wwPDB NMR Structure Validation Summary Report

Dec 24, 2024 – 02:52 PM EST

PDB ID	:	2LAP
BMRB ID	:	17532
Title	:	NMR structure of Ca2+-bound CaBP1 C-domain with RDC
Authors	:	Ames, J.
Deposited on	:	2011-03-16

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

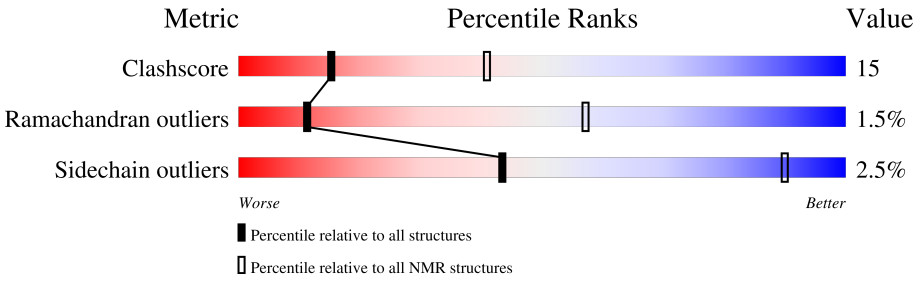
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 66%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	167	27% 7% 8% 58%

2 Ensemble composition and analysis

This entry contains 15 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:100-A:131, A:141-A:165 (57)	0.68	7

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 7, 8, 9, 10, 11, 12, 13, 14, 15
2	3, 4, 5
3	1, 6

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1120 atoms, of which 549 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	70	Total	C	H	N	O	S	0
			1118	346	549	106	113	4	

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9NZU7
A	2	GLY	-	expression tag	UNP Q9NZU7
A	3	ASN	-	expression tag	UNP Q9NZU7
A	4	CYS	-	expression tag	UNP Q9NZU7
A	5	VAL	-	expression tag	UNP Q9NZU7
A	6	LYS	-	expression tag	UNP Q9NZU7
A	7	TYR	-	expression tag	UNP Q9NZU7
A	8	PRO	-	expression tag	UNP Q9NZU7
A	9	LEU	-	expression tag	UNP Q9NZU7
A	10	ARG	-	expression tag	UNP Q9NZU7
A	11	ASN	-	expression tag	UNP Q9NZU7
A	12	LEU	-	expression tag	UNP Q9NZU7
A	13	SER	-	expression tag	UNP Q9NZU7
A	14	ARG	-	expression tag	UNP Q9NZU7
A	15	LYS	-	expression tag	UNP Q9NZU7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

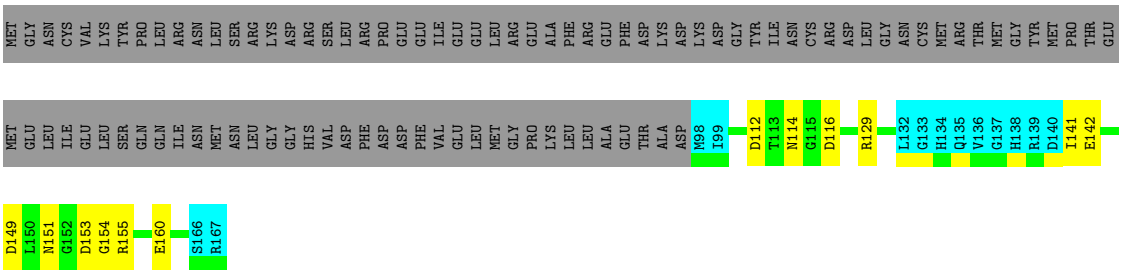
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Calcium-binding protein 1

Chain A:

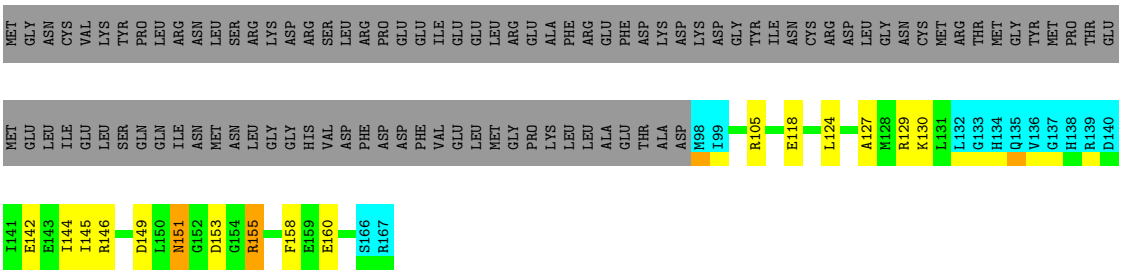


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 7. Colouring as in section 4.1 above.

• Molecule 1: Calcium-binding protein 1

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 15 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 solution	2.23
X-PLOR NIH	refinement	2.23

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	1354
Number of shifts mapped to atoms	605
Number of unparsed shifts	0
Number of shifts with mapping errors	749
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%

6 Model quality

6.1 Standard geometry

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

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

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	464	447	446	13±5
All	All	6990	6705	6703	200

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 15.

5 of 130 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ASN:HD22	1:A:153:ASP:H	0.66	1.31	7	1
1:A:114:ASN:HD22	1:A:114:ASN:N	0.65	1.89	15	1
1:A:141:ILE:HG22	1:A:141:ILE:O	0.63	1.91	12	4
1:A:105:ARG:NH2	1:A:109:ARG:NH2	0.63	2.47	15	1
1:A:151:ASN:HD22	1:A:151:ASN:H	0.63	1.37	2	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	57/167 (34%)	51±2 (90±3%)	5±2 (9±3%)	1±1 (2±2%)	11 57
All	All	855/2505 (34%)	766 (90%)	76 (9%)	13 (2%)	11 57

5 of 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	141	ILE	4
1	A	112	ASP	4
1	A	103	GLU	1
1	A	101	VAL	1
1	A	150	LEU	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	50/148 (34%)	49±1 (97±2%)	1±1 (3±2%)	43 90
All	All	750/2220 (34%)	731 (97%)	19 (3%)	43 90

