wwPDB NMR Structure Validation Summary Report

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PDB ID	:	8UOZ
BMRB ID	:	31121
Title	:	EmrE structure in the TPP-bound state (WT/E14Q heterodimer)
Authors	:	Li, J.; Sae Her, A.; Besch, A.; Ramirez, B.; Crames, M.; Banigan, J.R.; Mueller, C.; Marsiglia, W.M.; Zhang, Y.; Traaseth, N.J.
Deposited on	:	2023-10-20

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

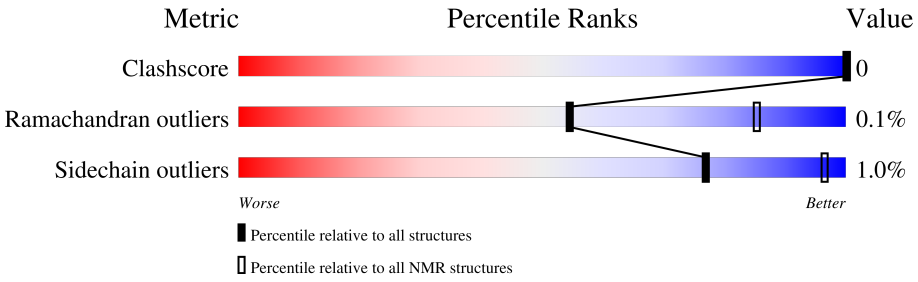
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR, SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 32%.

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	110	93% • 5%
2	B	110	96% •

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 4 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:2-A:106, B:1-B:110 (215)	0.84	4

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

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

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

Cluster number	Models
1	5, 6, 9, 10
2	2, 4
3	1, 8
Single-model clusters	3; 7

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3485 atoms, of which 1776 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SMR family multidrug efflux protein EmrE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	110	1719	564	877	130	141	7	0

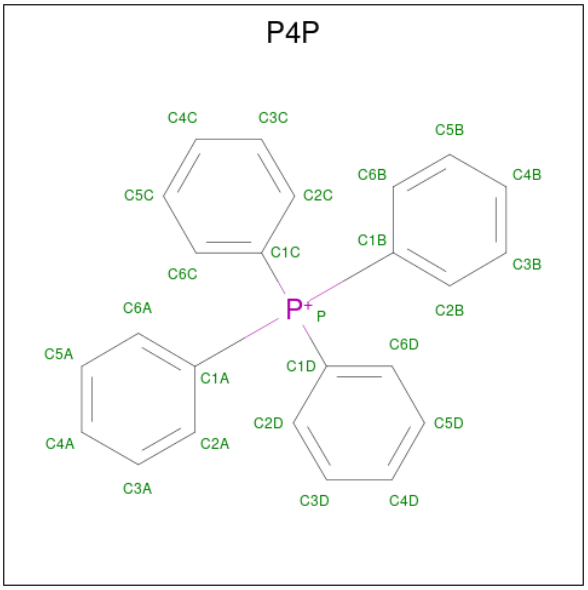
- Molecule 2 is a protein called SMR family multidrug efflux protein EmrE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	110	1721	564	879	131	140	7	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLN	GLU	engineered mutation	UNP A0A2X7QID6

- Molecule 3 is TETRAPHENYLPHOSPHONIUM (three-letter code: P4P) (formula: $C_{24}H_{20}P$).



Mol	Chain	Residues	Atoms			
			Total	C	H	P
3	A	1	45	24	20	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

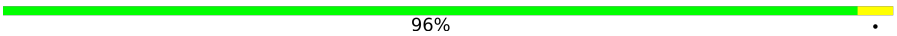
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: SMR family multidrug efflux protein EmrE

Chain A:

• Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:



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

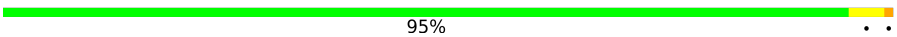
The representative model is number 4. Colouring as in section 4.1 above.

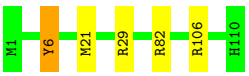
• Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:

• Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:





5 Refinement protocol and experimental data overview

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

Of the 100000 calculated structures, 10 were deposited, based on the following criterion: *back calculated data agree with experimental NMR data.*

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
GROMACS	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	1454
Number of shifts mapped to atoms	1444
Number of unparsed shifts	0
Number of shifts with mapping errors	10
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	32%

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

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P4P

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	0.73±0.01	0±0/825 (0.0± 0.0%)	0.99±0.03	4±1/1128 (0.3± 0.1%)
2	B	0.73±0.01	0±0/865 (0.0± 0.0%)	1.04±0.02	6±1/1180 (0.5± 0.1%)
All	All	0.73	0/16900 (0.0%)	1.01	97/23080 (0.4%)

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	A	0.0±0.0	0.3±0.5
2	B	0.0±0.0	0.2±0.4
All	All	0	5

There are no bond-length outliers.

5 of 17 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
2	B	29	ARG	NE-CZ-NH1	11.48	126.04	120.30	6	10
2	B	29	ARG	NE-CZ-NH2	-10.87	114.86	120.30	5	7
1	A	82	ARG	NE-CZ-NH1	10.45	125.53	120.30	10	8
1	A	106	ARG	NE-CZ-NH1	9.85	125.23	120.30	7	8
2	B	82	ARG	NE-CZ-NH1	9.20	124.90	120.30	7	10

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)
2	B	60	TYR	Sidechain	1
2	B	29	ARG	Sidechain	1
1	A	4	TYR	Sidechain	1
1	A	106	ARG	Sidechain	1
1	A	29	ARG	Sidechain	1

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	803	840	840	0±0
2	B	842	879	879	0±0
All	All	16700	17390	17390	-

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 -.

There are no clashes.

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	105/110 (95%)	102±1 (97±1%)	3±1 (3±1%)	0±0 (0±0%)	54 85
2	B	108/110 (98%)	105±1 (97±1%)	3±1 (3±1%)	0±0 (0±0%)	50 82
All	All	2130/2200 (97%)	2068 (97%)	59 (3%)	3 (0%)	54 85

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	25	GLU	2
1	A	27	PHE	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	84/89 (94%)	84±1 (99±1%)	0±1 (1±1%)	86 97
2	B	89/89 (100%)	88±1 (99±1%)	1±1 (1±1%)	70 96
All	All	1730/1780 (97%)	1713 (99%)	17 (1%)	77 96

5 of 10 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)
2	B	6	TYR	5
2	B	81	GLN	2
2	B	110	HIS	2
1	A	21	MET	2
1	A	56	THR	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 (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	P4P	A	201	-	28,28,28	1.94±0.04	12±0 (42±1%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	P4P	A	201	-	38,38,38	1.34±0.08	5±1 (12±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P4P	A	201	-	-	0±0,24,24,24	0±0,4,4,4

5 of 12 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
3	A	201	P4P	P-C1B	4.16	1.87	1.79	6	10
3	A	201	P4P	P-C1D	4.12	1.87	1.79	7	10
3	A	201	P4P	P-C1A	3.89	1.86	1.79	2	10
3	A	201	P4P	P-C1C	3.76	1.86	1.79	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	201	P4P	C6C-C1C	3.07	1.45	1.39	2	10

5 of 10 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
3	A	201	P4P	C2C-C1C-C6C	3.27	114.15	118.92	1	10
3	A	201	P4P	C1D-P-C1A	3.12	115.68	109.43	2	1
3	A	201	P4P	C2B-C1B-C6B	3.01	114.53	118.92	8	10
3	A	201	P4P	C2D-C1D-C6D	3.00	114.55	118.92	5	10
3	A	201	P4P	C1C-P-C1A	2.87	103.69	109.43	2	1

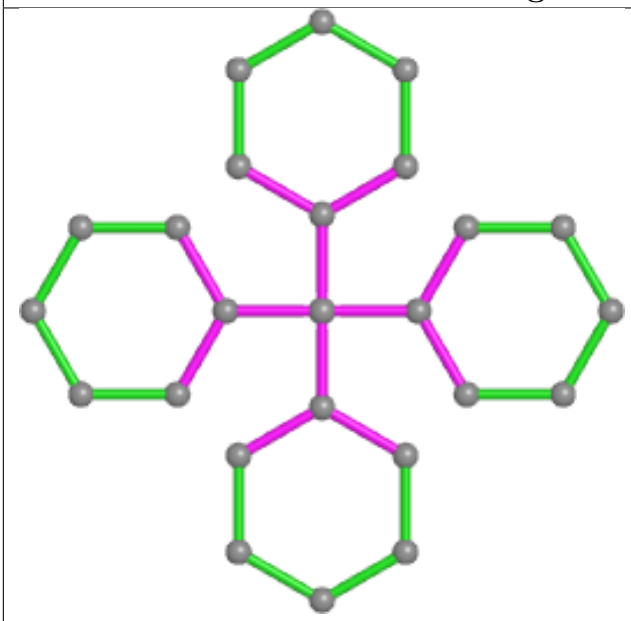
There are no chirality outliers.

There are no torsion outliers.

