	A	52	LYS	H	8.286	0.004	1
1	A	52	ASN	H	8.388	0.003	1
1	A	52	ILE	H	8.022	0.003	1
1	A	52	LEU	H	8.269	0.003	1
1	A	52	GLU	HA	4.248	0.000	1
1	A	52	PHE	HA	4.588	0.000	1
1	A	52	LYS	HA	4.33	0.000	1
1	A	52	ILE	HA	4.155	0.018	1
1	A	52	ASN	HA	4.724	0.000	1
1	A	52	THR	HA	4.394	0.007	1
1	A	52	ALA	HA	4.27	0.024	1
1	A	52	ASP	HA	4.52	0.005	1
1	A	52	GLY	HA2	3.886	0.000	2
1	A	52	GLY	HA3	3.886	0.000	2
1	A	52	ILE	HB	1.813	0.010	1
1	A	52	THR	HB	4.247	0.005	1
1	A	52	ALA	HB1	1.34	0.011	1
1	A	52	GLU	HB2	1.956	0.000	2
1	A	52	PHE	HB2	3.088	0.000	2
1	A	52	HIS	HB2	3.17	0.000	2
1	A	52	ASN	HB2	2.816	0.000	2
1	A	52	ALA	HB2	1.34	0.011	1
1	A	52	ASP	HB2	2.644	0.020	2
1	A	52	GLU	HB3	1.956	0.000	2
1	A	52	PHE	HB3	3.088	0.000	2
1	A	52	HIS	HB3	3.17	0.000	2
1	A	52	ASN	HB3	2.816	0.000	2
1	A	52	ALA	HB3	1.34	0.011	1
1	A	52	ASP	HB3	2.644	0.020	2
1	A	52	ILE	HD11	0.811	0.006	1
1	A	52	ILE	HD12	0.811	0.006	1
1	A	52	ILE	HD13	0.811	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	52	ILE	HG12	1.426	0.029	1
1	A	52	ILE	HG13	1.107	0.014	1
1	A	52	SER	HG2	2.285	0.000	2
1	A	52	GLU	HG2	2.252	0.000	2
1	A	52	THR	HG21	1.155	0.000	1
1	A	52	ILE	HG21	0.885	0.013	1
1	A	52	THR	HG22	1.155	0.000	1
1	A	52	ILE	HG22	0.885	0.013	1
1	A	52	THR	HG23	1.155	0.000	1
1	A	52	ILE	HG23	0.885	0.013	1
1	A	52	SER	HG3	2.285	0.000	2
1	A	52	GLU	HG3	2.252	0.000	2
1	A	52	GLU	CA	56.906	0.000	1
1	A	52	GLY	CA	45.382	0.045	1
1	A	52	ALA	CA	52.589	0.059	1
1	A	52	PHE	CA	57.772	0.013	1
1	A	52	HIS	CA	56.193	0.140	1
1	A	52	GLN	CA	56.239	0.028	1
1	A	52	THR	CA	61.895	0.108	1
1	A	52	TYR	CA	58.011	0.109	1
1	A	52	ASP	CA	54.326	0.046	1
1	A	52	LYS	CA	56.583	0.000	1
1	A	52	ASN	CA	53.289	0.014	1
1	A	52	ILE	CA	61.345	0.056	1
1	A	52	LEU	CA	55.288	0.005	1
1	A	52	GLU	CB	30.217	0.039	1
1	A	52	ALA	CB	19.181	0.016	1
1	A	52	PHE	CB	39.336	0.045	1
1	A	52	HIS	CB	30.022	0.065	1
1	A	52	GLN	CB	29.396	0.021	1
1	A	52	THR	CB	69.832	0.078	1
1	A	52	TYR	CB	38.852	0.035	1
1	A	52	ASP	CB	41.253	0.029	1
1	A	52	LYS	CB	32.82	0.000	1
1	A	52	ASN	CB	39.059	0.031	1
1	A	52	ILE	CB	38.686	0.071	1
1	A	52	LEU	CB	42.301	0.036	1
1	A	52	ILE	CD1	12.915	0.065	1
1	A	52	ILE	CG1	27.143	0.193	1
1	A	52	ILE	CG2	17.215	0.102	1
1	A	52	THR	CG2	21.608	0.015	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	52	GLU	N	121.243	0.030	1
1	A	52	GLY	N	110.002	0.040	1
1	A	52	ALA	N	123.533	0.043	1
1	A	52	PHE	N	118.997	0.024	1
1	A	52	HIS	N	119.659	0.033	1
1	A	52	GLN	N	121.934	0.046	1
1	A	52	THR	N	113.791	0.048	1
1	A	52	TYR	N	122.686	0.049	1
1	A	52	ASP	N	122.845	0.017	1
1	A	52	LYS	N	123.394	0.041	1
1	A	52	ASN	N	119.385	0.026	1
1	A	52	ILE	N	119.822	0.024	1
1	A	52	LEU	N	122.763	0.042	1
1	C	84	ARG	H	8.048	0.013	1
1	C	111	ALA	H	8.007	0.004	1
1	C	111	GLN	H	8.003	0.006	1
1	C	111	HIS	H	8.131	0.013	1
1	C	111	LEU	H	8.15	0.004	1
1	C	111	THR	H	8.189	0.003	1
1	C	111	VAL	H	8.089	0.003	1
1	C	111	ASN	H	8.451	0.004	1
