



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 25, 2026 – 07:20 AM UTC

PDB ID : 5IRT / pdb_00005irt
BMRB ID : 30035
Title : Dimerization interface of the noncrystalline HIV-1 capsid protein lattice from solid state NMR spectroscopy of tubular assemblies
Authors : Bayro, M.J.; Tycko, R.
Deposited on : 2016-03-14

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

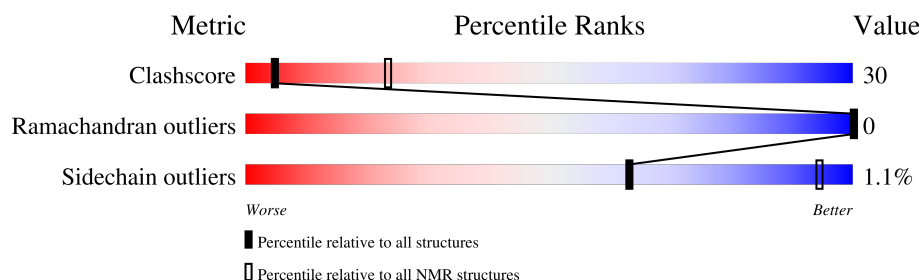
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 11%.

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	231	 . . . 92%
1	B	231	 . . . 92%

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:180-A:192, B:180-B:193 (27)	0.16	10

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 612 atoms, of which 300 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Capsid protein p24.

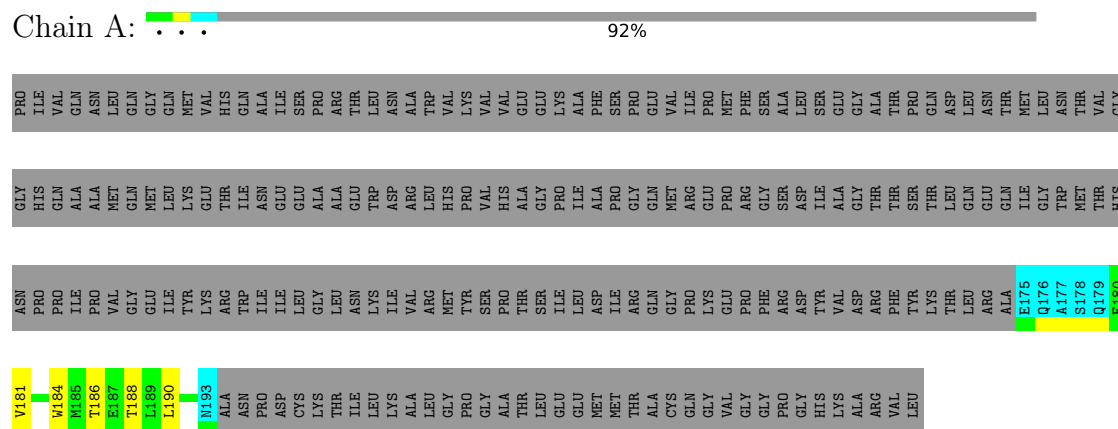
Mol	Chain	Residues	Atoms						Trace
1	A	19	Total	C	H	N	O	S	0
			306	96	150	26	33	1	
1	B	19	Total	C	H	N	O	S	0
			306	96	150	26	33	1	

4 Residue-property plots

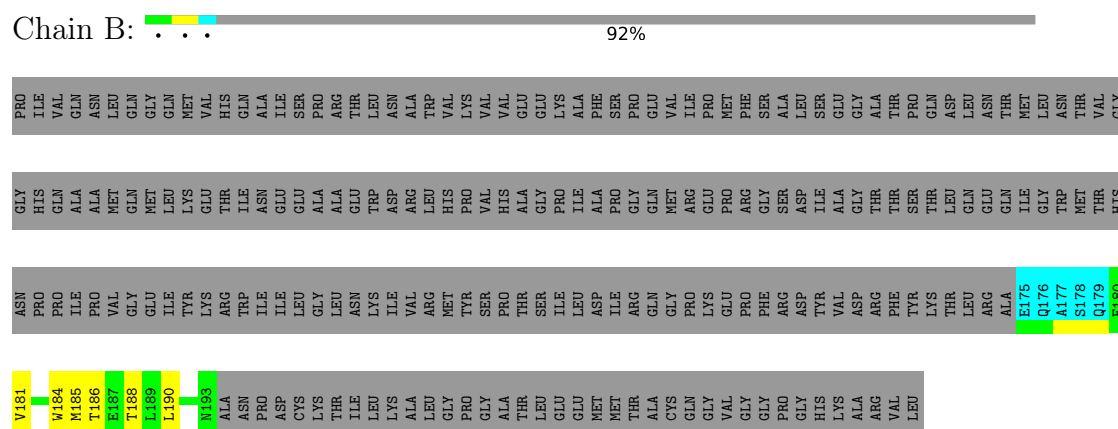
4.1 Average score per residue in the NMR ensemble

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: Capsid protein p24



- Molecule 1: Capsid protein p24



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

The representative model is number 10. Colouring as in section 4.1 above.

Chain A: 92%

Chain B: 92%

W184	ASN	GLY	PRO	ILE
T185	PRO	HIS	GLN	VAL
T186	ILE	ALA	ASN	GLN
E187	PRO	ALA	ALA	ASN
T188	VAL	MET	GLN	LEU
L189	GLY	GLN	MET	GLY
L190	ILE	LEU	LEU	GLN
	TYR	LYS	GLU	MET
M193	ASN	THR	THR	VAL
ALA	ARG	ILE	ILE	HIS
PRO	TRP	ASN	ASN	GLN
ASP	ILE	GLU	GLU	ALA
CYS	ILE	GLU	SER	ILE
LYS	LEU	ALA	GLY	GLY
THR	GLY	LEU	ALA	PRO
ILE	LEU	ALA	THR	ARG
THR	ASN	GLU	GLU	THR
LEU	LYS	TRP	LEU	THR
LYS	ALA	ASP	ASN	ASN
ALA	LEU	ARG	ALA	ALA
LEU	GLY	ARG	LEU	TRP
GLY	PRO	HIS	LEU	VAL
PRO	GLY	PRO	LYS	VAL
ALA	TYR	ILE	VAL	VAL
THR	SER	ALA	HIS	GLU
LEU	PRO	PRO	GLY	GLY
THR	THR	ILE	GLY	LYS
GLU	SER	GLY	ILE	ALA
GLU	THR	ALA	ALA	PHE
MET	ILE	ILE	PRO	SER
	THR	PRO	GLY	PRO
	SER	GLN	GLN	GLU
	GLY	MET	ARG	VAL
	PRO	ARG	ILE	ILE
	LYS	GLU	PRO	PRO
	GLY	PRO	ARG	PHE
	PHE	GLY	SER	SER
	ARG	SER	ALA	ALA
	ASP	ASP	LEU	LEU
	TYR	ILE	SER	GLY
	VAL	ALA	GLY	GLU
	ASP	THR	GLY	ALA
	ARG	THR	THR	THR
	PHE	THR	SER	PRO
	TYR	THR	THR	GLN
	LYS	LEU	ASP	LEU
	THR	GLN	LEU	LEU
	ARG	GLU	ASN	THR
	ALA	GLN	THR	ALA
		ILE	MET	GLY
		GLY	LEU	VAL
		TRP	ASN	THR
		THR	GLY	VAL
		THR	HIS	THR

5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
X-PLOR NIH	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	791
Number of shifts mapped to atoms	57
Number of unparsed shifts	0
Number of shifts with mapping errors	734
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	11%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	110	112	112	7±2
1	B	118	118	118	7±2
All	All	4560	4600	4600	274

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 30.

5 of 60 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:TRP:CD1	1:A:188:THR:HG1	0.93	1.80	4	17
1:B:184:TRP:CD1	1:B:188:THR:HG1	0.90	1.85	8	17
1:A:184:TRP:CD1	1:A:188:THR:HG21	0.68	2.24	6	3
1:B:184:TRP:CD1	1:B:188:THR:HG21	0.66	2.26	6	3
1:B:184:TRP:CD1	1:B:188:THR:OG1	0.63	2.52	18	17

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	13/231 (6%)	13±0 (100±2%)	0±0 (0±2%)	0±0 (0±0%)	100	100
1	B	13/231 (6%)	13±0 (100±2%)	0±0 (0±2%)	0±0 (0±0%)	100	100
All	All	520/9240 (6%)	518 (100%)	2 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains ⓘ

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	13/194 (7%)	13±0 (99±3%)	0±0 (1±3%)	61	94
1	B	14/194 (7%)	14±0 (99±3%)	0±0 (1±3%)	63	94
All	All	540/7760 (7%)	534 (99%)	6 (1%)	63	94

All 4 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	190	LEU	2
1	B	190	LEU	2
1	A	182	LYS	1
1	B	182	LYS	1