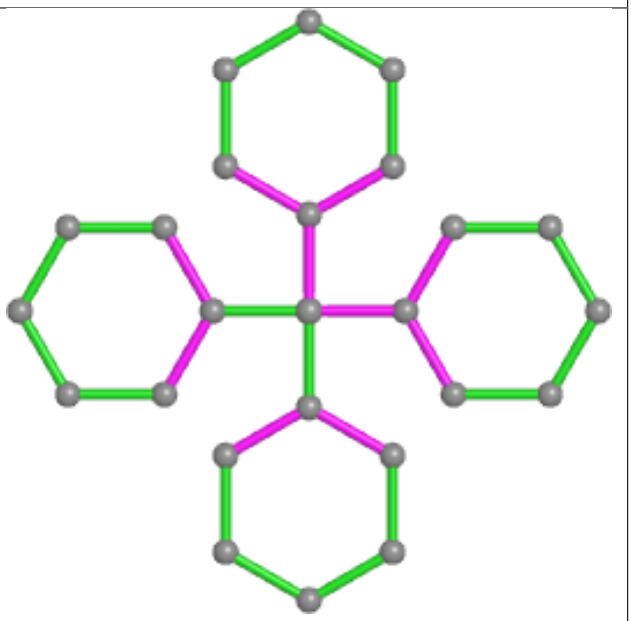
There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