5 of 11 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	128	MET	3
1	A	114	ASN	3
1	A	104	LEU	2
1	A	151	ASN	2
1	A	164	MET	2

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 66% for the well-defined parts and 62% 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	1354
Number of shifts mapped to atoms	605
Number of unparsed shifts	0
Number of shifts with mapping errors	749
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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 749) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	LYS	HA	4.313	0.04	1
1	A	15	LYS	HB2	1.87	0.04	2
1	A	15	LYS	HB3	1.8	0.04	2
1	A	15	LYS	C	176.111	0.2	1
1	A	15	LYS	CA	56.722	0.2	1
1	A	15	LYS	CB	32.883	0.2	1
1	A	16	ASP	H	8.219	0.04	1
1	A	16	ASP	HA	4.612	0.04	1
1	A	16	ASP	HB2	2.657	0.04	2
1	A	16	ASP	HB3	2.735	0.04	2
1	A	16	ASP	C	175.635	0.2	1
1	A	16	ASP	CA	54.049	0.2	1
1	A	16	ASP	CB	41.19	0.2	1
1	A	16	ASP	N	119.878	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	ARG	H	8.01	0.04	1
1	A	17	ARG	HA	4.405	0.04	1
1	A	17	ARG	HB2	1.94	0.04	2
1	A	17	ARG	C	174.866	0.2	1
1	A	17	ARG	CA	55.474	0.2	1
1	A	17	ARG	CB	30.781	0.2	1
1	A	17	ARG	N	119.816	0.2	1
1	A	18	SER	H	8.03	0.04	1
1	A	18	SER	HA	4.553	0.04	1
1	A	18	SER	HB2	3.782	0.04	2
1	A	18	SER	HB3	3.859	0.04	2
1	A	18	SER	C	174.494	0.2	1
1	A	18	SER	CA	57.617	0.2	1
1	A	18	SER	CB	64.608	0.2	1
1	A	18	SER	N	115.342	0.2	1
1	A	19	LEU	H	8.458	0.04	1
1	A	19	LEU	HA	4.373	0.04	1
1	A	19	LEU	HB2	1.687	0.04	2
1	A	19	LEU	HB3	1.4	0.04	2
1	A	19	LEU	HG	1.714	0.04	1
1	A	19	LEU	HD11	0.784	0.04	1
1	A	19	LEU	HD12	0.784	0.04	1
1	A	19	LEU	HD13	0.784	0.04	1
1	A	19	LEU	HD21	0.821	0.04	1
1	A	19	LEU	HD22	0.821	0.04	1
1	A	19	LEU	HD23	0.821	0.04	1
1	A	19	LEU	C	177.506	0.2	1
1	A	19	LEU	CA	55.36	0.2	1
1	A	19	LEU	CB	42.398	0.2	1
1	A	19	LEU	CD1	26.25	0.2	1
1	A	19	LEU	CD2	23.6	0.2	1
1	A	19	LEU	N	123.381	0.2	1
1	A	20	ARG	H	9.584	0.04	1
1	A	20	ARG	N	123.683	0.2	1
1	A	21	PRO	HA	4.281	0.04	1
1	A	21	PRO	HB2	2.486	0.04	2
1	A	21	PRO	HB3	2.055	0.04	2
1	A	21	PRO	C	179.232	0.2	1
1	A	21	PRO	CA	66.35	0.2	1
1	A	21	PRO	CB	31.74	0.2	1
1	A	22	GLU	H	9.993	0.04	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	GLU	HA	4.22	0.04	1
1	A	22	GLU	HB2	2.092	0.04	2
1	A	22	GLU	C	179.487	0.2	1
1	A	22	GLU	CA	59.799	0.2	1
1	A	22	GLU	CB	28.274	0.2	1
1	A	22	GLU	N	116.7	0.2	1
1	A	23	GLU	H	7.438	0.04	1
1	A	23	GLU	HA	4.28	0.04	1
1	A	23	GLU	HB2	2.654	0.04	2
1	A	23	GLU	HB3	2.203	0.04	2
1	A	23	GLU	C	178.784	0.2	1
1	A	23	GLU	CA	58.808	0.2	1
1	A	23	GLU	CB	30.357	0.2	1
1	A	23	GLU	N	120.542	0.2	1
1	A	24	ILE	H	7.792	0.04	1
1	A	24	ILE	HA	3.812	0.04	1
1	A	24	ILE	HB	2.203	0.04	1
1	A	24	ILE	HG12	1.659	0.04	1
1	A	24	ILE	HG21	1.117	0.04	1
1	A	24	ILE	HG22	1.117	0.04	1
1	A	24	ILE	HG23	1.117	0.04	1
1	A	24	ILE	HD11	0.85	0.04	1
1	A	24	ILE	HD12	0.85	0.04	1
1	A	24	ILE	HD13	0.85	0.04	1
1	A	24	ILE	C	178.421	0.2	1
1	A	24	ILE	CA	64.733	0.2	1
1	A	24	ILE	CB	36.916	0.2	1
1	A	24	ILE	CG1	29.23	0.2	1
1	A	24	ILE	CG2	17.51	0.2	1
1	A	24	ILE	CD1	12.04	0.2	1
1	A	24	ILE	N	120.005	0.2	1
1	A	25	GLU	H	8.062	0.04	1
1	A	25	GLU	HA	4.226	0.04	1
1	A	25	GLU	HB2	2.154	0.04	2
1	A	25	GLU	C	178.921	0.2	1
1	A	25	GLU	CA	59.247	0.2	1
1	A	25	GLU	CB	28.862	0.2	1
1	A	25	GLU	N	118.385	0.2	1
1	A	26	GLU	H	7.588	0.04	1
1	A	26	GLU	HA	4.231	0.04	1