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 [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 11% for the well-defined parts and 11% 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	791
Number of shifts mapped to atoms	57
Number of unparsed shifts	0
Number of shifts with mapping errors	734
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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 734) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	PRO	C	171.95	.	1
1	A	1	PRO	CA	60.85	.	1
1	A	1	PRO	CB	34.36	.	1
1	A	1	PRO	CD	50.21	.	1
1	A	1	PRO	CG	27.1	.	1
1	A	1	PRO	N	49.48	.	1
1	A	2	ILE	C	175.15	.	1
1	A	2	ILE	CA	59.95	.	1
1	A	2	ILE	CB	37.42	.	1
1	A	2	ILE	N	120.68	.	1
1	A	3	VAL	CA	60.55	.	1
1	A	3	VAL	CB	32.15	.	1
1	A	3	VAL	N	122.28	.	1
1	A	4	GLN	C	177.05	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	GLN	CA	54.92	.	1
1	A	4	GLN	CB	31.08	.	1
1	A	5	ASN	C	176.65	.	1
1	A	5	ASN	CA	50.85	.	1
1	A	5	ASN	CB	39.32	.	1
1	A	5	ASN	N	124.98	.	1
1	A	6	LEU	CA	57.02	.	1
1	A	6	LEU	CB	41.04	.	1
1	A	6	LEU	N	115.28	.	1
1	A	14	ALA	C	177.85	.	1
1	A	14	ALA	CA	51.74	.	1
1	A	14	ALA	CB	18.77	.	1
1	A	14	ALA	N	124.08	.	1
1	A	15	ILE	C	173.85	.	1
1	A	15	ILE	CA	61.81	.	1
1	A	15	ILE	CB	38.52	.	1
1	A	15	ILE	CG1	28.94	.	1
1	A	15	ILE	CG2	16.26	.	1
1	A	15	ILE	N	121.88	.	1
1	A	16	SER	C	174.45	.	1
1	A	16	SER	CA	55.5	.	1
1	A	16	SER	CB	63.64	.	1
1	A	16	SER	N	122.88	.	1
1	A	17	PRO	C	177.85	.	1
1	A	17	PRO	CA	65.05	.	1
1	A	17	PRO	CB	31.46	.	1
1	A	17	PRO	CD	50.63	.	1
1	A	17	PRO	CG	27.67	.	1
1	A	17	PRO	N	137.68	.	1
1	A	18	ARG	C	178.95	.	1
1	A	18	ARG	CA	58.96	.	1
1	A	18	ARG	CB	29.67	.	1
1	A	18	ARG	N	115.88	.	1
1	A	19	THR	C	175.45	.	1
1	A	19	THR	CA	66.34	.	1
1	A	19	THR	CB	68.07	.	1
1	A	19	THR	CG2	22.93	.	1
1	A	19	THR	N	119.78	.	1
1	A	20	LEU	C	178.05	.	1
1	A	20	LEU	CA	57.89	.	1
1	A	20	LEU	CB	40.21	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	LEU	N	120.28	.	1
1	A	21	ASN	C	177.25	.	1
1	A	21	ASN	CA	55.54	.	1
1	A	21	ASN	CB	38.33	.	1
1	A	21	ASN	N	115.18	.	1
1	A	22	ALA	C	179.85	.	1
1	A	22	ALA	CA	54.69	.	1
1	A	22	ALA	CB	17.97	.	1
1	A	22	ALA	N	121.38	.	1
1	A	23	TRP	C	175.35	.	1
1	A	23	TRP	CA	58.21	.	1
1	A	23	TRP	CB	29.35	.	1
1	A	23	TRP	CG	110.85	.	1
1	A	23	TRP	N	119.28	.	1
1	A	24	VAL	C	178.65	.	1
1	A	24	VAL	CA	66.38	.	1
1	A	24	VAL	CB	31.44	.	1
1	A	24	VAL	CG1	22.5	.	.
1	A	24	VAL	N	115.98	.	1
1	A	25	LYS	C	178.25	.	1
1	A	25	LYS	CA	58.46	.	1
1	A	25	LYS	CB	29.36	.	1
1	A	25	LYS	N	118.08	.	1
1	A	26	VAL	C	177.15	.	1
1	A	26	VAL	CA	65.6	.	1
1	A	26	VAL	CB	30.87	.	1
1	A	26	VAL	CG1	21.55	.	.
1	A	26	VAL	N	119.68	.	1
1	A	27	VAL	C	179.05	.	1
1	A	27	VAL	CA	65.64	.	1
1	A	27	VAL	CB	31.72	.	1
1	A	27	VAL	N	119.98	.	1
1	A	28	GLU	C	177.85	.	1
1	A	28	GLU	CA	58.64	.	1
1	A	28	GLU	CB	29.76	.	1
1	A	28	GLU	N	117.58	.	1
1	A	29	GLU	C	178.65	.	1
1	A	29	GLU	CA	58.09	.	1
1	A	29	GLU	CB	30.31	.	1
1	A	29	GLU	N	115.98	.	1
1	A	30	LYS	C	175.85	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	LYS	CA	56.39	.	1
1	A	30	LYS	N	116.68	.	1
1	A	31	ALA	N	121.38	.	1
1	A	32	PHE	C	176.75	.	1
1	A	32	PHE	CA	56.8	.	1
1	A	32	PHE	CB	39.5	.	1
1	A	32	PHE	N	111.88	.	1
1	A	33	SER	C	173.85	.	1
1	A	33	SER	CA	57.6	.	1
1	A	33	SER	CB	63.15	.	1
1	A	33	SER	N	113.68	.	1
1	A	34	PRO	C	178.35	.	1
1	A	34	PRO	CA	66.03	.	1
1	A	34	PRO	CB	31.82	.	1
1	A	34	PRO	CD	50.22	.	1
1	A	34	PRO	CG	27.64	.	1
1	A	34	PRO	N	134.58	.	1
1	A	35	GLU	C	179.05	.	1
1	A	35	GLU	CA	58.87	.	1
1	A	35	GLU	CB	29.58	.	1
1	A	35	GLU	N	118.18	.	1
1	A	36	VAL	C	176.45	.	1
1	A	36	VAL	CA	65.37	.	1
1	A	36	VAL	CB	31.55	.	1
1	A	36	VAL	CG1	21.41	.	.
1	A	36	VAL	N	115.38	.	1
1	A	37	ILE	C	175.05	.	1
1	A	37	ILE	CA	67.52	.	1
1	A	37	ILE	CB	34.52	.	1
1	A	37	ILE	CG1	30.36	.	1
1	A	37	ILE	CG2	18.25	.	1
1	A	37	ILE	N	118.68	.	1
1	A	38	PRO	C	179.15	.	1
1	A	38	PRO	CA	64.82	.	1
1	A	38	PRO	CB	30.21	.	1
1	A	38	PRO	CD	49.01	.	1
1	A	38	PRO	CG	27.82	.	1
1	A	38	PRO	N	134.58	.	1
1	A	39	MET	C	176.65	.	1
1	A	39	MET	CA	57.64	.	1
1	A	39	MET	CB	30.83	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	39	MET	N	116.48	.	1
1	A	40	PHE	C	178.55	.	1
1	A	40	PHE	CA	61.56	.	1
1	A	40	PHE	CB	37.87	.	1
1	A	40	PHE	N	121.08	.	1
1	A	41	SER	C	175.75	.	1
1	A	41	SER	CA	62.05	.	1
1	A	41	SER	CB	62.38	.	1
1	A	41	SER	N	114.48	.	1
1	A	42	ALA	C	180.25	.	1
1	A	42	ALA	CA	54.14	.	1
1	A	42	ALA	CB	18.99	.	1
1	A	42	ALA	N	121.48	.	1
1	A	43	LEU	C	175.85	.	1
1	A	43	LEU	CA	55.65	.	1
1	A	43	LEU	CB	41.9	.	1
1	A	43	LEU	N	115.88	.	1
1	A	44	SER	C	174.75	.	1
1	A	44	SER	CA	56.87	.	1
1	A	44	SER	CB	63.43	.	1
1	A	44	SER	N	109.08	.	1
1	A	45	GLU	C	178.05	.	1
1	A	45	GLU	CA	57.96	.	1
1	A	45	GLU	CB	29.11	.	1
1	A	45	GLU	CG	35.28	.	1
1	A	45	GLU	N	125.08	.	1
1	A	46	GLY	C	174.05	.	1
1	A	46	GLY	CA	45.72	.	1
1	A	46	GLY	N	115.78	.	1
1	A	47	ALA	C	178.15	.	1
1	A	47	ALA	CA	52.87	.	1
1	A	47	ALA	CB	20.08	.	1
1	A	47	ALA	N	119.78	.	1
1	A	48	THR	C	174.35	.	1
1	A	48	THR	CA	59.49	.	1
1	A	48	THR	CB	69.03	.	1
1	A	48	THR	CG2	21.86	.	1
1	A	48	THR	N	108.88	.	1
1	A	49	PRO	C	176.65	.	1
1	A	49	PRO	CA	66.83	.	1
1	A	49	PRO	CB	29.83	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	PRO	CD	49.77	.	1
1	A	49	PRO	CG	27.92	.	1
1	A	49	PRO	N	132.68	.	1
1	A	50	GLN	C	177.45	.	1
1	A	50	GLN	CA	58.8	.	1
1	A	50	GLN	CB	29.88	.	1
1	A	50	GLN	CG	32.73	.	1
1	A	50	GLN	N	116.28	.	1
1	A	51	ASP	C	179.55	.	1
1	A	51	ASP	CA	57.66	.	1
1	A	51	ASP	CB	41.83	.	1
1	A	51	ASP	N	117.68	.	1
1	A	52	LEU	C	178.35	.	1
1	A	52	LEU	CA	57.93	.	1
1	A	52	LEU	CB	42.04	.	1
1	A	52	LEU	N	120.38	.	1
1	A	53	ASN	C	177.85	.	1
1	A	53	ASN	CA	56.03	.	1
1	A	53	ASN	CB	38.32	.	1
1	A	53	ASN	N	115.58	.	1
1	A	54	THR	C	176.25	.	1
1	A	54	THR	CA	67.09	.	1
1	A	54	THR	CB	67.94	.	1
1	A	54	THR	CG2	23.24	.	1
1	A	54	THR	N	119.58	.	1
1	A	55	MET	C	179.45	.	1
1	A	55	MET	CA	60.02	.	1
1	A	55	MET	CB	32.71	.	1
1	A	55	MET	N	119.18	.	1
1	A	56	LEU	C	178.05	.	1
1	A	56	LEU	CA	58.7	.	1
1	A	56	LEU	CB	41.55	.	1
1	A	56	LEU	CG	26.78	.	1
1	A	56	LEU	N	121.98	.	1
1	A	57	ASN	C	176.75	.	1
1	A	57	ASN	CA	54.55	.	1
1	A	57	ASN	CB	38.1	.	1
1	A	57	ASN	N	115.48	.	1
1	A	58	THR	C	174.15	.	1
1	A	58	THR	CA	63.17	.	1
1	A	58	THR	N	107.98	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	59	VAL	C	176.55	.	1
1	A	59	VAL	CA	63.97	.	1
1	A	59	VAL	CB	32.16	.	1
1	A	59	VAL	CG1	22.06	.	.
1	A	59	VAL	N	120.88	.	1
1	A	60	GLY	C	174.15	.	1
1	A	60	GLY	CA	44.85	.	1
1	A	60	GLY	N	116.38	.	1
1	A	61	GLY	C	174.25	.	1
1	A	61	GLY	CA	45.14	.	1
1	A	62	HIS	N	119.48	.	1
1	A	63	GLN	C	178.85	.	1
1	A	63	GLN	CA	59.87	.	1
1	A	63	GLN	CB	30.06	.	1
1	A	63	GLN	N	119.98	.	1
1	A	64	ALA	C	178.55	.	1
1	A	64	ALA	CA	55.68	.	1
1	A	64	ALA	CB	18.36	.	1
1	A	64	ALA	N	124.18	.	1
1	A	65	ALA	C	179.45	.	1
1	A	65	ALA	CA	54.78	.	1
1	A	65	ALA	CB	18.29	.	1
1	A	65	ALA	N	121.08	.	1
1	A	66	MET	C	179.05	.	1
1	A	66	MET	CA	56.14	.	1
1	A	66	MET	CB	29.9	.	1
1	A	66	MET	N	113.08	.	1
1	A	67	GLN	N	121.08	.	1
1	A	69	LEU	C	181.25	.	1
1	A	69	LEU	CA	57.24	.	1
1	A	69	LEU	CB	41.53	.	1
1	A	69	LEU	N	117.88	.	1
1	A	70	LYS	C	178.35	.	1
1	A	70	LYS	CA	58.76	.	1
1	A	70	LYS	CB	31.52	.	1
1	A	70	LYS	N	119.48	.	1
1	A	71	GLU	C	178.65	.	1
1	A	71	GLU	CA	58.78	.	1
1	A	71	GLU	N	119.08	.	1
1	A	72	THR	C	176.45	.	1
1	A	72	THR	CA	66.87	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	THR	CB	67.99	.	1
1	A	72	THR	N	116.38	.	1
1	A	73	ILE	C	176.65	.	1
1	A	73	ILE	CA	65.58	.	1
1	A	73	ILE	CB	37.61	.	1
1	A	73	ILE	CG2	18.03	.	1
1	A	73	ILE	N	122.28	.	1
1	A	74	ASN	C	177.95	.	1
1	A	74	ASN	CA	55.69	.	1
1	A	74	ASN	CB	37.53	.	1
1	A	74	ASN	N	116.88	.	1
1	A	75	GLU	C	177.95	.	1
1	A	75	GLU	CA	57.92	.	1
1	A	75	GLU	CB	29.27	.	1
1	A	75	GLU	N	121.48	.	1
1	A	76	GLU	C	179.25	.	1
1	A	76	GLU	CA	57.74	.	1
1	A	76	GLU	CB	26.73	.	1
1	A	76	GLU	N	120.38	.	1
1	A	77	ALA	C	178.55	.	1
1	A	77	ALA	CA	54.55	.	1
1	A	77	ALA	CB	17.44	.	1
1	A	77	ALA	N	123.48	.	1
1	A	78	ALA	C	181.25	.	1
1	A	78	ALA	CA	54.4	.	1
1	A	78	ALA	CB	17.65	.	1
1	A	78	ALA	N	118.98	.	1
1	A	79	GLU	C	178.05	.	1
1	A	79	GLU	CA	58.57	.	1
1	A	79	GLU	CB	28.9	.	1
1	A	79	GLU	N	120.88	.	1
1	A	80	TRP	CA	61.92	.	1
1	A	80	TRP	CB	27.61	.	1
1	A	80	TRP	CG	109.95	.	1
1	A	80	TRP	N	121.38	.	1
1	A	81	ASP	C	177.65	.	1
1	A	81	ASP	CA	56.18	.	1
1	A	81	ASP	CB	37.25	.	1
1	A	81	ASP	N	116.88	.	1
1	A	82	ARG	C	177.65	.	1
1	A	82	ARG	CA	58.82	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	82	ARG	CB	30.26	.	1
1	A	82	ARG	CG	27.73	.	1
1	A	82	ARG	N	119.78	.	1
1	A	83	LEU	C	175.95	.	1
1	A	83	LEU	CA	54.97	.	1
1	A	83	LEU	CB	42.48	.	1
1	A	83	LEU	N	116.58	.	1
1	A	84	HIS	C	170.55	.	1
1	A	84	HIS	CA	52.76	.	1
1	A	84	HIS	CB	27.58	.	1
1	A	84	HIS	N	116.68	.	1
1	A	85	PRO	C	176.65	.	1
1	A	85	PRO	CA	62.76	.	1
1	A	85	PRO	CB	31.64	.	1
1	A	85	PRO	CD	49.98	.	1
1	A	85	PRO	CG	26.96	.	1
1	A	85	PRO	N	137.78	.	1
1	A	86	VAL	C	175.95	.	1
1	A	86	VAL	CA	62.03	.	1
1	A	86	VAL	CB	32.9	.	1
1	A	86	VAL	N	120.58	.	1
1	A	87	HIS	C	174.35	.	1
1	A	87	HIS	CA	55.43	.	1
1	A	87	HIS	N	122.38	.	1
1	A	88	ALA	C	177.35	.	1
1	A	88	ALA	CA	52.09	.	1
1	A	88	ALA	CB	19.08	.	1
1	A	88	ALA	N	127.28	.	1
1	A	89	GLY	C	171.25	.	1
1	A	89	GLY	CA	44.53	.	1
1	A	89	GLY	N	108.68	.	1
1	A	90	PRO	N	136.18	.	1
1	A	91	ILE	C	175.55	.	1
1	A	91	ILE	CA	59.9	.	1
1	A	91	ILE	N	121.38	.	1
1	A	92	ALA	C	174.85	.	1
1	A	92	ALA	CA	50.53	.	1
1	A	92	ALA	CB	17.88	.	1
1	A	92	ALA	N	130.08	.	1
1	A	93	PRO	C	178.05	.	1
1	A	93	PRO	CA	63.62	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	PRO	CB	32.42	.	1
1	A	93	PRO	N	133.98	.	1
1	A	94	GLY	C	174.25	.	1
1	A	94	GLY	CA	45.35	.	1
1	A	94	GLY	N	111.68	.	1
1	A	95	GLN	N	119.68	.	1
1	A	98	GLU	C	174.25	.	1
1	A	98	GLU	CA	54.19	.	1
1	A	98	GLU	CB	29.35	.	1
1	A	98	GLU	N	122.88	.	1
1	A	99	PRO	C	176.95	.	1
1	A	99	PRO	CA	62.33	.	1
1	A	99	PRO	CB	30.15	.	1
1	A	99	PRO	CD	48.82	.	1
1	A	99	PRO	CG	27.62	.	1
1	A	99	PRO	N	134.08	.	1
1	A	100	ARG	C	178.55	.	1
1	A	100	ARG	CA	52.89	.	1
1	A	100	ARG	CB	30.8	.	1
1	A	100	ARG	N	120.98	.	1
1	A	101	GLY	C	175.85	.	1
1	A	101	GLY	CA	48.29	.	1
1	A	101	GLY	N	116.48	.	1
1	A	102	SER	C	176.65	.	1
1	A	102	SER	CA	60.63	.	1
1	A	102	SER	CB	61.72	.	1
1	A	102	SER	N	114.58	.	1
1	A	103	ASP	C	179.65	.	1
1	A	103	ASP	CA	56.56	.	1