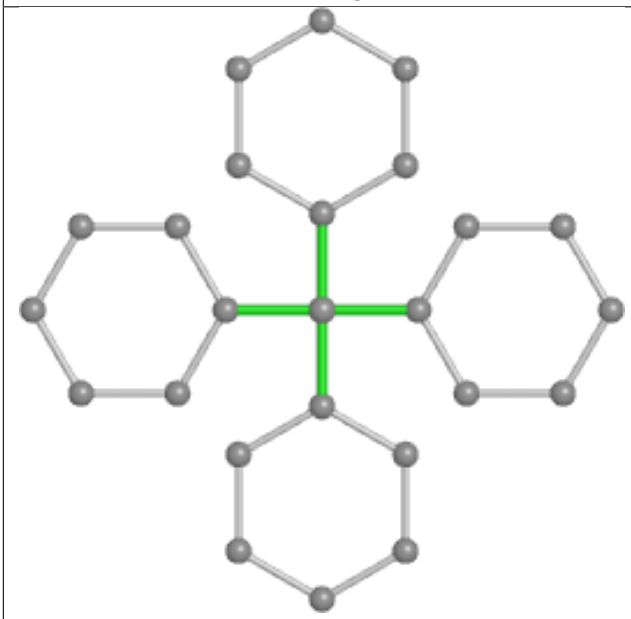
Ligand P4P A 201



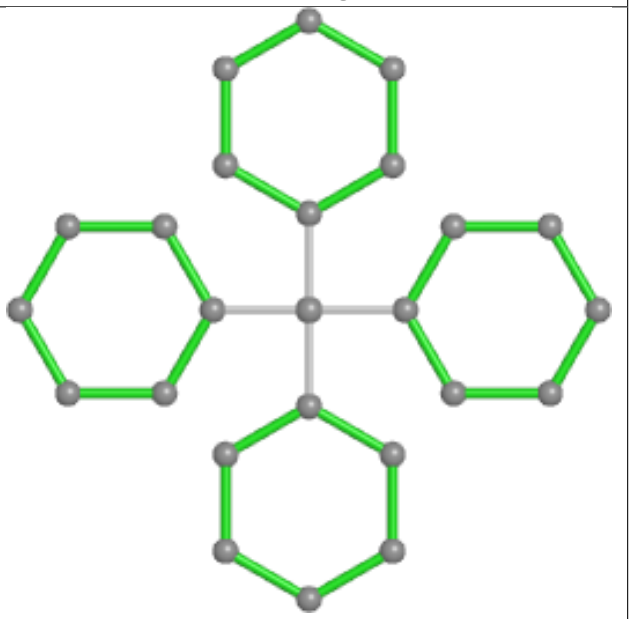
Bond lengths



Bond angles



Torsions



Rings

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 32% for the well-defined parts and 32% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1454
Number of shifts mapped to atoms	1444
Number of unparsed shifts	0
Number of shifts with mapping errors	10
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chemical shift has been reported more than once. First 5 (of 10) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	TYR	CA	62.190	.	.
1	A	4	TYR	C	177.827	.	.
1	A	4	TYR	N	117.100	.	.
1	A	5	ILE	CA	65.059	.	.
1	A	5	ILE	N	121.648	.	.
1	A	6	TYR	CA	62.611	.	.
1	A	6	TYR	N	116.948	.	.
1	A	7	LEU	CA	57.747	.	.
1	A	7	LEU	C	177.983	.	.
1	A	7	LEU	N	118.187	.	.
1	A	8	GLY	CA	47.681	.	.
1	A	8	GLY	C	175.103	.	.
1	A	8	GLY	N	105.222	.	.
1	A	9	GLY	CA	48.091	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	GLY	C	173.557	.	.
1	A	9	GLY	N	107.880	.	.
1	A	10	ALA	CA	55.572	.	.
1	A	10	ALA	C	180.583	.	.
1	A	10	ALA	N	125.582	.	.
1	A	11	ILE	CA	64.494	.	.
1	A	11	ILE	C	177.049	.	.
1	A	11	ILE	N	121.022	.	.
1	A	12	LEU	CA	57.699	.	.
1	A	12	LEU	C	177.840	.	.
1	A	12	LEU	N	117.990	.	.
1	A	13	ALA	CA	55.649	.	.
1	A	13	ALA	C	179.266	.	.
1	A	13	ALA	N	118.196	.	.
1	A	14	GLU	CA	61.513	.	.
1	A	14	GLU	N	118.642	.	.
1	A	15	VAL	CA	66.076	.	.
1	A	15	VAL	C	179.490	.	.
1	A	15	VAL	N	117.540	.	.
1	A	16	ILE	CA	66.412	.	.
1	A	16	ILE	C	177.764	.	.
1	A	16	ILE	N	122.486	.	.
1	A	17	GLY	CA	48.318	.	.
1	A	17	GLY	N	110.174	.	.
1	A	18	THR	C	175.562	.	.
1	A	19	THR	CA	67.953	.	.
1	A	19	THR	C	177.556	.	.
1	A	19	THR	N	121.899	.	.
1	A	20	LEU	CA	58.032	.	.
1	A	20	LEU	C	178.498	.	.
1	A	20	LEU	N	122.288	.	.
1	A	21	MET	CA	58.946	.	.
1	A	21	MET	C	182.274	.	.
1	A	21	MET	N	122.423	.	.
1	A	22	LYS	CA	60.193	.	.
1	A	22	LYS	C	178.389	.	.
1	A	22	LYS	N	125.930	.	.
1	A	23	PHE	CA	58.075	.	.
1	A	23	PHE	C	175.256	.	.
1	A	23	PHE	N	120.724	.	.
1	A	24	SER	CA	60.400	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	24	SER	C	173.420	.	.
1	A	24	SER	N	112.362	.	.
1	A	25	GLU	CA	55.928	.	.
1	A	25	GLU	CB	26.387	.	.
1	A	25	GLU	C	178.257	.	.
1	A	25	GLU	N	120.706	.	.
1	A	26	GLY	CA	46.139	.	.
1	A	26	GLY	C	175.288	.	.
1	A	26	GLY	N	112.795	.	.
1	A	27	PHE	CA	60.164	.	.
1	A	27	PHE	N	112.526	.	.
1	A	28	THR	CA	62.023	.	.
1	A	28	THR	C	175.043	.	.
1	A	28	THR	N	101.856	.	.
1	A	29	ARG	CA	54.308	.	.
1	A	29	ARG	CB	31.793	.	.
1	A	29	ARG	C	177.707	.	.
1	A	29	ARG	N	119.114	.	.
1	A	30	LEU	CA	59.916	.	.
1	A	30	LEU	CB	41.863	.	.
1	A	30	LEU	C	177.165	.	.
1	A	30	LEU	N	131.921	.	.
1	A	31	TRP	CA	61.940	.	.
1	A	31	TRP	N	119.196	.	.
1	A	32	PRO	CA	65.825	.	.
1	A	32	PRO	C	178.207	.	.
1	A	33	SER	CA	64.130	.	.
1	A	33	SER	C	175.388	.	.
1	A	33	SER	N	112.720	.	.
1	A	34	VAL	CA	67.114	.	.
1	A	34	VAL	C	178.125	.	.
1	A	34	VAL	N	122.434	.	.
1	A	35	GLY	CA	48.927	.	.
1	A	35	GLY	C	174.895	.	.
1	A	35	GLY	N	104.783	.	.
1	A	36	THR	CA	68.856	.	.
1	A	36	THR	C	175.316	.	.
1	A	36	THR	N	121.101	.	.
1	A	37	ILE	CA	66.549	.	.
1	A	37	ILE	N	123.500	.	.
1	A	38	ILE	CA	66.393	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	38	ILE	C	177.941	.	.
1	A	38	ILE	N	120.191	.	.
1	A	39	CYS	CA	65.739	.	.
1	A	39	CYS	C	177.904	.	.
1	A	39	CYS	N	116.864	.	.
1	A	40	TYR	CA	59.365	.	.
1	A	40	TYR	N	119.185	.	.
1	A	41	CYS	CA	65.755	.	.
1	A	42	ALA	CA	55.582	.	.
1	A	42	ALA	C	178.760	.	.
1	A	42	ALA	N	120.734	.	.
1	A	43	SER	CA	62.583	.	.
1	A	43	SER	C	177.483	.	.
1	A	43	SER	N	111.572	.	.
1	A	44	PHE	CA	64.087	.	.
1	A	44	PHE	C	175.184	.	.
1	A	44	PHE	N	115.282	.	.
1	A	47	LEU	CA	57.742	.	.
1	A	47	LEU	C	179.872	.	.
1	A	47	LEU	N	121.230	.	.
1	A	48	ALA	CA	54.711	.	.
1	A	48	ALA	C	178.789	.	.
1	A	48	ALA	N	122.975	.	.
1	A	49	GLN	CA	55.104	.	.
1	A	49	GLN	N	114.028	.	.
1	A	50	THR	CA	64.974	.	.
1	A	50	THR	C	177.439	.	.
1	A	51	LEU	CA	55.921	.	.
1	A	51	LEU	C	176.775	.	.
1	A	51	LEU	N	122.295	.	.
1	A	52	ALA	CA	52.921	.	.
1	A	52	ALA	C	177.688	.	.
1	A	52	ALA	N	119.929	.	.
1	A	53	TYR	CA	58.345	.	.
1	A	53	TYR	C	174.830	.	.
1	A	53	TYR	N	113.174	.	.
1	A	54	ILE	CA	57.780	.	.
1	A	54	ILE	N	120.393	.	.
1	A	56	THR	CA	66.093	.	.
1	A	56	THR	C	176.419	.	.
1	A	57	GLY	CA	47.201	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	GLY	C	176.779	.	.
1	A	57	GLY	N	109.130	.	.
1	A	58	ILE	CA	65.347	.	.
1	A	58	ILE	CB	37.662	.	.
1	A	58	ILE	C	176.718	.	.
1	A	58	ILE	N	120.998	.	.
1	A	59	ALA	CA	55.641	.	.
1	A	59	ALA	C	179.040	.	.
1	A	59	ALA	N	120.163	.	.
1	A	60	TYR	CA	61.679	.	.
1	A	60	TYR	C	179.256	.	.
1	A	60	TYR	N	117.070	.	.
1	A	61	ALA	CA	55.842	.	.
1	A	61	ALA	C	178.746	.	.
1	A	61	ALA	N	122.172	.	.
1	A	62	ILE	CA	65.830	.	.
1	A	62	ILE	C	178.495	.	.
1	A	62	ILE	N	116.081	.	.
1	A	63	TRP	CA	60.353	.	.
1	A	63	TRP	C	180.000	.	.
1	A	63	TRP	N	119.973	.	.
1	A	64	SER	CA	63.169	.	.
1	A	64	SER	C	176.187	.	.
1	A	64	SER	N	111.280	.	.
1	A	65	GLY	CA	47.982	.	.
1	A	65	GLY	C	173.458	.	.
1	A	65	GLY	N	105.841	.	.
1	A	66	VAL	CA	66.562	.	.
1	A	66	VAL	C	178.288	.	.
1	A	66	VAL	N	117.527	.	.
1	A	67	GLY	CA	47.307	.	.
1	A	67	GLY	C	175.089	.	.
1	A	67	GLY	N	109.251	.	.
1	A	68	ILE	CA	66.399	.	.
1	A	68	ILE	C	178.394	.	.
1	A	68	ILE	N	119.706	.	.
1	A	69	VAL	CA	66.228	.	.
1	A	69	VAL	N	118.930	.	.
1	A	70	LEU	CA	58.486	.	.
1	A	70	LEU	C	179.073	.	.
1	A	71	ILE	CA	62.008	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	ILE	C	179.501	.	.
1	A	71	ILE	N	119.256	.	.
1	A	72	SER	CA	63.234	.	.
1	A	72	SER	C	177.425	.	.
1	A	72	SER	N	119.633	.	.
1	A	73	LEU	CA	58.464	.	.
1	A	73	LEU	N	123.761	.	.
1	A	74	LEU	CA	58.265	.	.
1	A	74	LEU	CB	41.820	.	.
1	A	74	LEU	C	179.195	.	.
1	A	74	LEU	N	119.774	.	.
1	A	75	SER	CA	62.954	.	.
1	A	75	SER	C	177.875	.	.
1	A	75	SER	N	115.797	.	.
1	A	76	TRP	CA	57.964	.	.
1	A	76	TRP	C	178.947	.	.
1	A	76	TRP	N	125.676	.	.
1	A	77	GLY	CA	47.849	.	.
1	A	77	GLY	C	173.029	.	.
1	A	77	GLY	N	105.220	.	.
1	A	78	PHE	CA	61.290	.	.
1	A	78	PHE	C	176.554	.	.
1	A	78	PHE	N	112.513	.	.
1	A	79	PHE	CA	55.344	.	.
1	A	79	PHE	C	176.735	.	.
1	A	79	PHE	N	111.597	.	.
1	A	80	GLY	CA	46.699	.	.
1	A	80	GLY	C	174.739	.	.
1	A	80	GLY	N	109.745	.	.
1	A	81	GLN	CA	57.360	.	.
1	A	81	GLN	C	174.759	.	.
1	A	81	GLN	N	118.981	.	.
1	A	82	ARG	CA	55.168	.	.
1	A	82	ARG	CB	31.864	.	.
1	A	82	ARG	C	175.269	.	.
1	A	82	ARG	N	127.712	.	.
1	A	83	LEU	CA	52.679	.	.
1	A	83	LEU	C	175.080	.	.
1	A	84	ASP	CA	50.970	.	.
1	A	84	ASP	CB	41.550	.	.
1	A	84	ASP	C	175.185	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	84	ASP	N	119.842	.	.
1	A	85	LEU	CA	59.484	.	.
1	A	85	LEU	N	118.079	.	.
1	A	86	PRO	CA	66.216	.	.
1	A	86	PRO	C	177.918	.	.
1	A	87	ALA	CA	55.964	.	.
1	A	87	ALA	C	178.981	.	.
1	A	87	ALA	N	117.504	.	.
1	A	88	ILE	CA	65.426	.	.
1	A	88	ILE	N	117.667	.	.
1	A	89	ILE	CA	64.573	.	.
1	A	89	ILE	C	178.413	.	.
1	A	89	ILE	N	118.603	.	.
1	A	90	GLY	CA	47.904	.	.
1	A	90	GLY	C	176.044	.	.
1	A	90	GLY	N	107.189	.	.
1	A	91	MET	CA	60.447	.	.
1	A	91	MET	N	120.694	.	.
1	A	96	ALA	C	179.078	.	.
1	A	97	GLY	CA	49.082	.	.
1	A	97	GLY	N	104.855	.	.
1	A	98	VAL	CA	67.219	.	.
1	A	98	VAL	N	119.880	.	.
1	A	100	ILE	C	178.712	.	.
1	A	101	ILE	CA	65.618	.	.
1	A	101	ILE	C	177.202	.	.
1	A	101	ILE	N	117.848	.	.
1	A	102	ASN	CA	56.371	.	.
1	A	102	ASN	C	177.190	.	.
1	A	102	ASN	N	114.456	.	.
1	A	103	LEU	CA	55.988	.	.
1	A	103	LEU	N	114.137	.	.
1	A	104	LEU	CA	55.222	.	.
1	A	104	LEU	C	177.028	.	.
1	A	104	LEU	N	113.711	.	.
1	A	105	SER	CA	58.558	.	.
1	A	105	SER	CB	64.356	.	.
1	A	105	SER	C	176.338	.	.
1	A	105	SER	N	112.371	.	.
1	A	106	ARG	CA	54.478	.	.
1	A	106	ARG	CB	31.040	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	ARG	C	177.445	.	.
1	A	106	ARG	N	128.105	.	.
1	B	7	LEU	C	178.956	.	.
1	B	8	GLY	CA	47.735	.	.
1	B	8	GLY	C	175.753	.	.
1	B	8	GLY	N	106.933	.	.
1	B	9	GLY	CA	48.226	.	.
1	B	9	GLY	C	174.476	.	.
1	B	9	GLY	N	109.941	.	.
1	B	10	ALA	CA	55.518	.	.
1	B	10	ALA	C	182.562	.	.
1	B	10	ALA	N	124.576	.	.
1	B	11	ILE	CA	65.693	.	.
1	B	11	ILE	C	176.577	.	.
1	B	11	ILE	N	123.474	.	.
1	B	12	LEU	CA	58.540	.	.
1	B	12	LEU	C	178.283	.	.
1	B	12	LEU	N	121.103	.	.
1	B	13	ALA	CA	55.775	.	.
1	B	13	ALA	C	179.119	.	.
1	B	13	ALA	N	118.672	.	.
1	B	14	GLN	CA	59.869	.	.
1	B	14	GLN	C	176.722	.	.
1	B	14	GLN	N	116.282	.	.
1	B	15	VAL	CA	65.879	.	.
1	B	15	VAL	C	179.667	.	.
1	B	15	VAL	N	117.862	.	.
1	B	16	ILE	CA	65.930	.	.
1	B	16	ILE	N	122.791	.	.
1	B	17	GLY	CA	48.311	.	.
1	B	17	GLY	C	174.692	.	.
1	B	17	GLY	N	107.083	.	.
1	B	18	THR	CA	65.739	.	.
1	B	18	THR	N	119.925	.	.
1	B	19	THR	CA	67.989	.	.
1	B	19	THR	C	175.956	.	.
1	B	20	LEU	CA	58.181	.	.
1	B	20	LEU	C	179.203	.	.
1	B	20	LEU	N	120.595	.	.
1	B	21	MET	CA	59.443	.	.
1	B	21	MET	C	181.074	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	21	MET	N	120.995	.	.
1	B	22	LYS	CA	58.889	.	.
1	B	22	LYS	N	122.148	.	.
1	B	23	PHE	CA	58.496	.	.
1	B	23	PHE	CB	39.517	.	.
1	B	23	PHE	C	175.562	.	.
1	B	23	PHE	N	120.467	.	.
1	B	24	SER	CA	60.181	.	.
1	B	24	SER	C	173.528	.	.
1	B	24	SER	N	114.763	.	.
1	B	25	GLU	CA	55.913	.	.
1	B	25	GLU	CB	26.962	.	.
1	B	25	GLU	C	178.206	.	.
1	B	25	GLU	N	122.643	.	.
1	B	26	GLY	CA	47.423	.	.
1	B	26	GLY	C	174.665	.	.
1	B	26	GLY	N	113.283	.	.
1	B	27	PHE	CA	58.702	.	.
1	B	27	PHE	N	111.980	.	.
1	B	28	THR	CA	62.167	.	.
1	B	28	THR	C	175.177	.	.
1	B	28	THR	N	101.636	.	.
1	B	29	ARG	CA	53.982	.	.
1	B	29	ARG	CB	31.288	.	.
1	B	29	ARG	C	177.714	.	.
1	B	29	ARG	N	119.321	.	.
1	B	30	LEU	CA	59.929	.	.
1	B	30	LEU	CB	41.877	.	.
1	B	30	LEU	C	177.484	.	.
1	B	30	LEU	N	131.137	.	.
1	B	31	TRP	CA	62.000	.	.
1	B	31	TRP	CB	27.043	.	.
1	B	31	TRP	N	118.930	.	.
1	B	32	PRO	CA	65.711	.	.
1	B	32	PRO	C	179.117	.	.
1	B	33	SER	CA	63.918	.	.
1	B	33	SER	C	175.220	.	.
1	B	33	SER	N	115.348	.	.
1	B	34	VAL	CA	67.110	.	.
1	B	34	VAL	CB	32.053	.	.
1	B	34	VAL	C	178.394	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	34	VAL	N	122.603	.	.
1	B	35	GLY	CA	48.516	.	.
1	B	35	GLY	C	174.782	.	.
1	B	35	GLY	N	103.923	.	.
1	B	36	THR	CA	68.790	.	.
1	B	36	THR	N	120.536	.	.
1	B	37	ILE	CA	66.504	.	.
1	B	37	ILE	N	119.524	.	.
1	B	39	CYS	CA	65.576	.	.
1	B	40	TYR	CA	57.689	.	.
1	B	40	TYR	N	119.097	.	.
1	B	42	ALA	CA	55.421	.	.
1	B	42	ALA	C	178.656	.	.
1	B	43	SER	CA	63.250	.	.
1	B	43	SER	C	177.398	.	.
1	B	43	SER	N	111.444	.	.
1	B	44	PHE	CA	60.475	.	.
1	B	44	PHE	N	115.774	.	.
1	B	47	LEU	CA	57.541	.	.
1	B	47	LEU	C	179.730	.	.
1	B	48	ALA	CA	55.188	.	.
1	B	48	ALA	CB	18.483	.	.
1	B	48	ALA	C	180.360	.	.
1	B	48	ALA	N	121.033	.	.
1	B	49	GLN	CA	55.746	.	.
1	B	49	GLN	N	114.283	.	.
1	B	50	THR	C	177.236	.	.
1	B	51	LEU	CA	55.804	.	.
1	B	51	LEU	C	176.905	.	.
1	B	51	LEU	N	117.679	.	.
1	B	52	ALA	CA	52.937	.	.
1	B	52	ALA	C	177.541	.	.
1	B	52	ALA	N	119.912	.	.
1	B	53	TYR	CA	58.440	.	.
1	B	53	TYR	C	174.612	.	.
1	B	53	TYR	N	113.009	.	.
1	B	54	ILE	CA	57.985	.	.
1	B	54	ILE	N	120.300	.	.
1	B	55	PRO	CA	63.216	.	.
1	B	55	PRO	C	176.865	.	.
1	B	56	THR	CA	67.268	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	56	THR	C	176.513	.	.
1	B	56	THR	N	124.839	.	.
1	B	57	GLY	CA	47.659	.	.
1	B	57	GLY	N	106.646	.	.
1	B	58	ILE	CA	65.020	.	.
1	B	58	ILE	C	177.289	.	.
1	B	59	ALA	CA	55.994	.	.
1	B	59	ALA	CB	17.899	.	.
1	B	59	ALA	C	179.017	.	.
1	B	59	ALA	N	122.334	.	.
1	B	60	TYR	CA	62.197	.	.
1	B	60	TYR	N	117.458	.	.
1	B	61	ALA	CA	55.847	.	.
1	B	61	ALA	N	121.915	.	.
1	B	62	ILE	CA	66.912	.	.
1	B	62	ILE	C	177.465	.	.
1	B	62	ILE	N	117.179	.	.
1	B	63	TRP	CA	61.190	.	.
1	B	63	TRP	C	178.594	.	.
1	B	63	TRP	N	120.578	.	.
1	B	64	SER	CA	60.537	.	.
1	B	64	SER	C	177.227	.	.
1	B	64	SER	N	111.527	.	.
1	B	65	GLY	CA	47.161	.	.
1	B	65	GLY	C	175.098	.	.
1	B	65	GLY	N	108.792	.	.
1	B	66	VAL	CA	66.684	.	.
1	B	66	VAL	N	120.155	.	.
1	B	67	GLY	CA	47.627	.	.
1	B	67	GLY	C	174.805	.	.
1	B	68	ILE	CA	62.158	.	.
1	B	68	ILE	N	119.193	.	.
1	B	69	VAL	CA	65.663	.	.
1	B	69	VAL	N	117.803	.	.
1	B	70	LEU	CA	58.248	.	.
1	B	70	LEU	N	116.913	.	.
1	B	73	LEU	C	179.299	.	.
1	B	74	LEU	CA	57.828	.	.
1	B	74	LEU	C	179.028	.	.
1	B	74	LEU	N	120.995	.	.
1	B	75	SER	CA	62.312	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	75	SER	C	177.274	.	.
1	B	75	SER	N	116.476	.	.
1	B	76	TRP	CA	59.045	.	.
1	B	76	TRP	N	125.095	.	.
1	B	78	PHE	C	176.921	.	.
1	B	79	PHE	CA	56.006	.	.
1	B	79	PHE	N	113.689	.	.
1	B	83	LEU	C	174.931	.	.
1	B	84	ASP	CA	51.073	.	.
1	B	84	ASP	CB	41.435	.	.
1	B	84	ASP	C	175.159	.	.
1	B	84	ASP	N	119.990	.	.
1	B	85	LEU	CA	59.461	.	.
1	B	85	LEU	CB	38.626	.	.
1	B	85	LEU	N	118.407	.	.
1	B	86	PRO	CA	66.600	.	.
1	B	86	PRO	CB	31.482	.	.
1	B	86	PRO	C	177.594	.	.
1	B	87	ALA	CA	55.815	.	.
1	B	87	ALA	CB	17.747	.	.
1	B	87	ALA	C	179.220	.	.
1	B	87	ALA	N	117.509	.	.
1	B	88	ILE	CA	65.436	.	.
1	B	88	ILE	C	178.257	.	.
1	B	88	ILE	N	118.003	.	.
1	B	89	ILE	CA	65.953	.	.
1	B	89	ILE	C	178.134	.	.
1	B	89	ILE	N	118.428	.	.
1	B	90	GLY	CA	47.892	.	.
1	B	90	GLY	C	175.655	.	.
1	B	90	GLY	N	106.542	.	.
1	B	91	MET	CA	60.252	.	.
1	B	91	MET	N	119.789	.	.
1	B	95	CYS	CA	64.744	.	.
1	B	95	CYS	C	176.472	.	.
1	B	96	ALA	CA	55.390	.	.
1	B	96	ALA	N	119.791	.	.
1	B	100	ILE	C	179.052	.	.
1	B	101	ILE	CA	65.274	.	.
1	B	101	ILE	C	178.160	.	.
1	B	101	ILE	N	121.841	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	102	ASN	CA	56.677	.	.
1	B	102	ASN	CB	38.456	.	.
1	B	102	ASN	N	115.884	.	.
1	B	103	LEU	CA	55.716	.	.
1	B	103	LEU	C	178.141	.	.
1	B	104	LEU	CA	54.864	.	.
1	B	104	LEU	C	176.913	.	.
1	B	104	LEU	N	113.662	.	.
1	B	105	SER	CA	58.452	.	.
1	B	105	SER	CB	64.401	.	.
1	B	105	SER	C	176.135	.	.
1	B	105	SER	N	112.374	.	.
1	B	106	ARG	CA	54.515	.	.
1	B	106	ARG	N	127.884	.	.