1	A	26	GLU	HB2	2.284	0.04	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	GLU	C	180.202	0.2	1
1	A	26	GLU	CA	59.47	0.2	1
1	A	26	GLU	CB	29.486	0.2	1
1	A	26	GLU	N	120.114	0.2	1
1	A	27	LEU	H	8.084	0.04	1
1	A	27	LEU	HA	4.477	0.04	1
1	A	27	LEU	HB2	2.569	0.04	2
1	A	27	LEU	HB3	1.713	0.04	2
1	A	27	LEU	HG	2.018	0.04	1
1	A	27	LEU	HD11	0.817	0.04	1
1	A	27	LEU	HD12	0.817	0.04	1
1	A	27	LEU	HD13	0.817	0.04	1
1	A	27	LEU	HD21	0.803	0.04	1
1	A	27	LEU	HD22	0.803	0.04	1
1	A	27	LEU	HD23	0.803	0.04	1
1	A	27	LEU	C	178.746	0.2	1
1	A	27	LEU	CA	58.107	0.2	1
1	A	27	LEU	CB	41.595	0.2	1
1	A	27	LEU	CG	27.48	0.2	1
1	A	27	LEU	CD1	26.92	0.2	1
1	A	27	LEU	CD2	24.53	0.2	1
1	A	27	LEU	N	120.4	0.2	1
1	A	28	ARG	H	8.886	0.04	1
1	A	28	ARG	HA	3.719	0.04	1
1	A	28	ARG	HB2	1.843	0.04	2
1	A	28	ARG	HB3	1.768	0.04	2
1	A	28	ARG	C	178.664	0.2	1
1	A	28	ARG	CA	59.92	0.2	1
1	A	28	ARG	CB	29.953	0.2	1
1	A	28	ARG	N	121.879	0.2	1
1	A	29	GLU	H	8.128	0.04	1
1	A	29	GLU	HA	4.066	0.04	1
1	A	29	GLU	HB2	2.204	0.04	2
1	A	29	GLU	C	179.041	0.2	1
1	A	29	GLU	CA	59.364	0.2	1
1	A	29	GLU	CB	29.648	0.2	1
1	A	29	GLU	N	118.934	0.2	1
1	A	30	ALA	H	7.766	0.04	1
1	A	30	ALA	HA	4.351	0.04	1
1	A	30	ALA	HB1	1.774	0.04	1
1	A	30	ALA	HB2	1.774	0.04	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	ALA	HB3	1.774	0.04	1
1	A	30	ALA	C	178.784	0.2	1
1	A	30	ALA	CA	55.407	0.2	1
1	A	30	ALA	CB	18.774	0.2	1
1	A	30	ALA	N	122.423	0.2	1
1	A	31	PHE	H	8.57	0.04	1
1	A	31	PHE	HA	3.648	0.04	1
1	A	31	PHE	HB2	3.244	0.04	2
1	A	31	PHE	HB3	2.954	0.04	2
1	A	31	PHE	HD1	6.551	0.04	3
1	A	31	PHE	HD2	6.551	0.04	3
1	A	31	PHE	HE1	6.938	0.04	3
1	A	31	PHE	HE2	6.938	0.04	3
1	A	31	PHE	HZ	7.412	0.04	1
1	A	31	PHE	C	177.519	0.2	1
1	A	31	PHE	CA	62.131	0.2	1
1	A	31	PHE	CB	40.423	0.2	1
1	A	31	PHE	N	118.696	0.2	1
1	A	32	ARG	H	8.459	0.04	1
1	A	32	ARG	HA	3.976	0.04	1
1	A	32	ARG	C	179.02	0.2	1
1	A	32	ARG	CA	59.393	0.2	1
1	A	32	ARG	CB	30.406	0.2	1
1	A	32	ARG	N	115.937	0.2	1
1	A	33	GLU	H	7.566	0.04	1
1	A	33	GLU	HA	3.891	0.04	1
1	A	33	GLU	HB2	2.081	0.04	2
1	A	33	GLU	C	177.197	0.2	1
1	A	33	GLU	CA	58.589	0.2	1
1	A	33	GLU	CB	29.058	0.2	1
1	A	33	GLU	N	118.273	0.2	1
1	A	34	PHE	H	7.326	0.04	1
1	A	34	PHE	HA	4.262	0.04	1
1	A	34	PHE	HB2	2.607	0.04	2
1	A	34	PHE	HB3	3.042	0.04	2
1	A	34	PHE	HD1	7.534	0.04	3
1	A	34	PHE	HD2	7.534	0.04	3
1	A	34	PHE	HE1	7.438	0.04	3
1	A	34	PHE	HE2	7.438	0.04	3
1	A	34	PHE	HZ	7.24	0.04	1
1	A	34	PHE	C	175.852	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	34	PHE	CA	59.722	0.2	1
1	A	34	PHE	CB	39.757	0.2	1
1	A	34	PHE	N	114.06	0.2	1
1	A	35	ASP	H	7.768	0.04	1
1	A	35	ASP	HA	5.067	0.04	1
1	A	35	ASP	HB2	2.643	0.04	2
1	A	35	ASP	HB3	1.822	0.04	2
1	A	35	ASP	C	178.458	0.2	1
1	A	35	ASP	CA	52.535	0.2	1
1	A	35	ASP	CB	38.991	0.2	1
1	A	35	ASP	N	122.494	0.2	1
1	A	36	LYS	H	7.837	0.04	1
1	A	36	LYS	HA	3.984	0.04	1
1	A	36	LYS	HB2	1.891	0.04	2
1	A	36	LYS	C	177.34	0.2	1
1	A	36	LYS	CA	59.397	0.2	1
1	A	36	LYS	CB	32.345	0.2	1
1	A	36	LYS	N	122.532	0.2	1
1	A	37	ASP	H	8.26	0.04	1
1	A	37	ASP	HA	4.539	0.04	1
1	A	37	ASP	HB2	2.615	0.04	2
1	A	37	ASP	HB3	2.991	0.04	2
1	A	37	ASP	C	175.369	0.2	1
1	A	37	ASP	CA	52.845	0.2	1
1	A	37	ASP	CB	39.172	0.2	1
1	A	37	ASP	N	113.541	0.2	1
1	A	38	LYS	H	7.588	0.04	1
1	A	38	LYS	HA	3.946	0.04	1
1	A	38	LYS	C	175.784	0.2	1