1	A	103	ASP	CB	41.26	.	1
1	A	103	ASP	N	122.48	.	1
1	A	104	ILE	C	172.45	.	1
1	A	104	ILE	CA	65.58	.	1
1	A	104	ILE	CB	36.63	.	1
1	A	104	ILE	CG1	30.36	.	1
1	A	104	ILE	CG2	16.82	.	1
1	A	104	ILE	N	125.58	.	1
1	A	105	ALA	C	177.05	.	1
1	A	105	ALA	CA	50.35	.	1
1	A	105	ALA	CB	18.4	.	1
1	A	105	ALA	N	111.68	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	GLY	C	173.55	.	1
1	A	106	GLY	CA	45.3	.	1
1	A	106	GLY	N	101.98	.	1
1	A	107	THR	C	176.95	.	1
1	A	107	THR	CA	63.73	.	1
1	A	107	THR	CB	68.66	.	1
1	A	107	THR	CG2	22.54	.	1
1	A	107	THR	N	112.98	.	1
1	A	108	THR	C	173.05	.	1
1	A	108	THR	CA	60.69	.	1
1	A	108	THR	CB	69.15	.	1
1	A	108	THR	CG2	20.23	.	1
1	A	108	THR	N	105.68	.	1
1	A	109	SER	C	173.85	.	1
1	A	109	SER	CA	53.88	.	1
1	A	109	SER	CB	66.64	.	1
1	A	109	SER	N	111.98	.	1
1	A	110	THR	C	175.55	.	1
1	A	110	THR	CA	59.17	.	1
1	A	110	THR	CB	71.09	.	1
1	A	110	THR	CG2	21.84	.	1
1	A	110	THR	N	112.28	.	1
1	A	111	LEU	C	178.25	.	1
1	A	111	LEU	CA	57.8	.	1
1	A	111	LEU	CB	40.56	.	1
1	A	111	LEU	N	122.48	.	1
1	A	112	GLN	C	179.55	.	1
1	A	112	GLN	CA	59.39	.	1
1	A	112	GLN	CB	27.67	.	1
1	A	112	GLN	CG	34.06	.	1
1	A	112	GLN	N	115.48	.	1
1	A	113	GLU	C	179.15	.	1
1	A	113	GLU	CA	58.12	.	1
1	A	113	GLU	CB	26.94	.	1
1	A	113	GLU	N	120.28	.	1
1	A	114	GLN	CA	59.88	.	1
1	A	114	GLN	CB	29.72	.	1
1	A	114	GLN	CG	35.21	.	1
1	A	114	GLN	N	119.38	.	1
1	A	115	ILE	C	179.45	.	1
1	A	115	ILE	CA	65.44	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	115	ILE	CB	38.44	.	1
1	A	115	ILE	CG1	28.38	.	1
1	A	115	ILE	CG2	17.0	.	1
1	A	115	ILE	N	117.98	.	1
1	A	116	GLY	C	175.85	.	1
1	A	116	GLY	CA	47.0	.	1
1	A	116	GLY	N	110.48	.	1
1	A	117	TRP	C	178.65	.	1
1	A	117	TRP	CA	61.96	.	1
1	A	117	TRP	CB	27.37	.	1
1	A	117	TRP	CG	112.45	.	1
1	A	117	TRP	N	121.18	.	1
1	A	118	MET	C	177.25	.	1
1	A	118	MET	CA	59.41	.	1
1	A	118	MET	CB	34.82	.	1
1	A	118	MET	CG	32.81	.	1
1	A	118	MET	N	115.78	.	1
1	A	119	THR	C	173.45	.	1
1	A	119	THR	CA	60.75	.	1
1	A	119	THR	CB	69.77	.	1
1	A	119	THR	CG2	21.38	.	1
1	A	119	THR	N	104.18	.	1
1	A	120	HIS	C	172.35	.	1
1	A	120	HIS	CA	57.13	.	1
1	A	120	HIS	CB	28.76	.	1
1	A	120	HIS	N	123.78	.	1
1	A	121	ASN	C	172.35	.	1
1	A	121	ASN	CA	48.89	.	1
1	A	121	ASN	CB	39.74	.	1
1	A	121	ASN	CG	177.15	.	1
1	A	121	ASN	N	118.78	.	1
1	A	122	PRO	C	174.75	.	1
1	A	122	PRO	CA	61.98	.	1
1	A	122	PRO	CB	32.76	.	1
1	A	122	PRO	CD	50.28	.	1
1	A	122	PRO	CG	24.54	.	1
1	A	122	PRO	N	138.48	.	1
1	A	123	PRO	C	177.45	.	1
1	A	123	PRO	CA	63.84	.	1
1	A	123	PRO	CB	32.55	.	1
1	A	123	PRO	CD	50.25	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	123	PRO	CG	27.05	.	1
1	A	123	PRO	N	134.18	.	1
1	A	124	ILE	C	176.05	.	1
1	A	124	ILE	CA	59.08	.	1
1	A	124	ILE	CB	38.02	.	1
1	A	124	ILE	CG2	17.08	.	1
1	A	124	ILE	N	122.68	.	1
1	A	125	PRO	C	176.65	.	1
1	A	125	PRO	CA	62.46	.	1
1	A	125	PRO	CB	28.55	.	1
1	A	125	PRO	CD	50.94	.	1
1	A	125	PRO	CG	26.96	.	1
1	A	125	PRO	N	136.48	.	1
1	A	126	VAL	C	176.45	.	1
1	A	126	VAL	CA	65.5	.	1
1	A	126	VAL	CB	30.67	.	1
1	A	126	VAL	CG1	23.42	.	.
1	A	126	VAL	CG2	19.19	.	.
1	A	126	VAL	N	115.28	.	1
1	A	127	GLY	C	174.65	.	1
1	A	127	GLY	CA	47.04	.	1
1	A	127	GLY	N	106.48	.	1
1	A	128	GLU	C	179.25	.	1
1	A	128	GLU	CA	58.13	.	1
1	A	128	GLU	CB	29.12	.	1
1	A	128	GLU	N	121.48	.	1
1	A	129	ILE	C	175.85	.	1
1	A	129	ILE	CA	65.0	.	1
1	A	129	ILE	CB	37.87	.	1
1	A	129	ILE	CG2	17.74	.	1
1	A	129	ILE	N	120.58	.	1
1	A	130	TYR	C	178.15	.	1
1	A	130	TYR	CA	55.87	.	1
1	A	130	TYR	CB	37.63	.	1
1	A	130	TYR	N	116.58	.	1
1	A	131	LYS	N	121.48	.	1
1	A	133	TRP	C	178.05	.	1
1	A	133	TRP	CA	58.36	.	1
1	A	133	TRP	CB	29.84	.	1
1	A	133	TRP	CG	112.15	.	1
1	A	133	TRP	N	120.58	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	134	ILE	C	177.95	.	1
1	A	134	ILE	CA	65.05	.	1
1	A	134	ILE	CB	38.13	.	1
1	A	134	ILE	CG1	29.44	.	1
1	A	134	ILE	CG2	17.81	.	1
1	A	134	ILE	N	118.58	.	1
1	A	135	ILE	C	177.55	.	1
1	A	135	ILE	CA	66.16	.	1
1	A	135	ILE	CB	37.46	.	1
1	A	135	ILE	CG1	30.94	.	1
1	A	135	ILE	CG2	17.3	.	1
1	A	135	ILE	N	121.08	.	1
1	A	136	LEU	C	180.85	.	1
1	A	136	LEU	CA	58.54	.	1
1	A	136	LEU	CB	41.31	.	1
1	A	136	LEU	CG	26.82	.	1
1	A	136	LEU	N	121.48	.	1
1	A	137	GLY	C	175.65	.	1
1	A	137	GLY	CA	47.44	.	1
1	A	137	GLY	N	106.68	.	1
1	A	138	LEU	C	178.35	.	1
1	A	138	LEU	CA	57.82	.	1
1	A	138	LEU	CB	41.93	.	1
1	A	138	LEU	CG	26.0	.	1
1	A	138	LEU	N	123.08	.	1
1	A	139	ASN	C	178.05	.	1
1	A	139	ASN	CA	56.45	.	1
1	A	139	ASN	CB	38.4	.	1
1	A	139	ASN	N	118.28	.	1
1	A	140	LYS	N	118.28	.	1
1	A	146	SER	C	174.55	.	1
1	A	147	PRO	C	177.15	.	1
1	A	147	PRO	CA	62.43	.	1
1	A	147	PRO	N	133.78	.	1
1	A	148	THR	C	176.05	.	1
1	A	148	THR	CA	59.61	.	1
1	A	148	THR	CB	70.43	.	1
1	A	148	THR	N	112.88	.	1
1	A	149	SER	C	174.55	.	1
1	A	149	SER	CA	57.18	.	1
1	A	149	SER	CB	64.75	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	149	SER	N	116.88	.	1
1	A	150	ILE	C	178.35	.	1
1	A	150	ILE	CA	59.86	.	1
1	A	150	ILE	CB	37.35	.	1
1	A	150	ILE	N	121.18	.	1
1	A	151	LEU	C	179.35	.	1
1	A	151	LEU	CA	57.9	.	1
1	A	151	LEU	CB	41.05	.	1
1	A	151	LEU	CG	26.51	.	1
1	A	151	LEU	N	117.48	.	1
1	A	152	ASP	C	175.75	.	1
1	A	152	ASP	CA	53.91	.	1
1	A	152	ASP	CB	41.92	.	1
1	A	152	ASP	N	115.48	.	1
1	A	153	ILE	C	173.55	.	1
1	A	153	ILE	CA	58.9	.	1
1	A	153	ILE	CB	35.45	.	1
1	A	153	ILE	N	122.08	.	1
1	A	154	ARG	C	175.05	.	1
1	A	154	ARG	CA	53.88	.	1
1	A	154	ARG	CB	32.94	.	1
1	A	154	ARG	N	125.28	.	1
1	A	155	GLN	C	176.85	.	1
1	A	155	GLN	CA	55.49	.	1
1	A	155	GLN	CB	27.06	.	1
1	A	155	GLN	CG	32.34	.	1
1	A	155	GLN	N	127.48	.	1
1	A	156	GLY	C	173.15	.	1
1	A	156	GLY	CA	44.9	.	1
1	A	156	GLY	N	116.98	.	1
1	A	157	PRO	C	176.75	.	1
1	A	157	PRO	CA	65.23	.	1
1	A	157	PRO	CB	31.85	.	1
1	A	157	PRO	CD	49.89	.	1
1	A	157	PRO	CG	27.44	.	1
1	A	157	PRO	N	136.88	.	1
1	A	158	LYS	C	175.15	.	1
1	A	158	LYS	CA	53.92	.	1
1	A	158	LYS	CB	32.14	.	1
1	A	158	LYS	N	114.98	.	1
1	A	159	GLU	C	174.35	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	159	GLU	CA	53.17	.	1
1	A	159	GLU	CB	32.19	.	1
1	A	159	GLU	N	125.18	.	1
1	A	160	PRO	C	177.35	.	1
1	A	160	PRO	CA	62.91	.	1
1	A	160	PRO	CB	32.35	.	1
1	A	160	PRO	CD	51.31	.	1
1	A	160	PRO	CG	28.18	.	1
1	A	160	PRO	N	143.58	.	1
1	A	161	PHE	C	176.95	.	1
1	A	161	PHE	CA	62.32	.	1
1	A	161	PHE	CB	39.37	.	1
1	A	161	PHE	N	127.58	.	1
1	A	162	ARG	C	176.25	.	1
1	A	162	ARG	CA	59.67	.	1
1	A	162	ARG	N	115.88	.	1
1	A	163	ASP	C	178.25	.	1
1	A	163	ASP	CA	56.94	.	1
1	A	163	ASP	CB	39.91	.	1
1	A	163	ASP	N	116.68	.	1
1	A	164	TYR	C	175.95	.	1
1	A	164	TYR	CA	59.16	.	1
1	A	164	TYR	CG	126.75	.	1
1	A	164	TYR	N	123.28	.	1
1	A	165	VAL	CA	66.19	.	1
1	A	167	ARG	C	179.05	.	1
1	A	168	PHE	C	176.85	.	1
1	A	168	PHE	CA	62.24	.	1
1	A	168	PHE	CB	39.63	.	1
1	A	168	PHE	N	123.88	.	1
1	A	169	TYR	C	179.15	.	1
1	A	169	TYR	CA	63.47	.	1
1	A	169	TYR	CB	37.89	.	1
1	A	169	TYR	N	114.88	.	1
1	A	170	LYS	CA	60.04	.	1
1	A	170	LYS	N	123.58	.	1
1	A	171	THR	CA	64.6	.	1
1	A	171	THR	CB	68.94	.	1
1	A	171	THR	N	111.98	.	1
1	A	194	ALA	C	175.25	.	1
1	A	194	ALA	CA	51.68	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	194	ALA	CB	18.58	.	1
1	A	194	ALA	N	124.58	.	1
1	A	195	ASN	C	173.25	.	1
1	A	195	ASN	CA	51.39	.	1
1	A	195	ASN	CB	35.97	.	1
1	A	195	ASN	N	119.28	.	1
1	A	196	PRO	C	178.25	.	1
1	A	196	PRO	CA	66.43	.	1
1	A	196	PRO	CB	32.02	.	1
1	A	196	PRO	CD	49.62	.	1
1	A	196	PRO	CG	27.06	.	1
1	A	196	PRO	N	132.38	.	1
1	A	197	ASP	C	178.85	.	1
1	A	197	ASP	CA	56.78	.	1
1	A	197	ASP	CB	40.28	.	1
1	A	197	ASP	N	115.68	.	1
1	A	198	CYS	C	178.65	.	1
1	A	198	CYS	CA	59.65	.	1
1	A	198	CYS	CB	35.14	.	1
1	A	198	CYS	N	115.98	.	1
1	A	199	LYS	C	177.55	.	1
1	A	199	LYS	CA	60.8	.	1
1	A	199	LYS	CB	32.22	.	1
1	A	199	LYS	N	121.68	.	1
1	A	200	THR	C	176.05	.	1
1	A	200	THR	CA	66.51	.	1
1	A	200	THR	CB	68.83	.	1
1	A	200	THR	CG2	21.5	.	1
1	A	200	THR	N	112.08	.	1
1	A	201	ILE	C	178.25	.	1
1	A	201	ILE	CA	64.31	.	1
1	A	201	ILE	CB	37.95	.	1
1	A	201	ILE	CG1	29.1	.	1
1	A	201	ILE	CG2	18.25	.	1
1	A	201	ILE	N	122.98	.	1
1	A	202	LEU	C	178.05	.	1
1	A	202	LEU	CA	57.3	.	1
1	A	202	LEU	CB	41.29	.	1
1	A	202	LEU	N	118.18	.	1
1	A	203	LYS	C	178.35	.	1
1	A	203	LYS	CA	59.81	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	203	LYS	CB	31.68	.	1
1	A	203	LYS	N	119.68	.	1
1	A	204	ALA	C	178.15	.	1
1	A	204	ALA	CA	53.29	.	1
1	A	204	ALA	CB	18.11	.	1
1	A	204	ALA	N	120.08	.	1
1	A	205	LEU	C	178.75	.	1
1	A	205	LEU	CA	56.32	.	1
1	A	205	LEU	CB	42.38	.	1
1	A	205	LEU	N	116.98	.	1
1	A	206	GLY	C	171.55	.	1
1	A	206	GLY	CA	44.2	.	1
1	A	206	GLY	N	104.08	.	1
1	A	207	PRO	C	178.25	.	1
1	A	207	PRO	CA	62.98	.	1
1	A	207	PRO	CB	31.71	.	1
1	A	207	PRO	CD	49.51	.	1
1	A	207	PRO	CG	26.97	.	1
1	A	207	PRO	N	132.48	.	1
1	A	208	GLY	C	174.55	.	1
1	A	208	GLY	CA	45.29	.	1
1	A	208	GLY	N	109.98	.	1
1	A	209	ALA	C	177.55	.	1
1	A	209	ALA	CA	52.14	.	1
1	A	209	ALA	CB	19.53	.	1
1	A	209	ALA	N	123.48	.	1
1	A	210	THR	C	175.15	.	1
1	A	210	THR	CA	59.98	.	1
1	A	210	THR	CB	70.26	.	1
1	A	210	THR	CG2	21.9	.	1
1	A	210	THR	N	113.68	.	1
1	A	211	LEU	C	179.35	.	1
1	A	211	LEU	CA	58.18	.	1
1	A	211	LEU	CB	40.36	.	1
1	A	211	LEU	CG	26.94	.	1
1	A	211	LEU	N	125.18	.	1
1	A	212	GLU	C	179.35	.	1
1	A	212	GLU	CA	59.82	.	1
1	A	212	GLU	CB	28.99	.	1
1	A	212	GLU	N	119.28	.	1
1	A	213	GLU	C	178.35	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	213	GLU	CA	58.66	.	1
1	A	213	GLU	N	119.08	.	1
1	A	214	MET	C	179.05	.	1
1	A	214	MET	CA	59.66	.	1
1	A	214	MET	CB	31.53	.	1
1	A	214	MET	N	119.28	.	1
1	A	215	MET	C	179.15	.	1
1	A	215	MET	CA	58.58	.	1
1	A	215	MET	CB	32.41	.	1
1	A	215	MET	N	117.58	.	1
1	A	216	THR	C	175.95	.	1
1	A	216	THR	CA	65.87	.	1
1	A	216	THR	CB	68.52	.	1
1	A	216	THR	N	114.58	.	1
1	A	217	ALA	C	178.85	.	1
1	A	217	ALA	CA	54.76	.	1
1	A	217	ALA	CB	18.6	.	1
1	A	217	ALA	N	123.38	.	1
1	A	218	CYS	C	174.45	.	1
1	A	218	CYS	CA	56.57	.	1
1	A	218	CYS	CB	40.36	.	1
1	A	218	CYS	N	109.88	.	1
1	A	219	GLN	N	121.78	.	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
$^{13}\text{C}_\alpha$	184	-0.34 ± 0.56	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	158	0.64 ± 0.96	None needed (imprecise)
$^{13}\text{C}'$	179	-0.31 ± 0.68	None needed (< 0.5 ppm)
^{15}N	188	2.75 ± 1.04	Should be applied