1	C	111	SER	H	8.338	0.003	1
1	C	111	GLY	H	8.404	0.005	1
1	C	111	ALA	HA	4.201	0.008	1
1	C	111	GLN	HA	4.194	0.018	1
1	C	111	HIS	HA	4.591	0.005	1
1	C	111	PRO	HA	4.38	0.016	1
1	C	111	VAL	HA	4.095	0.011	1
1	C	111	ASN	HA	4.751	0.000	1
1	C	111	SER	HA	4.748	0.000	1
1	C	111	GLY	HA2	4.017	0.000	2
1	C	111	GLY	HA3	4.017	0.000	2
1	C	111	VAL	HB	2.041	0.010	1
1	C	111	ALA	HB1	1.381	0.009	1
1	C	111	ALA	HB2	1.381	0.009	1
1	C	111	GLN	HB2	1.977	0.003	2
1	C	111	HIS	HB2	3.173	0.005	1
1	C	111	PRO	HB2	1.876	0.003	1
1	C	111	SER	HB2	3.851	0.000	2
1	C	111	ALA	HB3	1.381	0.009	1
1	C	111	GLN	HB3	1.977	0.003	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	111	HIS	HB3	3.104	0.018	1
1	C	111	PRO	HB3	2.258	0.010	1
1	C	111	SER	HB3	3.851	0.000	2
1	C	111	PRO	HD2	3.646	0.013	1
1	C	111	PRO	HD3	3.817	0.022	1
1	C	111	VAL	HG11	0.896	0.011	2
1	C	111	VAL	HG12	0.896	0.011	2
1	C	111	VAL	HG13	0.896	0.011	2
1	C	111	GLN	HG2	2.322	0.016	2
1	C	111	PRO	HG2	1.907	0.002	1
1	C	111	THR	HG21	1.19	0.000	1
1	C	111	VAL	HG21	0.896	0.011	2
1	C	111	THR	HG22	1.19	0.000	1
1	C	111	VAL	HG22	0.896	0.011	2
1	C	111	THR	HG23	1.19	0.000	1
1	C	111	VAL	HG23	0.896	0.011	2
1	C	111	GLN	HG3	2.322	0.016	2
1	C	111	PRO	HG3	1.999	0.005	1
1	C	111	ALA	CA	52.82	0.086	1
1	C	111	GLN	CA	56.569	0.017	1
1	C	111	HIS	CA	56.381	0.121	1
1	C	111	PRO	CA	63.308	0.036	1
1	C	111	LEU	CA	52.857	0.000	1
1	C	111	THR	CA	62.066	0.027	1
1	C	111	VAL	CA	62.248	0.039	1
1	C	111	ASN	CA	52.942	0.027	1
1	C	111	SER	CA	56.502	0.000	1
1	C	111	GLY	CA	45.346	0.027	1
1	C	111	ALA	CB	18.935	0.004	1
1	C	111	HIS	CB	30.084	0.091	1
1	C	111	PRO	CB	31.543	0.339	1
1	C	111	LEU	CB	41.72	0.000	1
1	C	111	THR	CB	69.823	0.002	1
1	C	111	VAL	CB	32.822	0.101	1
1	C	111	ASN	CB	39.07	0.030	1
1	C	111	SER	CB	63.539	0.000	1
1	C	111	GLN	CB	29.364	0.020	1
1	C	111	PRO	CD	50.942	0.110	1
1	C	111	GLN	CG	33.709	0.032	1
1	C	111	PRO	CG	27.315	0.024	1
1	C	111	VAL	CG1	20.866	0.082	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	111	ALA	N	123.121	0.028	1
1	C	111	GLN	N	117.87	0.004	1
1	C	111	HIS	N	119.534	0.000	1
1	C	111	LEU	N	122.551	0.037	1
1	C	111	THR	N	115.823	0.033	1
1	C	111	VAL	N	122.399	0.037	1
1	C	111	ASN	N	122.555	0.030	1
1	C	111	SER	N	117.564	0.057	1
1	C	111	GLY	N	110.902	0.032	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	142	-0.34 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	126	0.16 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	143	-0.02 ± 0.14	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 67%, i.e. 992 atoms were assigned a chemical shift out of a possible 1473. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	372/504 (74%)	188/203 (93%)	91/206 (44%)	93/95 (98%)
Sidechain	620/886 (70%)	431/579 (74%)	189/274 (69%)	0/33 (0%)
Aromatic	0/83 (0%)	0/40 (0%)	0/42 (0%)	0/1 (0%)
Overall	992/1473 (67%)	619/822 (75%)	280/522 (54%)	93/129 (72%)