1	A	38	LYS	CA	57.538	0.2	1
1	A	38	LYS	CB	29.258	0.2	1
1	A	38	LYS	N	114.73	0.2	1
1	A	39	ASP	H	8.301	0.04	1
1	A	39	ASP	HA	4.756	0.04	1
1	A	39	ASP	HB2	2.634	0.04	2
1	A	39	ASP	HB3	3.198	0.04	2
1	A	39	ASP	C	177.146	0.2	1
1	A	39	ASP	CA	53.432	0.2	1
1	A	39	ASP	CB	41.107	0.2	1
1	A	39	ASP	N	118.583	0.2	1
1	A	40	GLY	H	10.14	0.04	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	40	GLY	HA2	4.12	0.04	2
1	A	40	GLY	HA3	3.545	0.04	2
1	A	40	GLY	C	173.383	0.2	1
1	A	40	GLY	CA	45.033	0.2	1
1	A	40	GLY	N	111.561	0.2	1
1	A	41	TYR	H	7.989	0.04	1
1	A	41	TYR	HA	5.64	0.04	1
1	A	41	TYR	HB2	2.662	0.04	2
1	A	41	TYR	HB3	2.833	0.04	2
1	A	41	TYR	HD1	6.69	0.04	3
1	A	41	TYR	HD2	6.69	0.04	3
1	A	41	TYR	HE1	6.819	0.04	3
1	A	41	TYR	HE2	6.819	0.04	3
1	A	41	TYR	C	176.661	0.2	1
1	A	41	TYR	CA	56.74	0.2	1
1	A	41	TYR	CB	42.766	0.2	1
1	A	41	TYR	N	115.987	0.2	1
1	A	42	ILE	H	9.347	0.04	1
1	A	42	ILE	HA	4.859	0.04	1
1	A	42	ILE	HB	1.941	0.04	1
1	A	42	ILE	HG12	1.209	0.04	2
1	A	42	ILE	HG13	0.932	0.04	2
1	A	42	ILE	HG21	0.298	0.04	1
1	A	42	ILE	HG22	0.298	0.04	1
1	A	42	ILE	HG23	0.298	0.04	1
1	A	42	ILE	HD11	0.335	0.04	1
1	A	42	ILE	HD12	0.335	0.04	1
1	A	42	ILE	HD13	0.335	0.04	1
1	A	42	ILE	C	174.798	0.2	1
1	A	42	ILE	CA	60.017	0.2	1
1	A	42	ILE	CB	40.728	0.2	1
1	A	42	ILE	CG1	25.56	0.2	1
1	A	42	ILE	CG2	16.3	0.2	1
1	A	42	ILE	CD1	13.87	0.2	1
1	A	42	ILE	N	118.7	0.2	1
1	A	43	ASN	H	8.852	0.04	1
1	A	43	ASN	HA	5.073	0.04	1
1	A	43	ASN	HB2	3.058	0.04	2
1	A	43	ASN	HB3	3.092	0.04	2
1	A	43	ASN	C	176.122	0.2	1
1	A	43	ASN	CA	52.189	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	43	ASN	CB	39.963	0.2	1
1	A	43	ASN	N	120.7	0.2	1
1	A	44	CYS	H	8.519	0.04	1
1	A	44	CYS	HA	3.946	0.04	1
1	A	44	CYS	HB2	3.02	0.04	2
1	A	44	CYS	HB3	2.878	0.04	2
1	A	44	CYS	CA	62.439	0.2	1
1	A	44	CYS	CB	26.68	0.2	1
1	A	44	CYS	N	118.771	0.2	1
1	A	45	ARG	C	178.109	0.2	1
1	A	45	ARG	CA	58.78	0.2	1
1	A	45	ARG	CB	29.45	0.2	1
1	A	46	ASP	H	8.165	0.04	1
1	A	46	ASP	HA	4.7	0.04	1
1	A	46	ASP	HB2	2.736	0.04	2
1	A	46	ASP	HB3	2.86	0.04	2
1	A	46	ASP	CA	56.116	0.2	1
1	A	46	ASP	CB	41.874	0.2	1
1	A	46	ASP	N	118.981	0.2	1
1	A	47	LEU	H	7.946	0.04	1
1	A	47	LEU	HA	3.786	0.04	1
1	A	47	LEU	HB2	1.909	0.04	2
1	A	47	LEU	HB3	1.626	0.04	2
1	A	47	LEU	HG	1.735	0.04	1
1	A	47	LEU	HD11	1.051	0.04	1
1	A	47	LEU	HD12	1.051	0.04	1
1	A	47	LEU	HD13	1.051	0.04	1
1	A	47	LEU	HD21	0.946	0.04	1
1	A	47	LEU	HD22	0.946	0.04	1
1	A	47	LEU	HD23	0.946	0.04	1
1	A	47	LEU	C	178.476	0.2	1
1	A	47	LEU	CA	59.027	0.2	1
1	A	47	LEU	CB	41.908	0.2	1
1	A	47	LEU	CG	27.13	0.2	1
1	A	47	LEU	CD1	24.95	0.2	1
1	A	47	LEU	CD2	26.05	0.2	1
1	A	47	LEU	N	120.831	0.2	1
1	A	48	GLY	H	8.425	0.04	1
1	A	48	GLY	HA2	3.896	0.04	2
1	A	48	GLY	HA3	3.685	0.04	2
1	A	48	GLY	C	175.488	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	48	GLY	CA	47.923	0.2	1
1	A	48	GLY	N	106.142	0.2	1
1	A	49	ASN	H	7.851	0.04	1
1	A	49	ASN	HA	4.497	0.04	1
1	A	49	ASN	HB2	2.703	0.04	2
1	A	49	ASN	C	177.492	0.2	1
1	A	49	ASN	CA	55.812	0.2	1
1	A	49	ASN	CB	37.888	0.2	1
1	A	49	ASN	N	119.524	0.2	1
1	A	50	CYS	H	8.186	0.04	1
1	A	50	CYS	HA	3.529	0.04	1
1	A	50	CYS	HB2	2.661	0.04	2
1	A	50	CYS	HB3	2.215	0.04	2
1	A	50	CYS	C	176.805	0.2	1
1	A	50	CYS	CA	63.013	0.2	1
1	A	50	CYS	CB	26.453	0.2	1
1	A	50	CYS	N	122.947	0.2	1
1	A	51	MET	H	8.436	0.04	1
1	A	51	MET	HA	3.988	0.04	1