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 10) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	31	TRP	HE	10.432	.	.
1	A	31	TRP	NE	130.154	.	.
1	A	45	TRP	HE	10.494	.	.
1	A	45	TRP	NE	131.304	.	.
1	A	63	TRP	HE	11.48	.	.
1	A	63	TRP	NE	136.449	.	.
1	A	76	TRP	HE	10.372	.	.
1	A	76	TRP	NE	130.641	.	.
1	B	63	TRP	HE	8.676	.	.
1	B	63	TRP	NE	124.872	.	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	219	-0.82 ± 0.13	Should be checked
$^{13}C_{\beta}$	158	0.55 ± 0.13	Should be checked
$^{13}C'$	196	-0.47 ± 0.06	None needed (< 0.5 ppm)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	206	0.65 ± 0.28	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 32%, i.e. 939 atoms were assigned a chemical shift out of a possible 2972. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	786/1081 (73%)	181/445 (41%)	407/430 (95%)	198/206 (96%)
Sidechain	153/1598 (10%)	0/1081 (0%)	153/488 (31%)	0/29 (0%)
Aromatic	0/293 (0%)	0/142 (0%)	0/142 (0%)	0/9 (0%)
Overall	939/2972 (32%)	181/1668 (11%)	560/1060 (53%)	198/244 (81%)

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.