7.1.4 Statistically unusual chemical shifts ⓘ

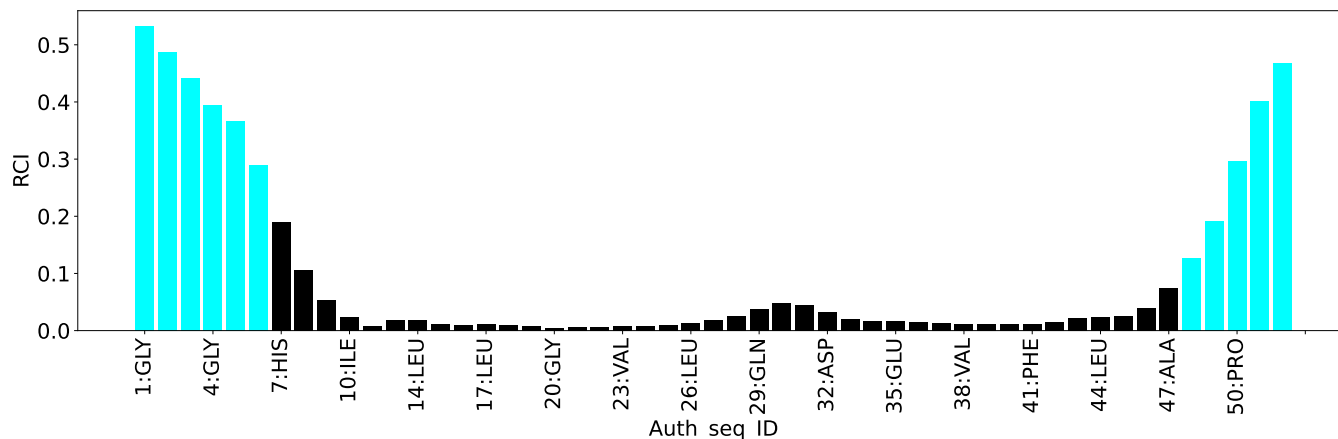
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	16	GLU	CB	63.77	21.56 – 38.37	20.1
1	A	20	GLY	CA	62.24	38.93 – 51.79	13.1
1	A	17	LEU	CB	19.17	33.11 – 51.34	-12.7
1	A	11	PRO	CB	18.16	26.06 – 37.61	-11.8
1	A	11	PRO	CA	50.60	55.85 – 70.84	-8.5
1	B	8	ILE	CG2	28.02	10.93 – 24.12	8.0
1	A	19	GLN	CB	42.22	20.34 – 37.98	7.4
1	A	45	ARG	CB	19.17	21.74 – 39.52	-6.5
1	A	24	GLU	CB	19.25	21.56 – 38.37	-6.4