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 11%, i.e. 43 atoms were assigned a chemical shift out of a possible 396. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	30/135 (22%)	0/54 (0%)	20/54 (37%)	10/27 (37%)
Sidechain	13/237 (5%)	0/154 (0%)	13/76 (17%)	0/7 (0%)
Aromatic	0/24 (0%)	0/12 (0%)	0/10 (0%)	0/2 (0%)
Overall	43/396 (11%)	0/220 (0%)	33/140 (24%)	10/36 (28%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts [i](#)

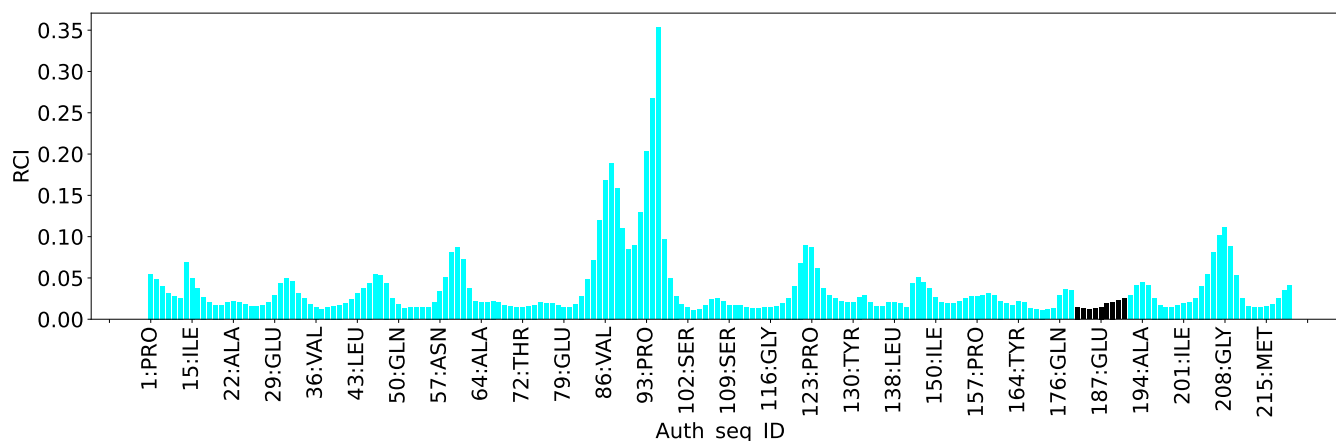
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	1	PRO	N	49.48	108.67 – 162.11	-16.1