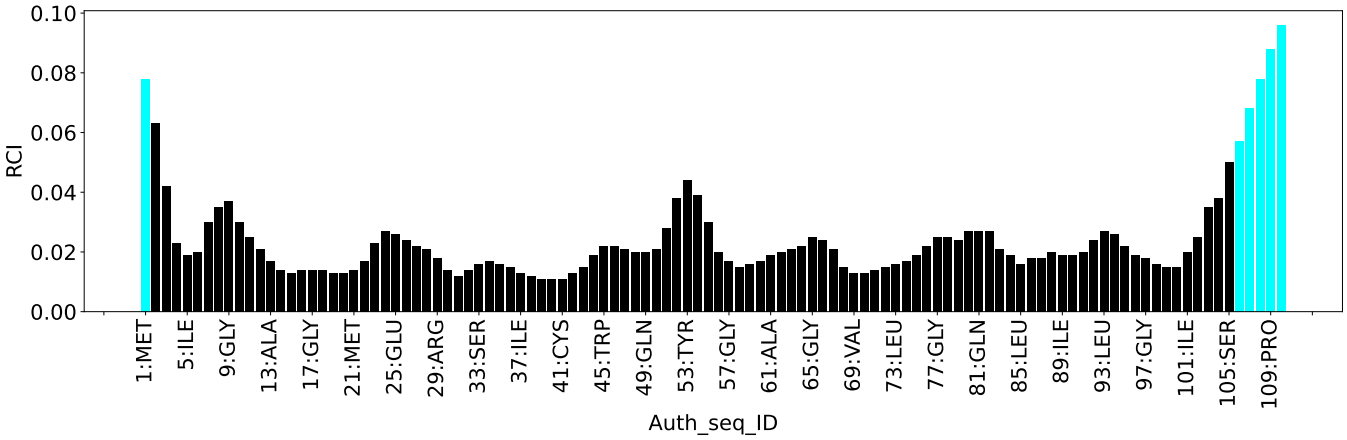
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

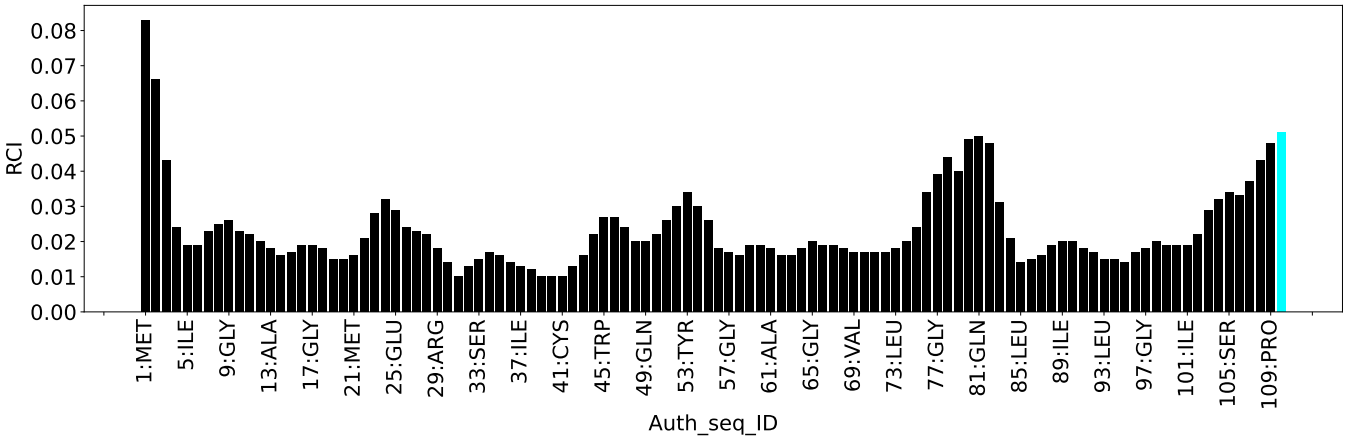
7.1.5 Random Coil Index (RCI) plots

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:



Random coil index (RCI) for chain B:



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	1452
Intra-residue (|i-j|=0)	1
Sequential (|i-j|=1)	40
Medium range (|i-j|>1 and |i-j|<5)	131
Long range (|i-j|≥5)	576
Inter-chain	488
Hydrogen bond restraints	216
Disulfide bond restraints	0
Total dihedral-angle restraints	390
Number of unmapped restraints	7
Number of restraints per residue	8.3
Number of long range restraints per residue[1]	2.6

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å
are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	7.4	0.2
0.2-0.5 (Medium)	25.8	0.5
>0.5 (Large)	98.8	6.85

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)	11.5	9.64
10.0-20.0 (Medium)	5.6	19.87
>20.0 (Large)	7.1	158.86

9 Distance violation analysis (i)

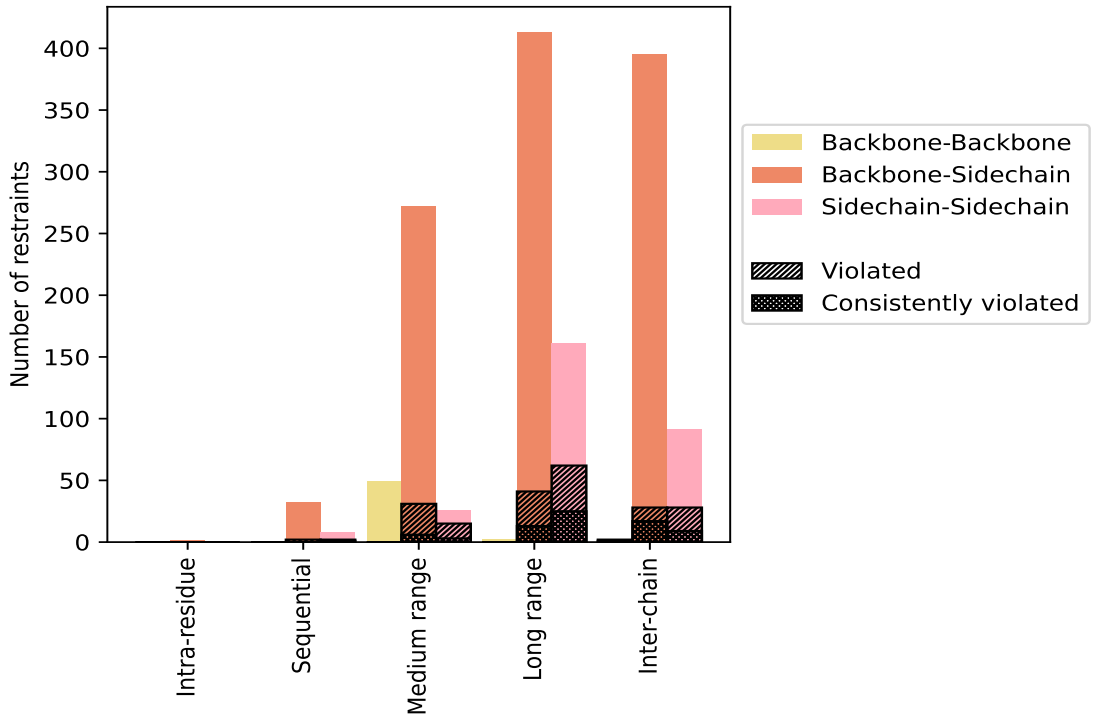
9.1 Summary of distance violations (i)

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)	1	0.1	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	1	0.1	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
Sequential (|i-j|=1)	40	2.8	4	10.0	0.3	1	2.5	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	32	2.2	2	6.2	0.1	0	0.0	0.0
Sidechain-Sidechain	8	0.6	2	25.0	0.1	1	12.5	0.1
Medium range (|i-j|>1 & |i-j|<5)	131	9.0	22	16.8	1.5	5	3.8	0.3
Backbone-Backbone	49	3.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	56	3.9	7	12.5	0.5	2	3.6	0.1
Sidechain-Sidechain	26	1.8	15	57.7	1.0	3	11.5	0.2
Long range (|i-j|≥5)	576	39.7	103	17.9	7.1	38	6.6	2.6
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	413	28.4	41	9.9	2.8	13	3.1	0.9
Sidechain-Sidechain	161	11.1	62	38.5	4.3	25	15.5	1.7
Inter-chain	488	33.6	58	11.9	4.0	27	5.5	1.9
Backbone-Backbone	2	0.1	2	100.0	0.1	1	50.0	0.1
Backbone-Sidechain	395	27.2	28	7.1	1.9	17	4.3	1.2
Sidechain-Sidechain	91	6.3	28	30.8	1.9	9	9.9	0.6
Hydrogen bond	216	14.9	24	11.1	1.7	4	1.9	0.3
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1452	100.0	211	14.5	14.5	75	5.2	5.2
Backbone-Backbone	53	3.7	2	3.8	0.1	1	1.9	0.1
Backbone-Sidechain	1113	76.7	102	9.2	7.0	36	3.2	2.5
Sidechain-Sidechain	286	19.7	107	37.4	7.4	38	13.3	2.6