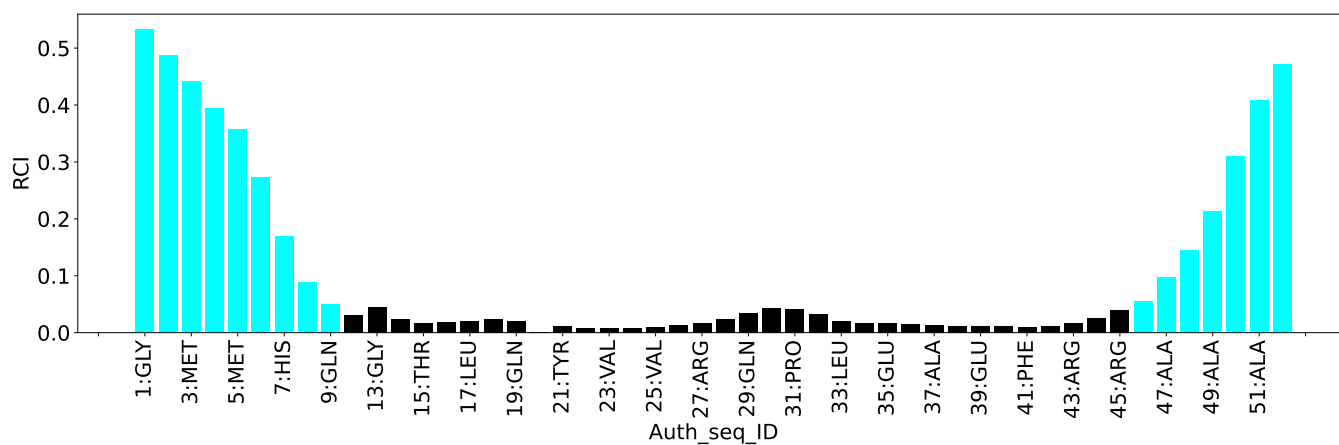
7.1.5 Random Coil Index (RCI) plots [i](#)

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

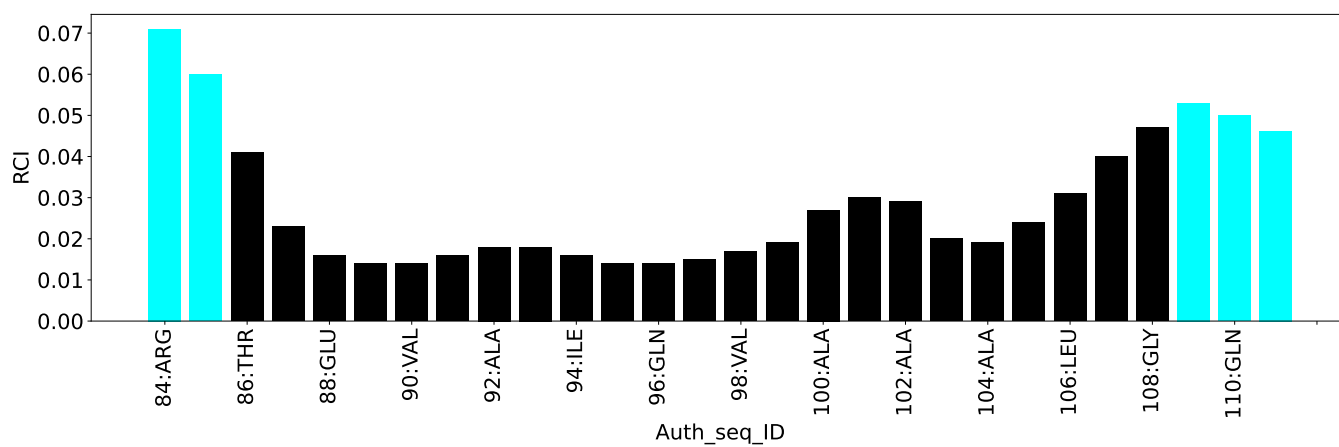
Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:



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	0
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	174
Number of unmapped restraints	0
Number of restraints per residue	0
Number of long range restraints per residue ¹	0

¹Long 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. There are no distance restraints

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)	11.7	7.14

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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

No distance restraints data found

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

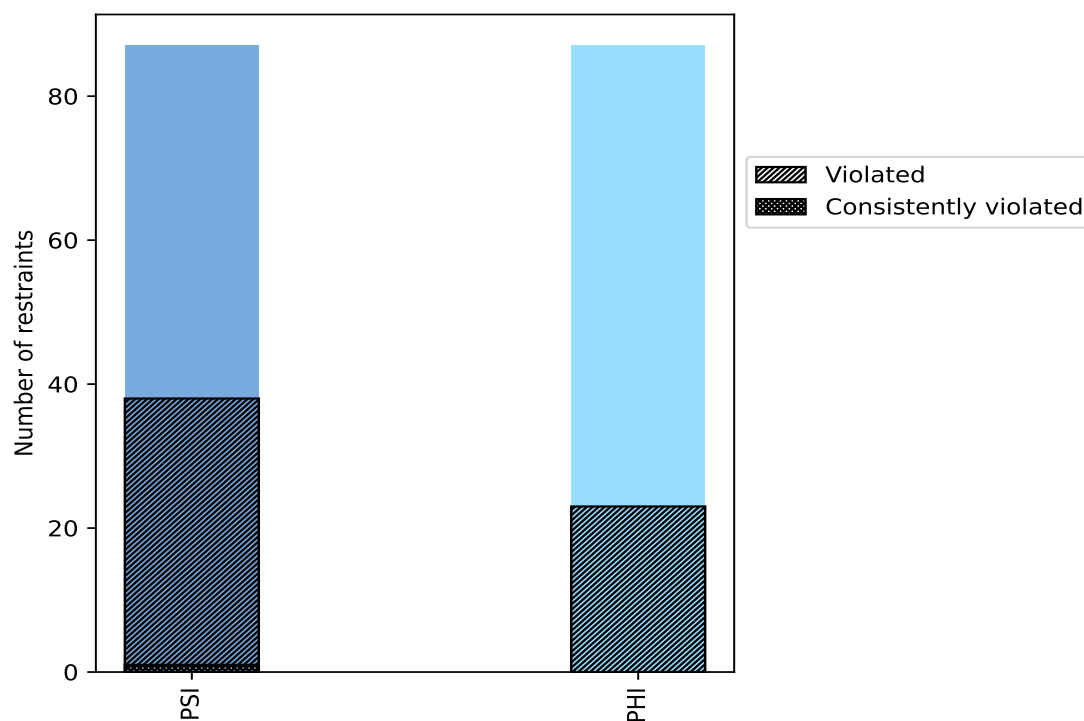
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	87	50.0	38	43.7	21.8	1	1.1	0.6
PHI	87	50.0	23	26.4	13.2	0	0.0	0.0
Total	174	100.0	61	35.1	35.1	1	0.6	0.6