1	A	51	MET	HB2	2.36	0.04	2
1	A	51	MET	HB3	2.581	0.04	2
1	A	51	MET	C	178.111	0.2	1
1	A	51	MET	CA	60.917	0.2	1
1	A	51	MET	CB	33.146	0.2	1
1	A	51	MET	N	117.78	0.2	1
1	A	52	ARG	H	7.961	0.04	1
1	A	52	ARG	HA	4.444	0.04	1
1	A	52	ARG	HB2	2.002	0.04	2
1	A	52	ARG	C	181.061	0.2	1
1	A	52	ARG	CA	59.549	0.2	1
1	A	52	ARG	CB	30.289	0.2	1
1	A	52	ARG	N	117.844	0.2	1
1	A	53	THR	H	8.118	0.04	1
1	A	53	THR	HA	4.195	0.04	1
1	A	53	THR	HB	4.585	0.04	1
1	A	53	THR	HG21	1.59	0.04	1
1	A	53	THR	HG22	1.59	0.04	1
1	A	53	THR	HG23	1.59	0.04	1
1	A	53	THR	C	175.566	0.2	1
1	A	53	THR	CA	66.342	0.2	1
1	A	53	THR	CB	69.113	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	THR	CG2	21.78	0.2	1
1	A	53	THR	N	116.83	0.2	1
1	A	54	MET	H	7.599	0.04	1
1	A	54	MET	HA	4.63	0.04	1
1	A	54	MET	HB2	2.435	0.04	2
1	A	54	MET	HB3	2.304	0.04	2
1	A	54	MET	C	175.777	0.2	1
1	A	54	MET	CA	55.894	0.2	1
1	A	54	MET	CB	33.038	0.2	1
1	A	54	MET	N	118.06	0.2	1
1	A	55	GLY	H	7.776	0.04	1
1	A	55	GLY	HA2	4.286	0.04	2
1	A	55	GLY	HA3	3.682	0.04	2
1	A	55	GLY	C	173.298	0.2	1
1	A	55	GLY	CA	45.239	0.2	1
1	A	55	GLY	N	105.74	0.2	1
1	A	56	TYR	H	7.854	0.04	1
1	A	56	TYR	HA	4.556	0.04	1
1	A	56	TYR	HB2	2.605	0.04	2
1	A	56	TYR	HB3	2.808	0.04	2
1	A	56	TYR	CA	57.243	0.2	1
1	A	56	TYR	CB	39.752	0.2	1
1	A	56	TYR	N	122.043	0.2	1
1	A	58	PRO	HA	4.732	0.04	1
1	A	58	PRO	HB2	2.204	0.04	2
1	A	58	PRO	HB3	1.999	0.04	2
1	A	58	PRO	C	177.733	0.2	1
1	A	58	PRO	CA	61.95	0.2	1
1	A	58	PRO	CB	31.98	0.2	1
1	A	59	THR	H	8.636	0.04	1
1	A	59	THR	HA	4.5	0.04	1
1	A	59	THR	HB	4.734	0.04	1
1	A	59	THR	HG21	1.402	0.04	1
1	A	59	THR	HG22	1.402	0.04	1
1	A	59	THR	HG23	1.402	0.04	1
1	A	59	THR	C	175.209	0.2	1
1	A	59	THR	CA	60.747	0.2	1
1	A	59	THR	CB	70.849	0.2	1
1	A	59	THR	CG2	21.94	0.2	1
1	A	59	THR	N	112.866	0.2	1
1	A	60	GLU	H	8.839	0.04	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	GLU	HA	4.052	0.04	1
1	A	60	GLU	HB2	2.331	0.04	2
1	A	60	GLU	HB3	2.097	0.04	2
1	A	60	GLU	C	179.393	0.2	1
1	A	60	GLU	CA	60.166	0.2	1
1	A	60	GLU	CB	29.382	0.2	1
1	A	60	GLU	N	121.022	0.2	1
1	A	61	MET	H	8.363	0.04	1
1	A	61	MET	HA	4.296	0.04	1
1	A	61	MET	HB2	2.076	0.04	2
1	A	61	MET	C	178.435	0.2	1
1	A	61	MET	CA	58.262	0.2	1
1	A	61	MET	CB	31.967	0.2	1
1	A	61	MET	N	116.428	0.2	1
1	A	62	GLU	H	7.849	0.04	1
1	A	62	GLU	HA	4.129	0.04	1
1	A	62	GLU	HB2	2.332	0.04	2
1	A	62	GLU	HB3	2.084	0.04	2
1	A	62	GLU	C	179.314	0.2	1
1	A	62	GLU	CA	59.167	0.2	1
1	A	62	GLU	CB	30.26	0.2	1
1	A	62	GLU	N	120.855	0.2	1
1	A	63	LEU	H	7.946	0.04	1
1	A	63	LEU	HA	4.14	0.04	1
1	A	63	LEU	HB2	1.899	0.04	2
1	A	63	LEU	HB3	1.647	0.04	2
1	A	63	LEU	HD11	0.902	0.04	1
1	A	63	LEU	HD12	0.902	0.04	1
1	A	63	LEU	HD13	0.902	0.04	1
1	A	63	LEU	HD21	0.864	0.04	1
1	A	63	LEU	HD22	0.864	0.04	1
1	A	63	LEU	HD23	0.864	0.04	1
1	A	63	LEU	C	180.109	0.2	1
1	A	63	LEU	CA	57.76	0.2	1
1	A	63	LEU	CB	41.335	0.2	1
1	A	63	LEU	CD1	24.92	0.2	1
1	A	63	LEU	CD2	22.91	0.2	1
1	A	63	LEU	N	119.06	0.2	1
1	A	64	ILE	H	8.188	0.04	1
1	A	64	ILE	HA	3.769	0.04	1
1	A	64	ILE	HB	2.058	0.04	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	64	ILE	HG12	1.82	0.04	2
1	A	64	ILE	HG13	1.183	0.04	2
1	A	64	ILE	HG21	0.937	0.04	1
1	A	64	ILE	HG22	0.937	0.04	1
1	A	64	ILE	HG23	0.937	0.04	1
1	A	64	ILE	HD11	0.909	0.04	1
1	A	64	ILE	HD12	0.909	0.04	1
1	A	64	ILE	HD13	0.909	0.04	1