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

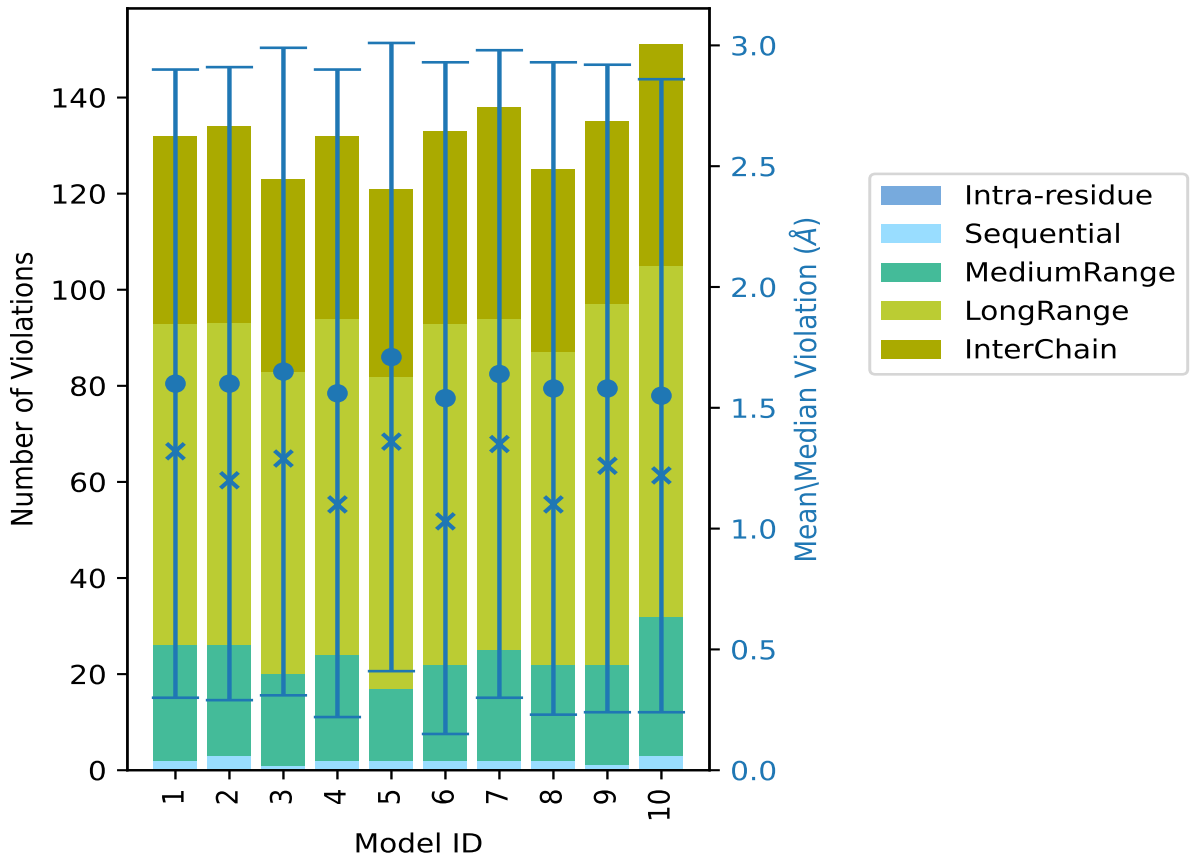
9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	2	24	67	39	132	1.6	5.9	1.3	1.32
2	0	3	23	67	41	134	1.6	6.13	1.31	1.2
3	0	1	19	63	40	123	1.65	6.39	1.34	1.29
4	0	2	22	70	38	132	1.56	5.75	1.34	1.1
5	0	2	15	65	39	121	1.71	5.59	1.3	1.36
6	0	2	20	71	40	133	1.54	5.45	1.39	1.03
7	0	2	23	69	44	138	1.64	5.74	1.34	1.35
8	0	2	20	65	38	125	1.58	6.0	1.35	1.1
9	0	1	21	75	38	135	1.58	6.81	1.34	1.26
10	0	3	29	73	46	151	1.55	6.85	1.31	1.22

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1049(IR:1, SQ:36, MR:109, LR:473, IC:430) 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	2	5	9	3	19	1	10.0
0	0	1	10	4	15	2	20.0
0	0	3	11	9	23	3	30.0

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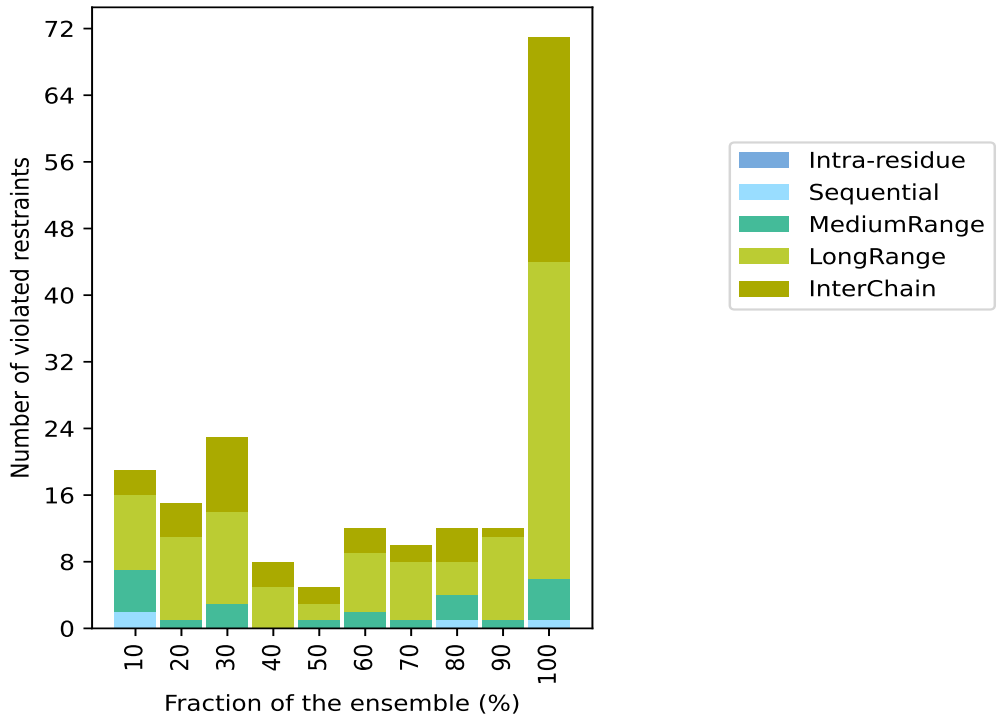
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	5	3	8	4	40.0
0	0	1	2	2	5	5	50.0
0	0	2	7	3	12	6	60.0
0	0	1	7	2	10	7	70.0
0	1	3	4	4	12	8	80.0
0	0	1	10	1	12	9	90.0
0	1	5	38	27	71	10	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble

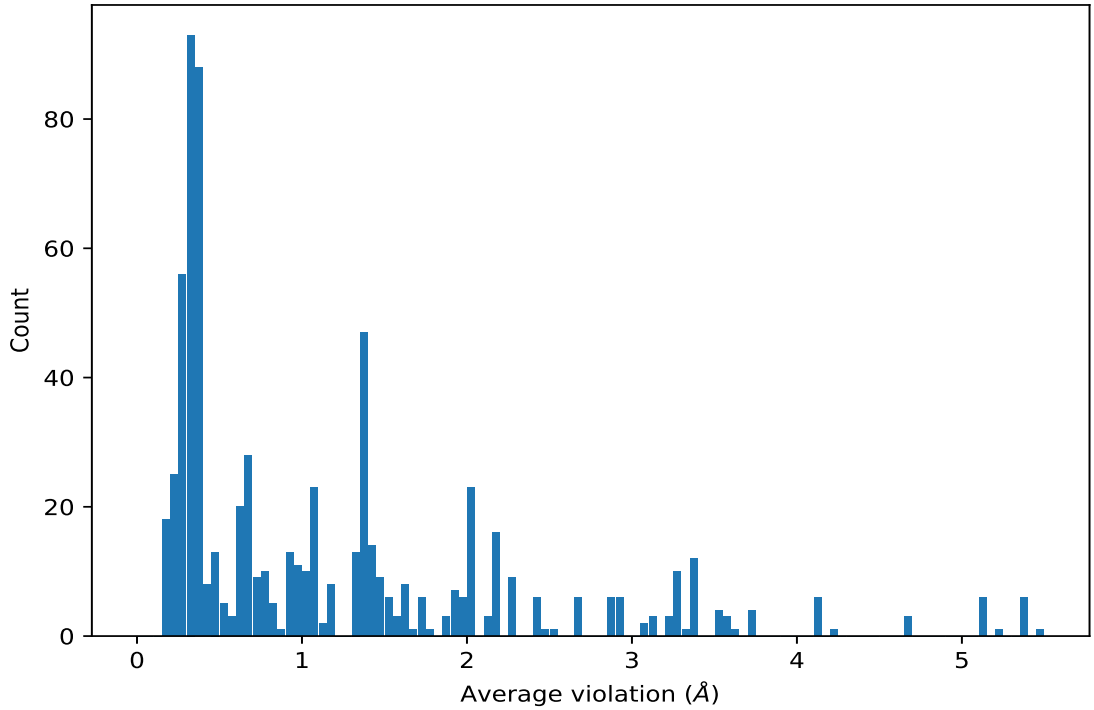


9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

in the ensemble



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	10	5.45	0.34	5.48
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	10	5.37	0.82	5.2
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	10	5.37	0.82	5.2
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	10	5.37	0.82	5.2
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	10	5.37	0.82	5.2
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	10	5.37	0.82	5.2
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	10	5.37	0.82	5.2
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	10	5.22	0.54	5.17
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	10	5.14	0.77	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	10	5.14	0.77	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	10	5.14	0.77	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	10	5.14	0.77	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	10	5.14	0.77	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	10	5.14	0.77	5.22
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	10	4.66	0.83	4.93