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

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



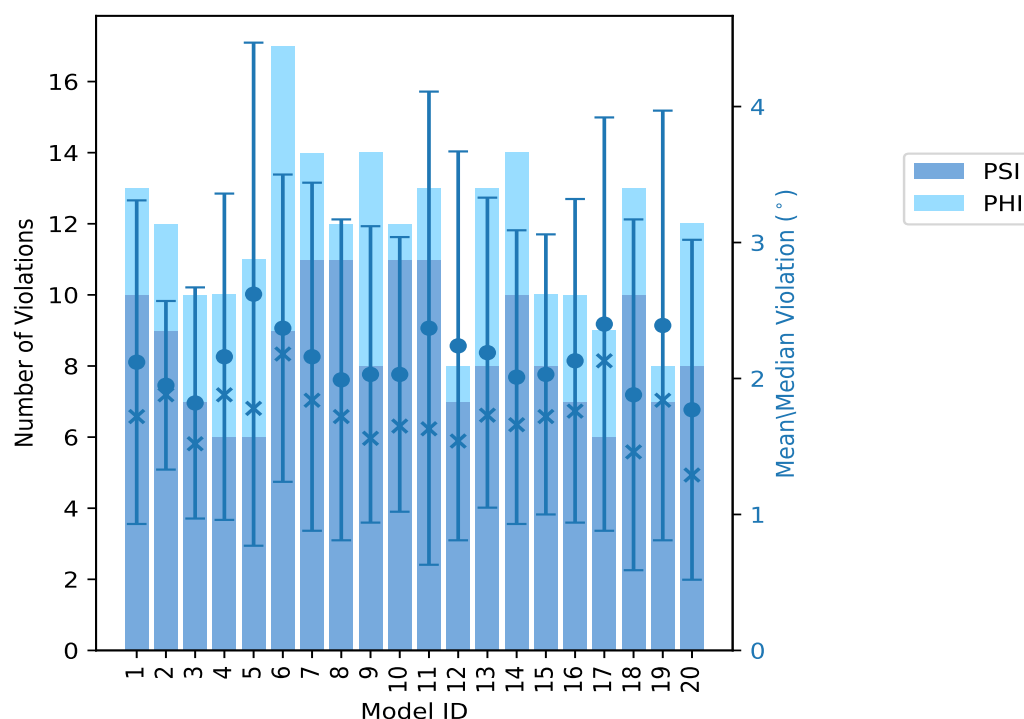
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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	10	3	13	2.12	5.34	1.19	1.72
2	9	3	12	1.95	3.12	0.62	1.88
3	7	3	10	1.82	4.05	0.85	1.52
4	6	4	10	2.16	5.2	1.2	1.88
5	6	5	11	2.62	7.14	1.85	1.78
6	9	8	17	2.37	4.59	1.13	2.18
7	11	3	14	2.16	5.3	1.28	1.84
8	11	1	12	1.99	5.75	1.18	1.72
9	8	6	14	2.03	4.63	1.09	1.56
10	11	1	12	2.03	4.49	1.01	1.65
11	11	2	13	2.37	6.34	1.74	1.63
12	7	1	8	2.24	5.45	1.43	1.54
13	8	5	13	2.19	5.4	1.14	1.73
14	10	4	14	2.01	5.07	1.08	1.66
15	8	2	10	2.03	4.79	1.03	1.72
16	7	3	10	2.13	5.37	1.19	1.76
17	6	3	9	2.4	6.44	1.52	2.13
18	10	3	13	1.88	5.84	1.29	1.46
19	7	1	8	2.39	6.11	1.58	1.84
20	8	4	12	1.77	5.74	1.25	1.29

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	%
8	9	17	1	5.0
11	9	20	2	10.0
6	1	7	3	15.0
1	2	3	4	20.0
4	0	4	5	25.0
0	0	0	6	30.0
2	0	2	7	35.0
0	1	1	8	40.0
0	0	0	9	45.0
1	0	1	10	50.0
0	0	0	11	55.0