1	A	64	ILE	C	178.748	0.2	1
1	A	64	ILE	CA	65.336	0.2	1
1	A	64	ILE	CB	37.936	0.2	1
1	A	64	ILE	CG2	17.09	0.2	1
1	A	64	ILE	CD1	13.25	0.2	1
1	A	64	ILE	N	123.431	0.2	1
1	A	65	GLU	H	8.002	0.04	1
1	A	65	GLU	HA	4.086	0.04	1
1	A	65	GLU	HB2	2.218	0.04	2
1	A	65	GLU	C	179.579	0.2	1
1	A	65	GLU	CA	59.758	0.2	1
1	A	65	GLU	CB	29.627	0.2	1
1	A	65	GLU	N	121.012	0.2	1
1	A	66	LEU	H	8.381	0.04	1
1	A	66	LEU	HA	4.182	0.04	1
1	A	66	LEU	HB2	1.878	0.04	2
1	A	66	LEU	HB3	1.559	0.04	2
1	A	66	LEU	C	178.783	0.2	1
1	A	66	LEU	CA	57.985	0.2	1
1	A	66	LEU	CB	42.436	0.2	1
1	A	66	LEU	N	120.046	0.2	1
1	A	67	SER	H	8.257	0.04	1
1	A	67	SER	HA	4.245	0.04	1
1	A	67	SER	HB2	3.937	0.04	2
1	A	67	SER	HB3	3.937	0.04	2
1	A	67	SER	C	176.098	0.2	1
1	A	67	SER	CA	61.88	0.2	1
1	A	67	SER	CB	62.959	0.2	1
1	A	67	SER	N	114.185	0.2	1
1	A	68	GLN	H	7.942	0.04	1
1	A	68	GLN	HA	4.198	0.04	1
1	A	68	GLN	HB2	2.256	0.04	2
1	A	68	GLN	C	178.26	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	68	GLN	CA	59.027	0.2	1
1	A	68	GLN	CB	28.269	0.2	1
1	A	68	GLN	N	120.772	0.2	1
1	A	69	GLN	H	7.849	0.04	1
1	A	69	GLN	HA	4.131	0.04	1
1	A	69	GLN	HB2	2.272	0.04	2
1	A	69	GLN	C	178.706	0.2	1
1	A	69	GLN	CA	59.081	0.2	1
1	A	69	GLN	CB	28.577	0.2	1
1	A	69	GLN	N	118.945	0.2	1
1	A	70	ILE	H	8.537	0.04	1
1	A	70	ILE	HA	3.752	0.04	1
1	A	70	ILE	HB	1.914	0.04	1
1	A	70	ILE	HG12	1.782	0.04	2
1	A	70	ILE	HG13	1.05	0.04	2
1	A	70	ILE	HG21	0.732	0.04	1
1	A	70	ILE	HG22	0.732	0.04	1
1	A	70	ILE	HG23	0.732	0.04	1
1	A	70	ILE	HD11	0.78	0.04	1
1	A	70	ILE	HD12	0.78	0.04	1
1	A	70	ILE	HD13	0.78	0.04	1
1	A	70	ILE	C	179.185	0.2	1
1	A	70	ILE	CA	64.358	0.2	1
1	A	70	ILE	CB	38.049	0.2	1
1	A	70	ILE	CG2	17.78	0.2	1
1	A	70	ILE	CD1	14.81	0.2	1
1	A	70	ILE	N	119.589	0.2	1
1	A	71	ASN	H	8.609	0.04	1
1	A	71	ASN	HA	4.361	0.04	1
1	A	71	ASN	HB2	2.773	0.04	2
1	A	71	ASN	HB3	2.955	0.04	2
1	A	71	ASN	C	176.871	0.2	1
1	A	71	ASN	CA	56.098	0.2	1
1	A	71	ASN	CB	37.98	0.2	1
1	A	71	ASN	N	119.932	0.2	1
1	A	72	MET	H	8.203	0.04	1
1	A	72	MET	HA	4.414	0.04	1
1	A	72	MET	HB2	2.151	0.04	2
1	A	72	MET	HB3	2.089	0.04	2
1	A	72	MET	C	177.643	0.2	1
1	A	72	MET	CA	57.838	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	MET	CB	33.106	0.2	1
1	A	72	MET	N	117.207	0.2	1
1	A	73	ASN	H	8.224	0.04	1
1	A	73	ASN	HA	4.996	0.04	1
1	A	73	ASN	HB2	2.908	0.04	2
1	A	73	ASN	C	176.247	0.2	1
1	A	73	ASN	CA	54.514	0.2	1
1	A	73	ASN	CB	40.081	0.2	1
1	A	73	ASN	N	114.487	0.2	1
1	A	74	LEU	H	7.619	0.04	1
1	A	74	LEU	HA	4.852	0.04	1
1	A	74	LEU	HB2	2.411	0.04	2
1	A	74	LEU	HB3	2.028	0.04	2
1	A	74	LEU	HG	1.635	0.04	1
1	A	74	LEU	HD11	1.018	0.04	1
1	A	74	LEU	HD12	1.018	0.04	1
1	A	74	LEU	HD13	1.018	0.04	1
1	A	74	LEU	HD21	1.008	0.04	1
1	A	74	LEU	HD22	1.008	0.04	1
1	A	74	LEU	HD23	1.008	0.04	1
1	A	74	LEU	C	177.946	0.2	1
1	A	74	LEU	CA	54.64	0.2	1
1	A	74	LEU	CB	42.995	0.2	1
1	A	74	LEU	CG	27.26	0.2	1
1	A	74	LEU	CD1	25.78	0.2	1
1	A	74	LEU	CD2	23.08	0.2	1
1	A	74	LEU	N	118.929	0.2	1
1	A	75	GLY	H	7.923	0.04	1
1	A	75	GLY	HA2	4.044	0.04	2
1	A	75	GLY	HA3	4.044	0.04	2
1	A	75	GLY	C	175.578	0.2	1
1	A	75	GLY	CA	46.576	0.2	1
1	A	75	GLY	N	107.269	0.2	1
1	A	76	GLY	H	8.121	0.04	1
1	A	76	GLY	HA2	4.232	0.04	2
1	A	76	GLY	HA3	3.734	0.04	2
1	A	76	GLY	C	172.881	0.2	1
1	A	76	GLY	CA	45.74	0.2	1
1	A	76	GLY	N	104.615	0.2	1
1	A	77	HIS	H	7.496	0.04	1