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	24
Intra-residue ($ i-j =0$)	6
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	8
Inter-chain	10
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	50
Number of unmapped restraints	0
Number of restraints per residue	0.2
Number of long range restraints per residue ¹	0.0

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

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)	4.0	0.2
0.2-0.5 (Medium)	1.9	0.23
>0.5 (Large)	None	None

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)	2.4	9.26
10.0-20.0 (Medium)	0.7	19.59
>20.0 (Large)	4.1	149.49

9 Distance violation analysis ⓘ

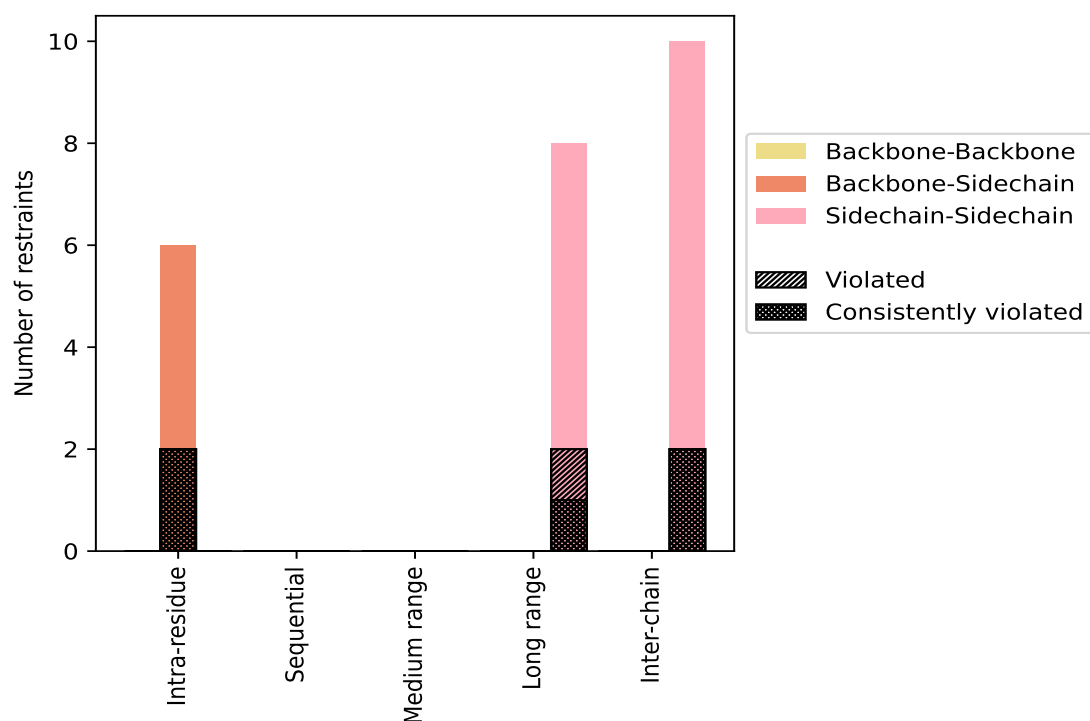
9.1 Summary of distance violations ⓘ

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)	6	25.0	2	33.3	8.3	2	33.3	8.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	25.0	2	33.3	8.3	2	33.3	8.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	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
Medium range (i-j >1 & i-j <5)	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
Long range (i-j ≥5)	8	33.3	2	25.0	8.3	1	12.5	4.2
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	8	33.3	2	25.0	8.3	1	12.5	4.2
Inter-chain	10	41.7	2	20.0	8.3	2	20.0	8.3
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	10	41.7	2	20.0	8.3	2	20.0	8.3
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	24	100.0	6	25.0	25.0	5	20.8	20.8
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	25.0	2	33.3	8.3	2	33.3	8.3
Sidechain-Sidechain	18	75.0	4	22.2	16.7	3	16.7	12.5