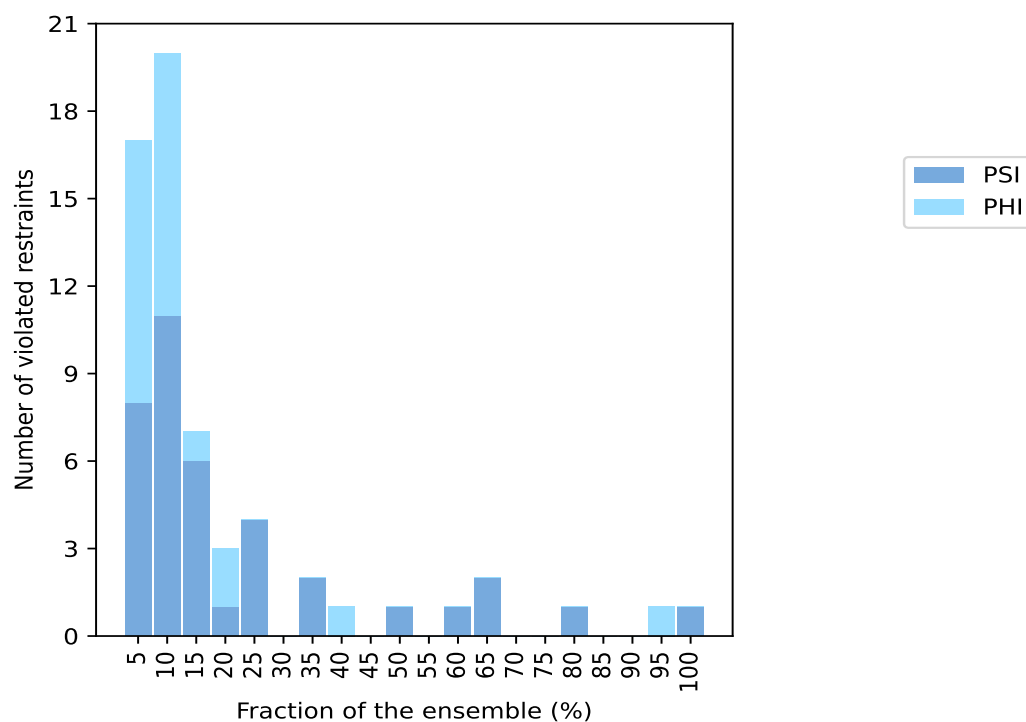
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
1	0	1	12	60.0
2	0	2	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	1	1	19	95.0
1	0	1	20	100.0