1	A	77	HIS	HA	5.204	0.04	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	77	HIS	HB2	2.936	0.04	2
1	A	77	HIS	HB3	3.159	0.04	2
1	A	77	HIS	C	172.514	0.2	1
1	A	77	HIS	CA	53.91	0.2	1
1	A	77	HIS	CB	32.248	0.2	1
1	A	77	HIS	N	117.092	0.2	1
1	A	78	VAL	H	8.889	0.04	1
1	A	78	VAL	HA	5.036	0.04	1
1	A	78	VAL	HB	2.438	0.04	1
1	A	78	VAL	HG11	1.157	0.04	1
1	A	78	VAL	HG12	1.157	0.04	1
1	A	78	VAL	HG13	1.157	0.04	1
1	A	78	VAL	HG21	1.032	0.04	1
1	A	78	VAL	HG22	1.032	0.04	1
1	A	78	VAL	HG23	1.032	0.04	1
1	A	78	VAL	C	175.349	0.2	1
1	A	78	VAL	CA	60.494	0.2	1
1	A	78	VAL	CB	34.753	0.2	1
1	A	78	VAL	CG1	22.75	0.2	1
1	A	78	VAL	CG2	21.07	0.2	1
1	A	78	VAL	N	115.571	0.2	1
1	A	79	ASP	H	9.188	0.04	1
1	A	79	ASP	HA	5.506	0.04	1
1	A	79	ASP	HB2	2.508	0.04	2
1	A	79	ASP	HB3	3.006	0.04	2
1	A	79	ASP	C	176.4	0.2	1
1	A	79	ASP	CA	51.767	0.2	1
1	A	79	ASP	CB	41.112	0.2	1
1	A	79	ASP	N	126.427	0.2	1
1	A	80	PHE	H	8.472	0.04	1
1	A	80	PHE	HA	3.35	0.04	1
1	A	80	PHE	HB2	2.486	0.04	2
1	A	80	PHE	HB3	2.131	0.04	2
1	A	80	PHE	HD1	6.693	0.04	3
1	A	80	PHE	HD2	6.693	0.04	3
1	A	80	PHE	HE1	7.063	0.04	3
1	A	80	PHE	HE2	7.063	0.04	3
1	A	80	PHE	HZ	7.217	0.04	1
1	A	80	PHE	C	176.411	0.2	1
1	A	80	PHE	CA	62.142	0.2	1
1	A	80	PHE	CB	38.557	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	PHE	N	118.573	0.2	1
1	A	81	ASP	H	7.697	0.04	1
1	A	81	ASP	HA	4.048	0.04	1
1	A	81	ASP	HB2	2.593	0.04	2
1	A	81	ASP	HB3	2.74	0.04	2
1	A	81	ASP	C	179.52	0.2	1
1	A	81	ASP	CA	57.661	0.2	1
1	A	81	ASP	CB	40.051	0.2	1
1	A	81	ASP	N	117.736	0.2	1
1	A	82	ASP	H	8.552	0.04	1
1	A	82	ASP	HA	4.382	0.04	1
1	A	82	ASP	HB2	2.977	0.04	2
1	A	82	ASP	HB3	2.593	0.04	2
1	A	82	ASP	C	178.307	0.2	1
1	A	82	ASP	CA	57.299	0.2	1
1	A	82	ASP	CB	41.123	0.2	1
1	A	82	ASP	N	121.901	0.2	1
1	A	83	PHE	H	8.555	0.04	1
1	A	83	PHE	HA	4.104	0.04	1
1	A	83	PHE	HB2	3.406	0.04	2
1	A	83	PHE	HB3	3.192	0.04	2
1	A	83	PHE	HD1	7.09	0.04	3
1	A	83	PHE	HD2	7.09	0.04	3
1	A	83	PHE	HE1	7.473	0.04	3
1	A	83	PHE	HE2	7.473	0.04	3
1	A	83	PHE	HZ	7.29	0.04	1
1	A	83	PHE	C	176.688	0.2	1
1	A	83	PHE	CA	61.154	0.2	1
1	A	83	PHE	CB	39.758	0.2	1
1	A	83	PHE	N	122.051	0.2	1
1	A	84	VAL	H	8.255	0.04	1
1	A	84	VAL	HA	2.986	0.04	1
1	A	84	VAL	HB	1.812	0.04	1
1	A	84	VAL	HG11	0.684	0.04	1
1	A	84	VAL	HG12	0.684	0.04	1
1	A	84	VAL	HG13	0.684	0.04	1
1	A	84	VAL	HG21	0.334	0.04	1
1	A	84	VAL	HG22	0.334	0.04	1
1	A	84	VAL	HG23	0.334	0.04	1
1	A	84	VAL	C	178.681	0.2	1
1	A	84	VAL	CA	67.086	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	84	VAL	CB	31.555	0.2	1
1	A	84	VAL	CG1	21.39	0.2	1
1	A	84	VAL	CG2	24.06	0.2	1
1	A	84	VAL	N	119.936	0.2	1
1	A	85	GLU	H	7.579	0.04	1
1	A	85	GLU	HA	3.952	0.04	1
1	A	85	GLU	HB2	2.14	0.04	2
1	A	85	GLU	C	178.419	0.2	1
1	A	85	GLU	CA	59.161	0.2	1
1	A	85	GLU	CB	29.486	0.2	1
1	A	85	GLU	N	120.098	0.2	1
1	A	86	LEU	H	7.823	0.04	1
1	A	86	LEU	HA	4.142	0.04	1
1	A	86	LEU	HB2	1.743	0.04	2
1	A	86	LEU	HB3	1.389	0.04	2
1	A	86	LEU	HG	1.818	0.04	1
1	A	86	LEU	HD11	0.816	0.04	1
1	A	86	LEU	HD12	0.816	0.04	1
1	A	86	LEU	HD13	0.816	0.04	1
1	A	86	LEU	HD21	0.852	0.04	1
1	A	86	LEU	HD22	0.852	0.04	1
1	A	86	LEU	HD23	0.852	0.04	1
1	A	86	LEU	C	178.465	0.2	1
1	A	86	LEU	CA	56.959	0.2	1
1	A	86	LEU	CB	43.038	0.2	1
1	A	86	LEU	CG	26.78	0.2	1
1	A	86	LEU	CD1	25.67	0.2	1
1	A	86	LEU	CD2	24.2	0.2	1
1	A	86	LEU	N	117.34	0.2	1