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

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	2	0	0	2	2	6	0.18	0.22	0.03	0.18
2	2	0	0	2	2	6	0.18	0.23	0.04	0.18
3	2	0	0	2	2	6	0.17	0.23	0.04	0.16
4	2	0	0	2	2	6	0.19	0.22	0.03	0.2
5	2	0	0	2	2	6	0.16	0.23	0.04	0.16
6	2	0	0	2	2	6	0.16	0.22	0.04	0.15
7	2	0	0	2	2	6	0.17	0.22	0.04	0.16
8	2	0	0	2	2	6	0.19	0.22	0.03	0.2
9	2	0	0	2	2	6	0.16	0.22	0.05	0.15
10	2	0	0	2	2	6	0.17	0.23	0.05	0.17

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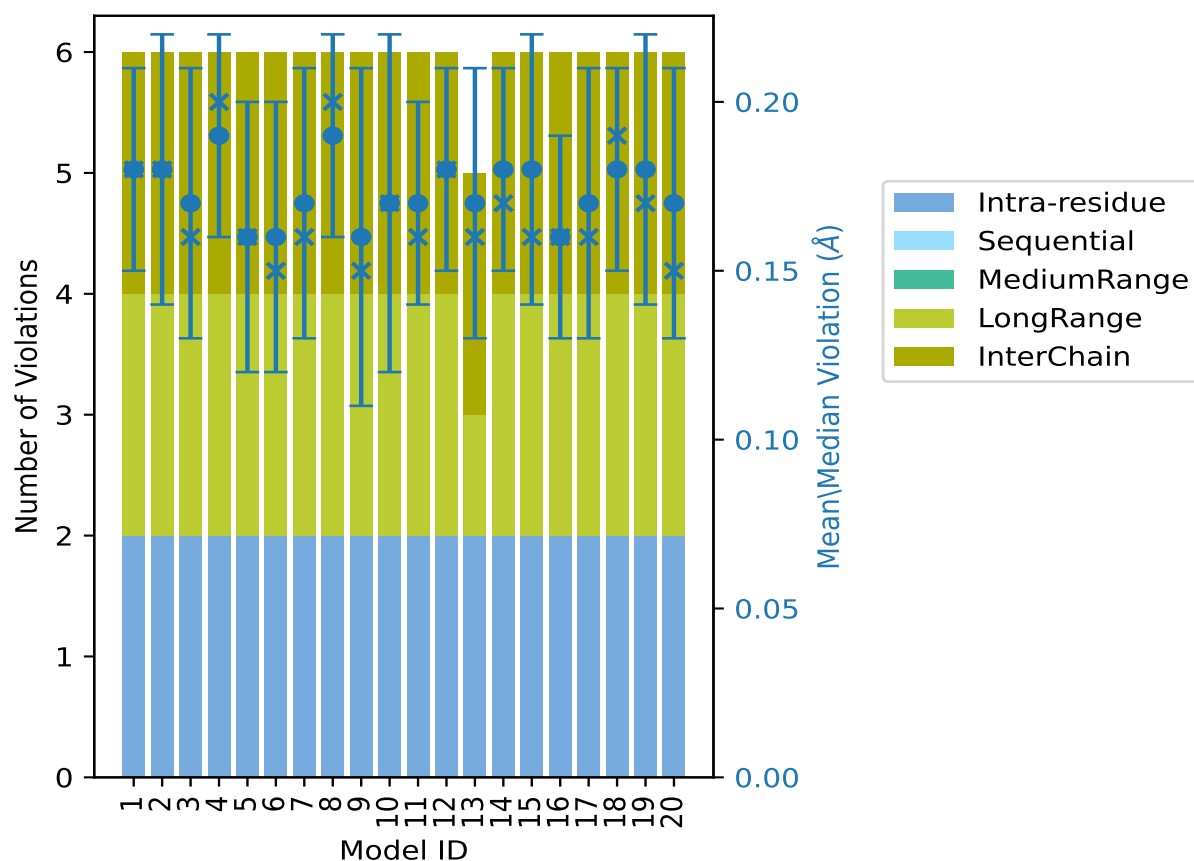
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2	0	0	2	2	6	0.17	0.23	0.03	0.16
12	2	0	0	2	2	6	0.18	0.23	0.03	0.18
13	2	0	0	1	2	5	0.17	0.23	0.04	0.16
14	2	0	0	2	2	6	0.18	0.22	0.03	0.17
15	2	0	0	2	2	6	0.18	0.23	0.04	0.16
16	2	0	0	2	2	6	0.16	0.21	0.03	0.16
17	2	0	0	2	2	6	0.17	0.22	0.04	0.16
18	2	0	0	2	2	6	0.18	0.21	0.03	0.19
19	2	0	0	2	2	6	0.18	0.23	0.04	0.17
20	2	0	0	2	2	6	0.17	0.22	0.04	0.15

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard 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 ⓘ

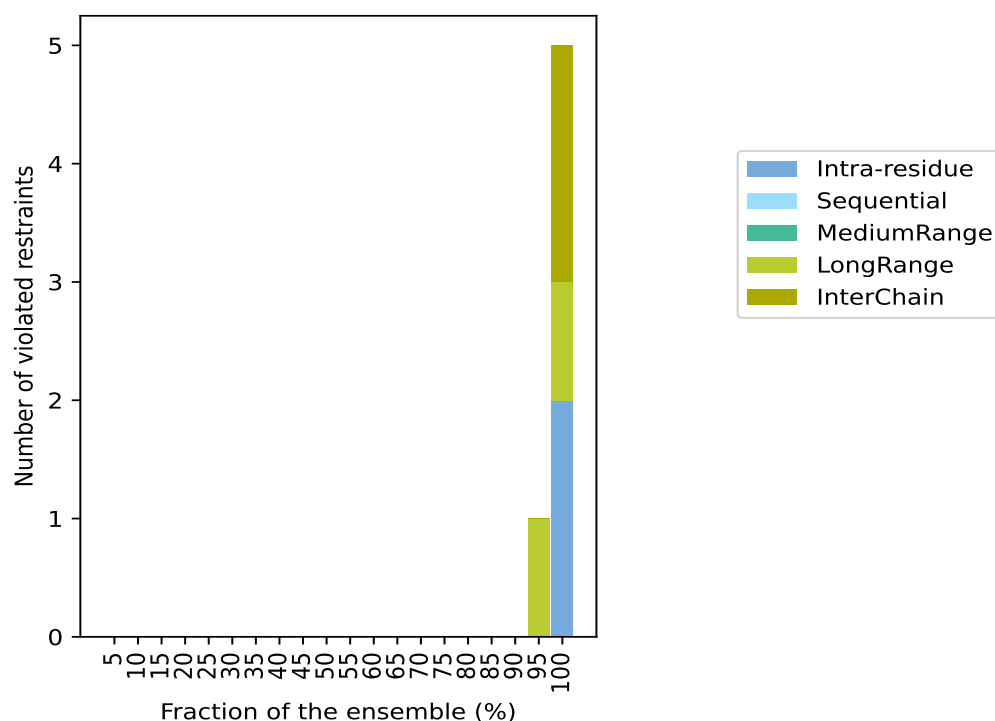
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 18(IR:4, SQ:0, MR:0, LR:6, IC:8) restraints are not violated 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	0	0	0	0	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	1	0	1	19	95.0
2	0	0	1	2	5	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

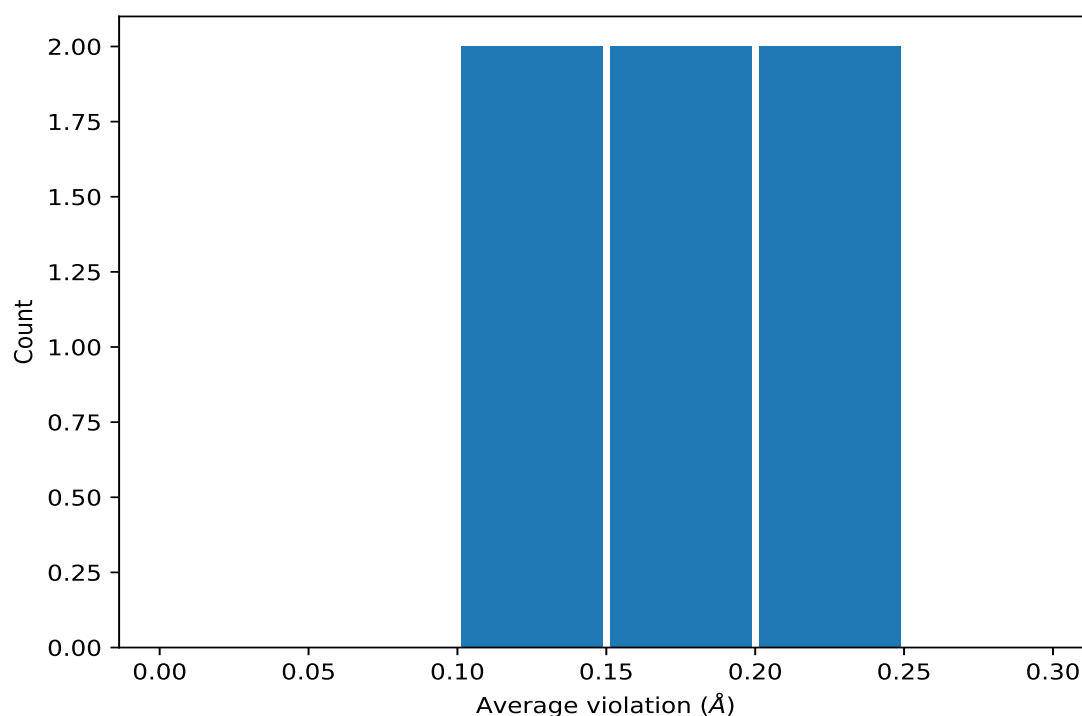
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