¹ Number of models with violations

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

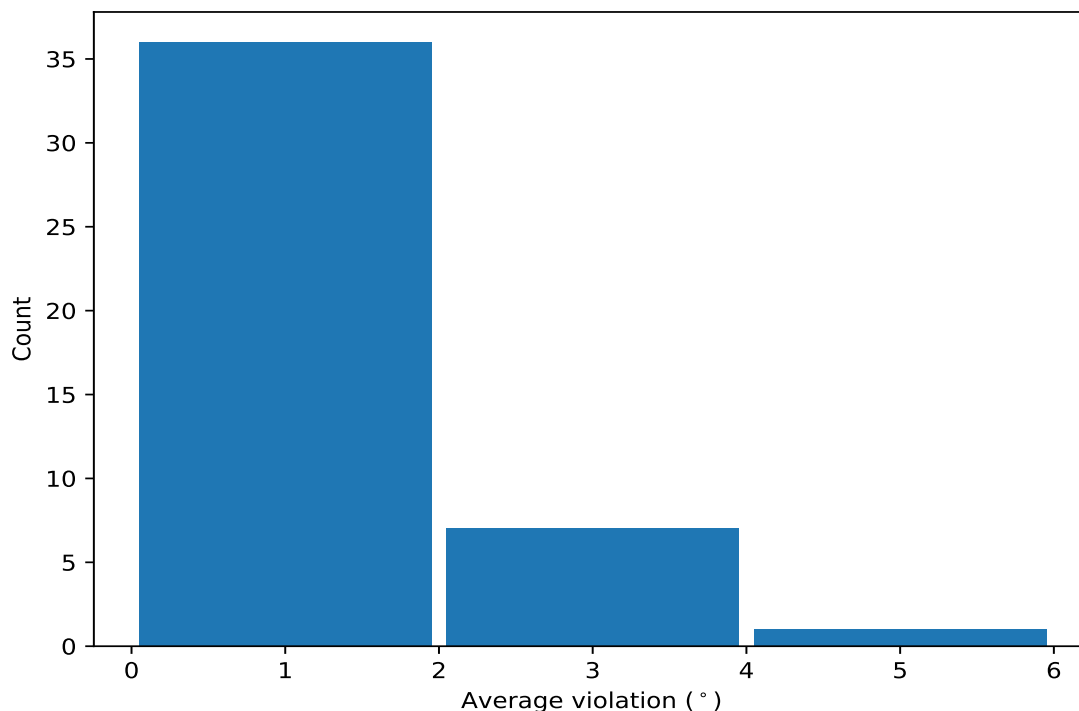


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

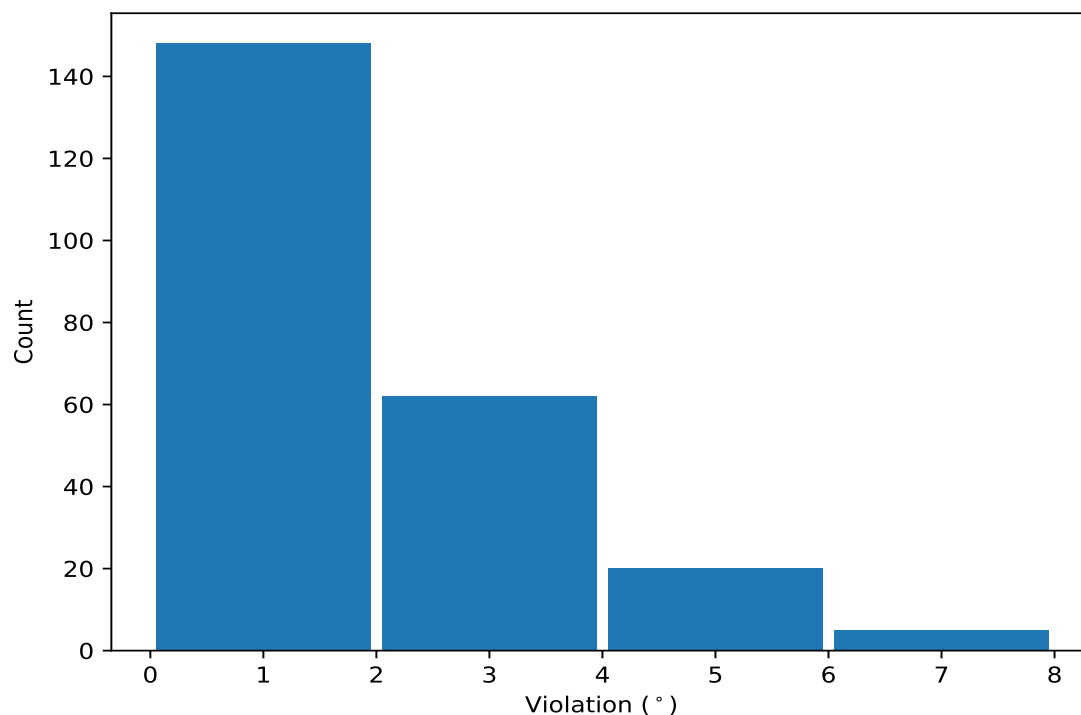
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	20	5.31	0.88	5.36
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	19	1.81	0.68	1.67
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	16	2.03	0.62	2.02
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	13	2.67	0.76	2.9
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	13	1.86	0.46	1.89
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	12	3.14	1.67	2.61
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	10	1.96	0.83	1.7
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	8	1.78	0.63	1.56
(1,170)	2:105:C:VAL:N	2:105:C:VAL:CA	2:105:C:VAL:C	2:106:C:LEU:N	7	1.61	0.49	1.56
(1,14)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:LEU:N	7	1.55	0.23	1.53

¹ Number of violated models, ²Standard 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 (°)
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	5	7.14
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	17	6.44
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	11	6.34
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	11	6.33
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	19	6.11
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	18	5.84
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	8	5.75
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	20	5.74
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	12	5.45
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	13	5.4