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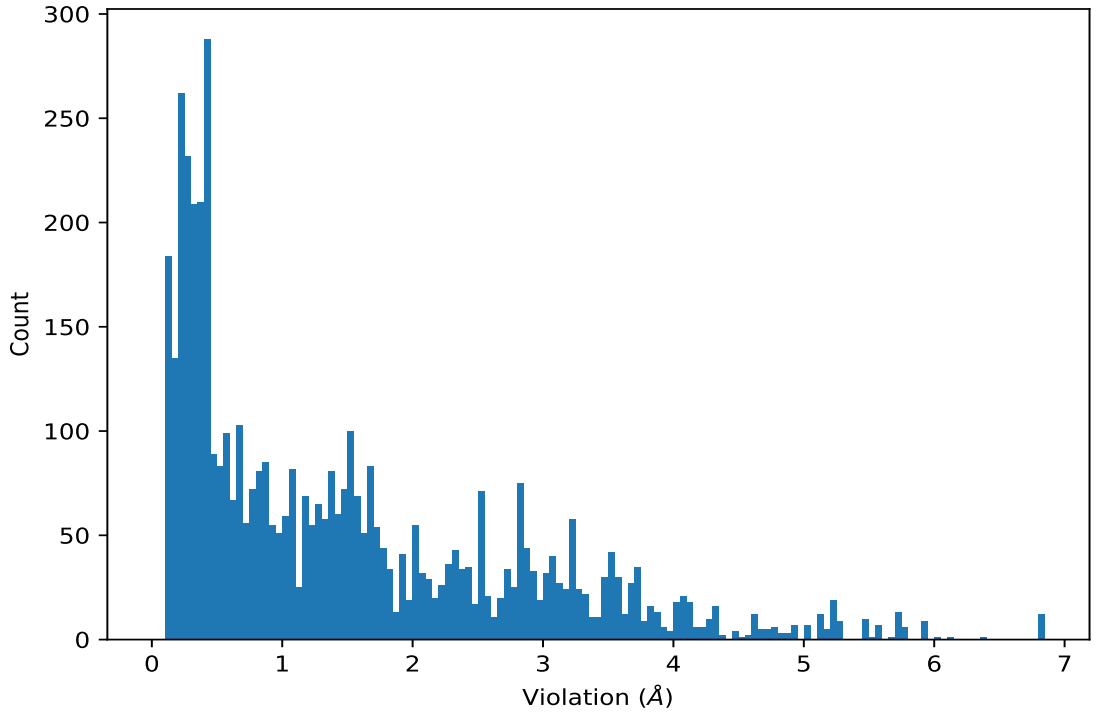
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	10	4.66	0.83	4.93
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	10	4.66	0.83	4.93
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	10	4.2	0.3	4.29
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	10	4.14	0.1	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	10	4.14	0.1	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	10	4.14	0.1	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	10	4.14	0.1	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	10	4.14	0.1	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	10	4.14	0.1	4.1
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	10	3.74	0.62	3.51
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	10	3.74	0.62	3.51
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	10	3.74	0.62	3.51
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	10	3.72	0.55	3.68
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	10	3.62	1.01	3.77

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	9	6.81
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	9	6.81
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	9	6.81
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	9	6.81
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	9	6.81
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	9	6.81
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	3	6.39
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	2	6.13
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	8	6.0
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	2	5.94
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	2	5.94
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	2	5.94
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	2	5.94
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	2	5.94
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	2	5.94
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	1	5.9
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	1	5.9
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	1	5.9
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	4	5.75
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	4	5.75
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	4	5.75
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	4	5.75
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	4	5.75
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	4	5.75
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	7	5.74
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	9	5.7

10 Dihedral-angle violation analysis

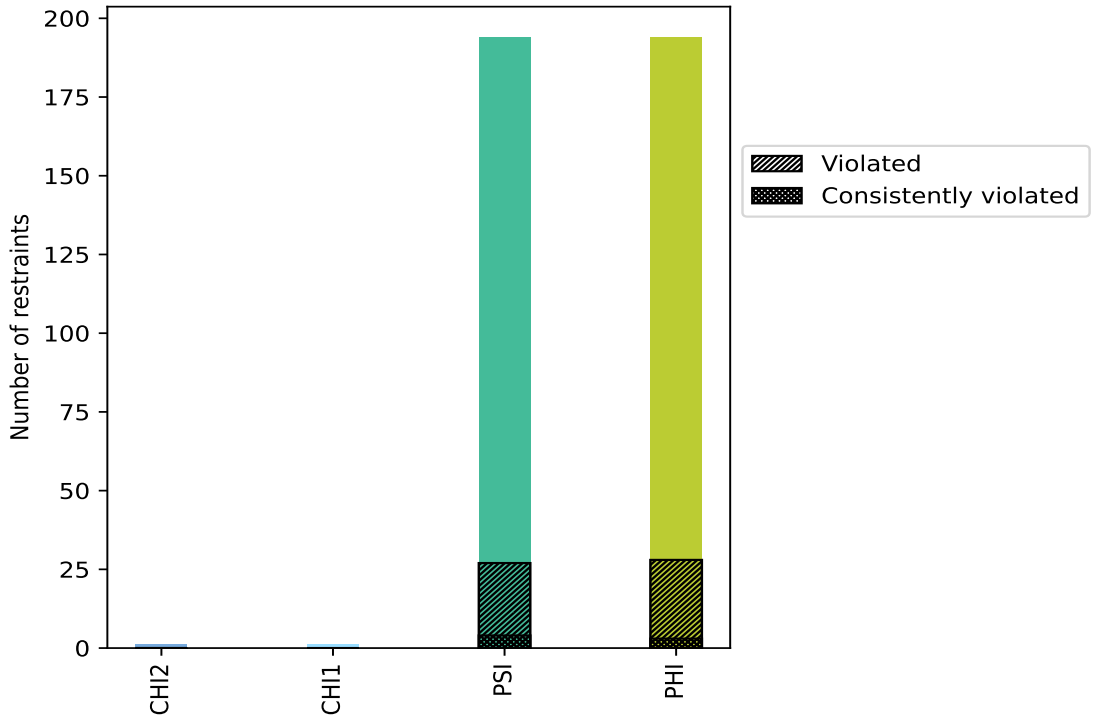
10.1 Summary of dihedral-angle violations

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]
CHI2	1	0.3	0	0.0	0.0	0	0.0	0.0
CHI1	1	0.3	0	0.0	0.0	0	0.0	0.0
PSI	194	49.7	27	13.9	6.9	4	2.1	1.0
PHI	194	49.7	28	14.4	7.2	3	1.5	0.8
Total	390	100.0	55	14.1	14.1	7	1.8	1.8

[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



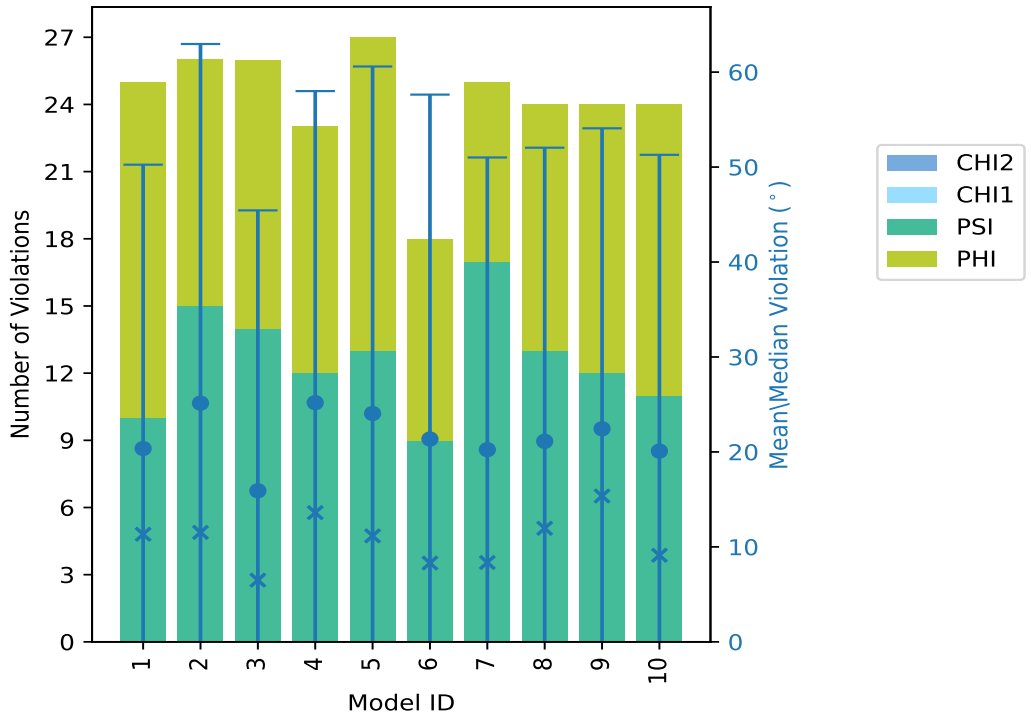
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	CHI2	CHI1	PSI	PHI	Total				
1	0	0	10	15	25	20.36	158.29	29.89	11.33
2	0	0	15	11	26	25.14	157.15	37.82	11.53
3	0	0	14	12	26	15.91	155.1	29.53	6.5
4	0	0	12	11	23	25.19	156.3	32.81	13.61
5	0	0	13	14	27	24.05	155.99	36.54	11.16
6	0	0	9	9	18	21.36	157.48	36.27	8.3
7	0	0	17	8	25	20.24	158.57	30.77	8.36
8	0	0	13	11	24	21.12	157.3	30.92	11.96
9	0	0	12	12	24	22.44	158.86	31.64	15.36
10	0	0	11	13	24	20.09	157.45	31.2	9.12