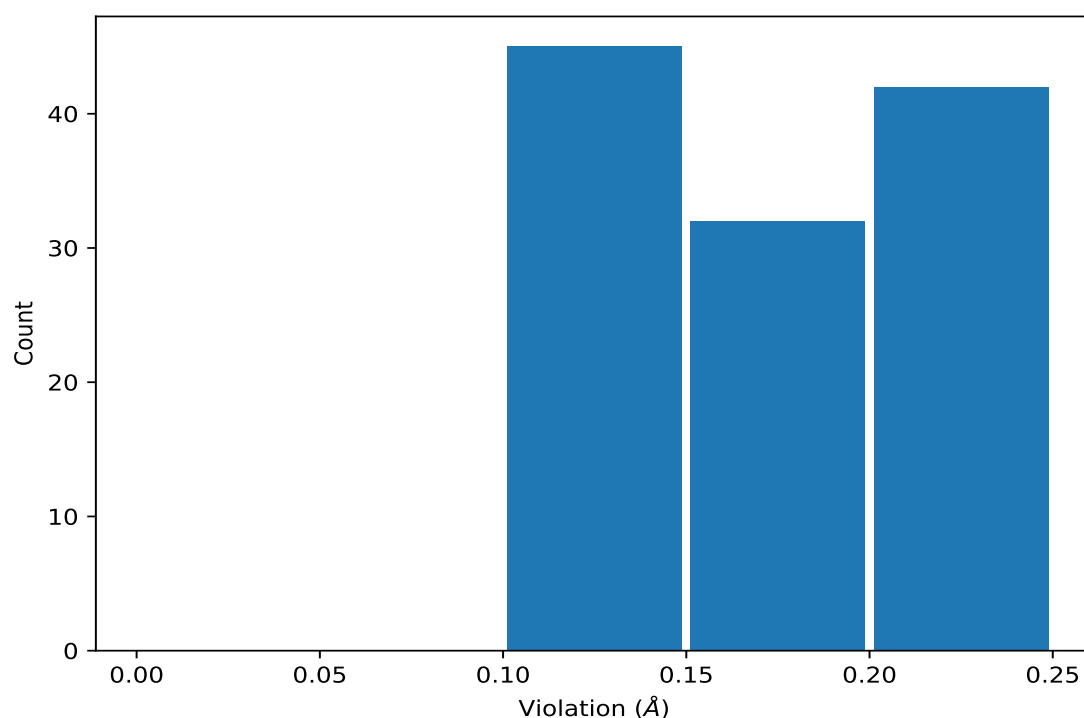
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,8)	1:184:B:TRP:NE1	1:185:A:MET:CE	20	0.22	0.01	0.22
(1,7)	1:184:A:TRP:NE1	1:185:B:MET:CE	20	0.22	0.01	0.22
(1,1)	1:185:A:MET:N	1:185:A:MET:CE	20	0.17	0.02	0.17
(1,2)	1:185:B:MET:N	1:185:B:MET:CE	20	0.17	0.01	0.16
(1,13)	1:184:A:TRP:CD1	1:189:A:LEU:CG	20	0.13	0.01	0.13
(1,14)	1:184:B:TRP:CD1	1:189:B:LEU:CG	19	0.13	0.01	0.13

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:184:B:TRP:NE1	1:185:A:MET:CE	3	0.23
(1,8)	1:184:B:TRP:NE1	1:185:A:MET:CE	11	0.23
(1,8)	1:184:B:TRP:NE1	1:185:A:MET:CE	13	0.23
(1,8)	1:184:B:TRP:NE1	1:185:A:MET:CE	19	0.23
(1,7)	1:184:A:TRP:NE1	1:185:B:MET:CE	2	0.23
(1,7)	1:184:A:TRP:NE1	1:185:B:MET:CE	3	0.23
(1,7)	1:184:A:TRP:NE1	1:185:B:MET:CE	5	0.23
(1,7)	1:184:A:TRP:NE1	1:185:B:MET:CE	10	0.23
(1,7)	1:184:A:TRP:NE1	1:185:B:MET:CE	12	0.23
(1,7)	1:184:A:TRP:NE1	1:185:B:MET:CE	15	0.23

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

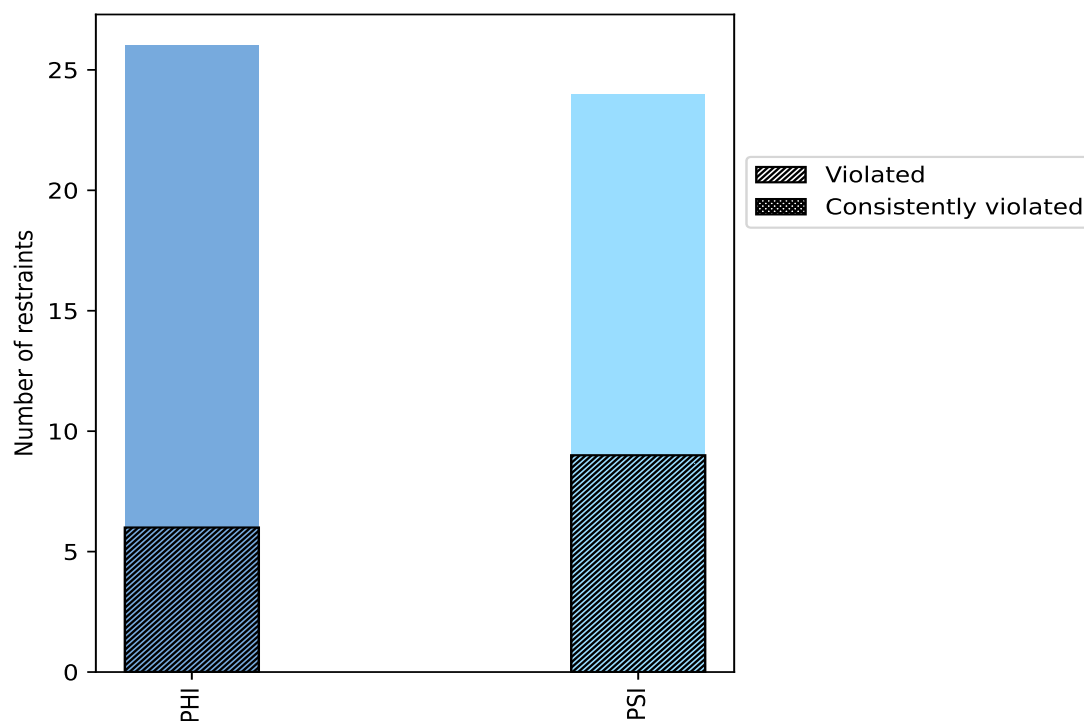
10.1 Summary of dihedral-angle violations [i](#)

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
PHI	26	52.0	6	23.1	12.0	0	0.0	0.0
PSI	24	48.0	9	37.5	18.0	0	0.0	0.0
Total	50	100.0	15	30.0	30.0	0	0.0	0.0

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

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



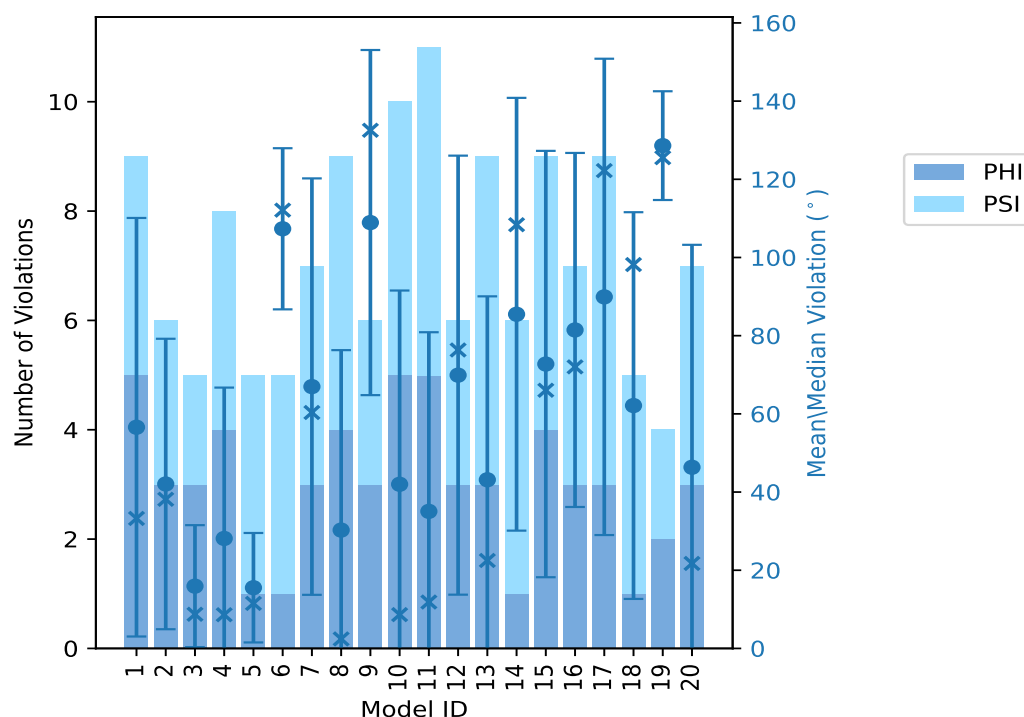
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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 (°)
	PHI	PSI	Total				
1	5	4	9	56.58	136.72	53.53	33.25
2	3	3	6	42.06	91.54	37.15	38.15
3	3	2	5	15.93	44.66	15.6	8.74
4	4	4	8	28.13	95.0	38.59	8.62
5	1	4	5	15.53	36.84	14.0	11.52
6	1	4	5	107.34	139.64	20.61	112.11
7	3	4	7	66.97	145.23	53.26	60.35
8	4	5	9	30.27	116.88	46.03	2.43
9	3	3	6	108.93	139.85	44.14	132.54
10	5	5	10	41.99	136.12	49.56	8.65
11	5	6	11	35.06	129.08	45.82	11.87
12	3	3	6	69.9	127.83	56.15	76.34
13	3	6	9	43.14	126.54	46.92	22.5
14	1	5	6	85.48	143.5	55.35	108.38
15	4	5	9	72.74	146.21	54.53	66.04
16	3	4	7	81.46	148.56	45.28	72.02
17	3	6	9	89.92	147.37	60.92	122.23
18	1	4	5	62.12	106.82	49.46	98.19
19	2	2	4	128.61	149.49	13.91	125.53
20	3	4	7	46.34	135.81	56.9	21.74

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	
PHI	PSI	Total	Count ¹	%
0	3	3	1	5.0
0	0	0	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	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	1	1	10	50.0
1	2	3	11	55.0

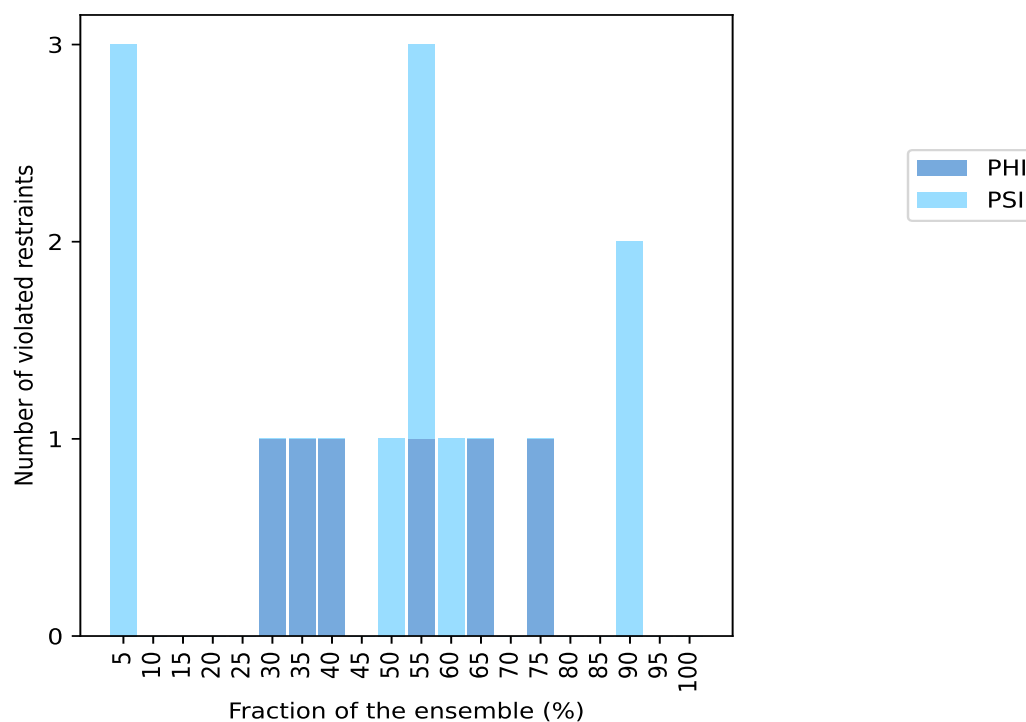
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	1	1	12	60.0
1	0	1	13	65.0
0	0	0	14	70.0
1	0	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	2	2	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

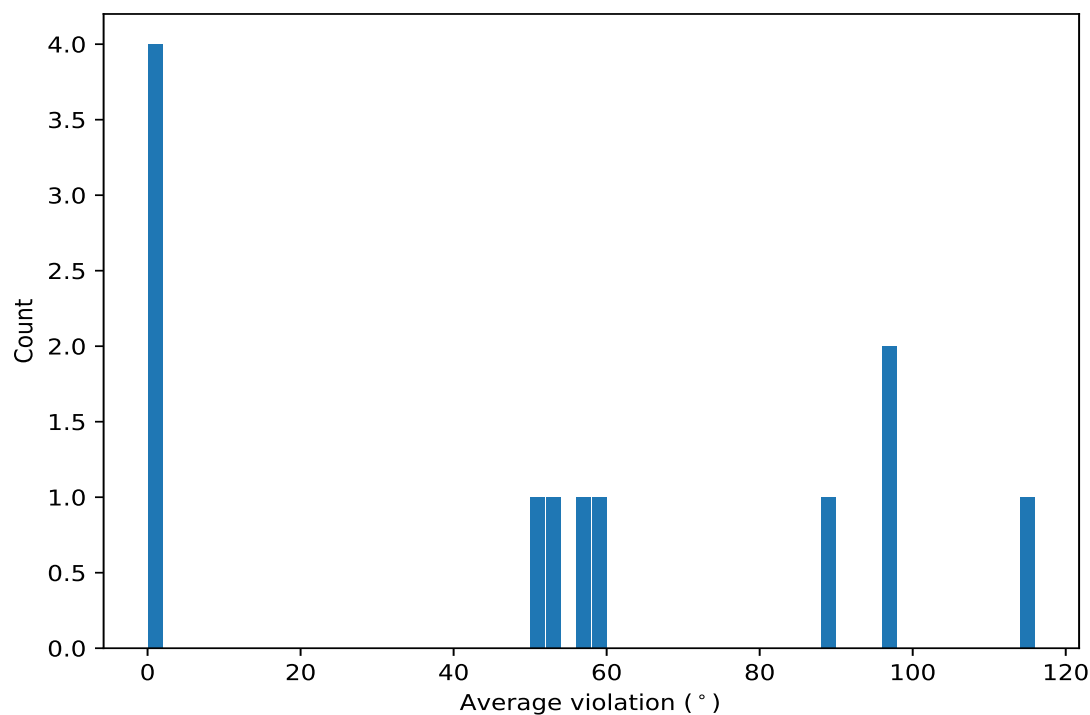


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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 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.

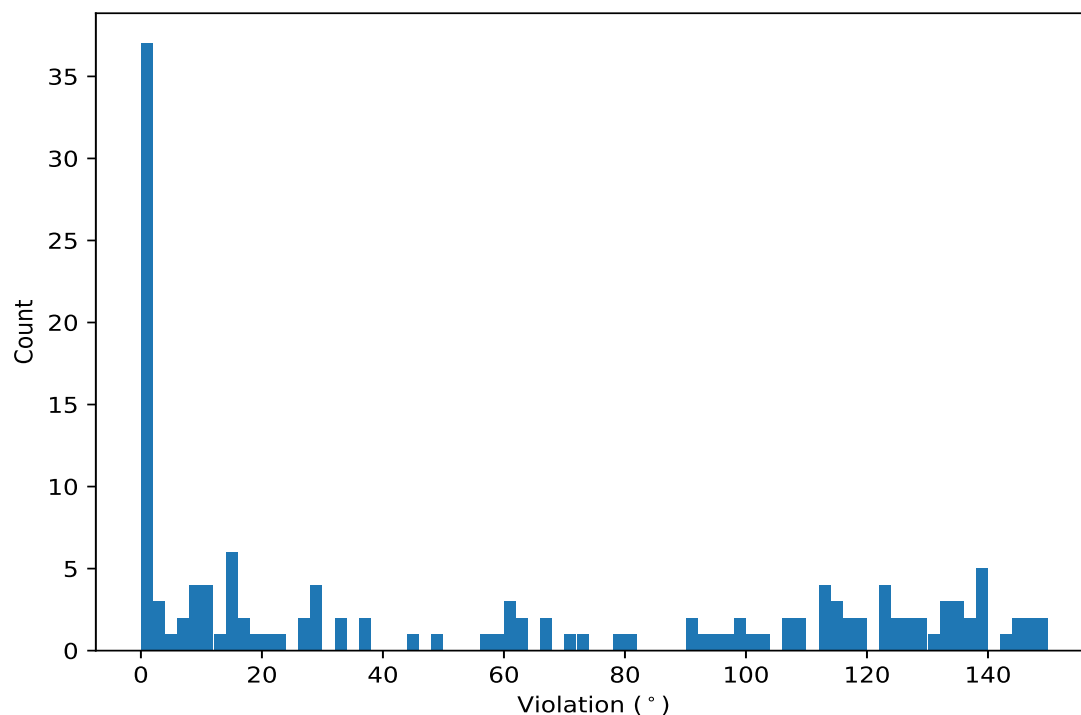
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,40)	1:177:B:ALA:N	1:177:B:ALA:CA	1:177:B:ALA:C	1:178:B:SER:N	18	96.96	37.01	111.3
(1,15)	1:177:A:ALA:N	1:177:A:ALA:CA	1:177:A:ALA:C	1:178:A:SER:N	18	96.01	37.76	110.02
(1,2)	1:176:A:GLN:C	1:177:A:ALA:N	1:177:A:ALA:CA	1:177:A:ALA:C	15	51.97	51.85	28.44
(1,27)	1:176:B:GLN:C	1:177:B:ALA:N	1:177:B:ALA:CA	1:177:B:ALA:C	13	58.37	54.54	21.74
(1,14)	1:176:A:GLN:N	1:176:A:GLN:CA	1:176:A:GLN:C	1:177:A:ALA:N	12	89.93	55.46	128.26
(1,39)	1:176:B:GLN:N	1:176:B:GLN:CA	1:176:B:GLN:C	1:177:B:ALA:N	11	114.22	46.13	139.64
(1,1)	1:175:A:GLU:C	1:176:A:GLN:N	1:176:A:GLN:CA	1:176:A:GLN:C	11	52.5	34.81	60.04
(1,16)	1:183:A:ASN:N	1:183:A:ASN:CA	1:183:A:ASN:C	1:184:A:TRP:N	11	1.44	0.31	1.36
(1,41)	1:183:B:ASN:N	1:183:B:ASN:CA	1:183:B:ASN:C	1:184:B:TRP:N	10	1.54	0.21	1.59
(1,30)	1:184:B:TRP:C	1:185:B:MET:N	1:185:B:MET:CA	1:185:B:MET:C	8	1.39	0.28	1.34

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 (°)
(1,27)	1:176:B:GLN:C	1:177:B:ALA:N	1:177:B:ALA:CA	1:177:B:ALA:C	19	149.49
(1,39)	1:176:B:GLN:N	1:176:B:GLN:CA	1:176:B:GLN:C	1:177:B:ALA:N	16	148.56
(1,39)	1:176:B:GLN:N	1:176:B:GLN:CA	1:176:B:GLN:C	1:177:B:ALA:N	17	147.37
(1,14)	1:176:A:GLN:N	1:176:A:GLN:CA	1:176:A:GLN:C	1:177:A:ALA:N	15	146.21
(1,39)	1:176:B:GLN:N	1:176:B:GLN:CA	1:176:B:GLN:C	1:177:B:ALA:N	7	145.23
(1,39)	1:176:B:GLN:N	1:176:B:GLN:CA	1:176:B:GLN:C	1:177:B:ALA:N	15	145.14
(1,39)	1:176:B:GLN:N	1:176:B:GLN:CA	1:176:B:GLN:C	1:177:B:ALA:N	14	143.5
(1,15)	1:177:A:ALA:N	1:177:A:ALA:CA	1:177:A:ALA:C	1:178:A:SER:N	17	139.88
(1,2)	1:176:A:GLN:C	1:177:A:ALA:N	1:177:A:ALA:CA	1:177:A:ALA:C	9	139.85
(1,39)	1:176:B:GLN:N	1:176:B:GLN:CA	1:176:B:GLN:C	1:177:B:ALA:N	6	139.64