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

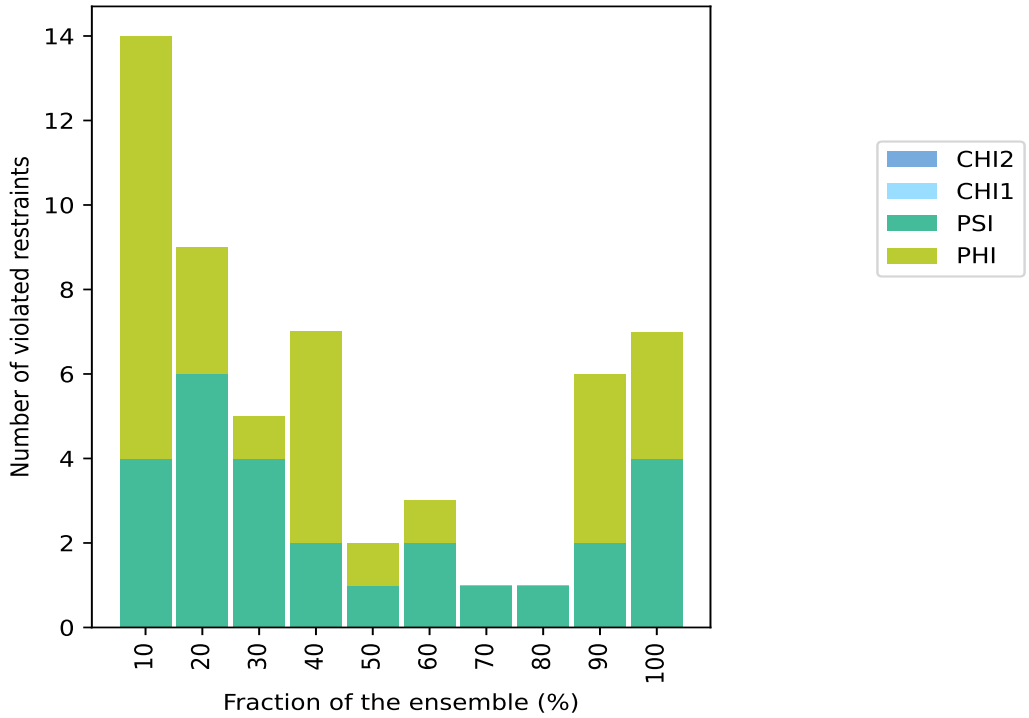
10.3 Dihedral-angle violation statistics for the ensemble

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	
CHI2	CHI1	PSI	PHI	Total	Count[1]	%
0	0	4	10	14	1	10.0
0	0	6	3	9	2	20.0
0	0	4	1	5	3	30.0
0	0	2	5	7	4	40.0
0	0	1	1	2	5	50.0
0	0	2	1	3	6	60.0
0	0	1	0	1	7	70.0
0	0	1	0	1	8	80.0
0	0	2	4	6	9	90.0
0	0	4	3	7	10	100.0

[1] Number of models with violations

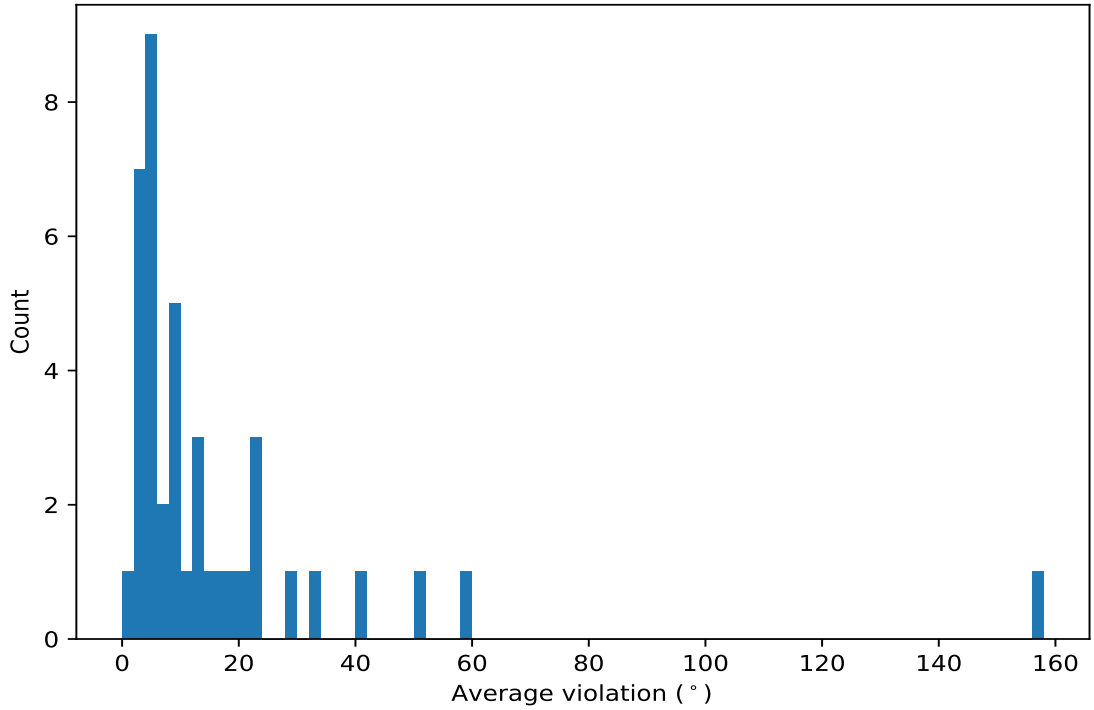
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

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



10.4.2 Table: Most violated dihedral-angle restraints (i)

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

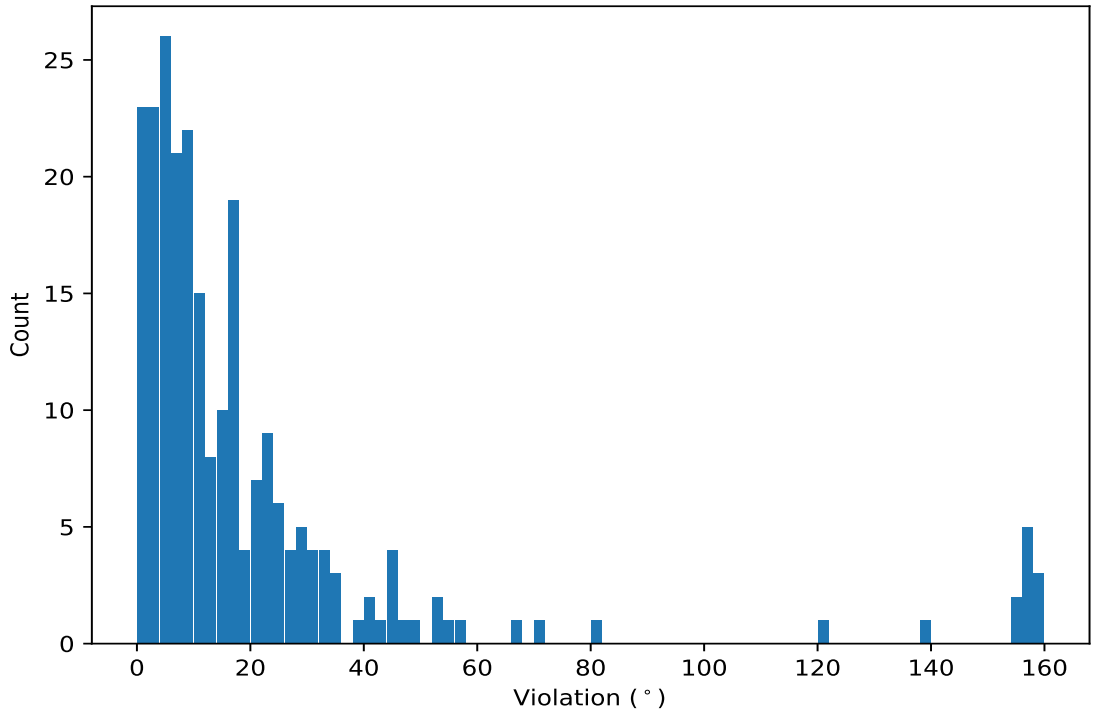
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	10	157.25	1.12	157.38
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	10	29.41	2.47	28.58
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	10	22.91	9.6	25.58
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	10	20.38	5.03	20.98
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	10	16.44	1.15	16.62
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	10	8.19	1.82	8.53
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	10	6.27	1.21	6.3
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	9	40.65	8.95	43.01
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	9	32.74	18.57	23.63
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	9	13.91	6.59	11.16

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (i)

The following table 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 (°)
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	9	158.86
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	7	158.57
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	1	158.29
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	6	157.48
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	10	157.45
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	8	157.3
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	2	157.15
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	4	156.3
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	5	155.99
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	3	155.1