1	A	87	MET	H	8.196	0.04	1
1	A	87	MET	HA	4.348	0.04	1
1	A	87	MET	HB2	1.524	0.04	2
1	A	87	MET	HB3	1.447	0.04	2
1	A	87	MET	C	178.592	0.2	1
1	A	87	MET	CA	54.447	0.2	1
1	A	87	MET	CB	32.065	0.2	1
1	A	87	MET	N	114.402	0.2	1
1	A	88	GLY	H	8.296	0.04	1
1	A	88	GLY	HA2	4.195	0.04	2
1	A	88	GLY	HA3	3.616	0.04	2
1	A	88	GLY	CA	49.091	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	88	GLY	N	108.218	0.2	1
1	A	89	PRO	HA	4.209	0.04	1
1	A	89	PRO	HB2	2.421	0.04	2
1	A	89	PRO	HB3	1.842	0.04	2
1	A	89	PRO	C	178.721	0.2	1
1	A	89	PRO	CA	65.11	0.2	1
1	A	89	PRO	CB	32.22	0.2	1
1	A	90	LYS	H	7.043	0.04	1
1	A	90	LYS	HA	4.029	0.04	1
1	A	90	LYS	C	178.018	0.2	1
1	A	90	LYS	CA	57.619	0.2	1
1	A	90	LYS	CB	31.758	0.2	1
1	A	90	LYS	N	114.717	0.2	1
1	A	91	LEU	H	7.687	0.04	1
1	A	91	LEU	HA	4.121	0.04	1
1	A	91	LEU	HB2	1.611	0.04	2
1	A	91	LEU	C	179.155	0.2	1
1	A	91	LEU	CA	57.228	0.2	1
1	A	91	LEU	CB	41.79	0.2	1
1	A	91	LEU	N	119.101	0.2	1
1	A	92	LEU	H	7.837	0.04	1
1	A	92	LEU	HA	4.199	0.04	1
1	A	92	LEU	HB2	1.652	0.04	2
1	A	92	LEU	HB3	1.51	0.04	2
1	A	92	LEU	HG	1.668	0.04	1
1	A	92	LEU	HD11	0.754	0.04	1
1	A	92	LEU	HD12	0.754	0.04	1
1	A	92	LEU	HD13	0.754	0.04	1
1	A	92	LEU	HD21	0.748	0.04	1
1	A	92	LEU	HD22	0.748	0.04	1
1	A	92	LEU	HD23	0.748	0.04	1
1	A	92	LEU	C	177.405	0.2	1
1	A	92	LEU	CA	55.906	0.2	1
1	A	92	LEU	CB	41.937	0.2	1
1	A	92	LEU	CD1	25.27	0.2	1
1	A	92	LEU	CD2	22.99	0.2	1
1	A	92	LEU	N	117.988	0.2	1
1	A	93	ALA	H	7.429	0.04	1
1	A	93	ALA	HA	4.282	0.04	1
1	A	93	ALA	HB1	1.515	0.04	1
1	A	93	ALA	HB2	1.515	0.04	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	ALA	HB3	1.515	0.04	1
1	A	93	ALA	C	177.4	0.2	1
1	A	93	ALA	CA	53.285	0.2	1
1	A	93	ALA	CB	19.251	0.2	1
1	A	93	ALA	N	121.849	0.2	1
1	A	94	GLU	H	8.127	0.04	1
1	A	94	GLU	HA	4.423	0.04	1
1	A	94	GLU	HB2	2.162	0.04	2
1	A	94	GLU	C	176.9	0.2	1
1	A	94	GLU	CA	57.1	0.2	1
1	A	94	GLU	CB	30.15	0.2	1
1	A	94	GLU	N	118.932	0.2	1
1	A	95	THR	H	7.93	0.04	1
1	A	95	THR	HA	4.417	0.04	1
1	A	95	THR	HB	4.352	0.04	1
1	A	95	THR	HG21	1.28	0.04	1
1	A	95	THR	HG22	1.28	0.04	1
1	A	95	THR	HG23	1.28	0.04	1
1	A	95	THR	C	174.663	0.2	1
1	A	95	THR	CA	61.848	0.2	1
1	A	95	THR	CB	70.11	0.2	1
1	A	95	THR	CG2	21.83	0.2	1
1	A	95	THR	N	113.151	0.2	1
1	A	96	ALA	H	8.216	0.04	1
1	A	96	ALA	HA	4.305	0.04	1
1	A	96	ALA	HB1	1.444	0.04	1
1	A	96	ALA	HB2	1.444	0.04	1
1	A	96	ALA	HB3	1.444	0.04	1
1	A	96	ALA	C	177.477	0.2	1
1	A	96	ALA	CA	53.206	0.2	1
1	A	96	ALA	CB	19.436	0.2	1
1	A	96	ALA	N	125.432	0.2	1
1	A	97	ASP	H	8.211	0.04	1
1	A	97	ASP	C	176.233	0.2	1
1	A	97	ASP	CA	54.743	0.2	1
1	A	97	ASP	CB	41.246	0.2	1
1	A	97	ASP	N	118.477	0.2	1
1	A	98	MET	H	8.106	0.04	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	147	-0.22 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	134	0.28 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	138	-0.41 ± 0.06	None needed (< 0.5 ppm)
^{15}N	139	0.24 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 66%, i.e. 525 atoms were assigned a chemical shift out of a possible 799. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	282/290 (97%)	116/119 (97%)	112/114 (98%)	54/57 (95%)
Sidechain	228/469 (49%)	152/298 (51%)	76/146 (52%)	0/25 (0%)
Aromatic	15/40 (38%)	15/20 (75%)	0/20 (0%)	0/0 (—%)
Overall	525/799 (66%)	283/437 (65%)	188/280 (67%)	54/82 (66%)

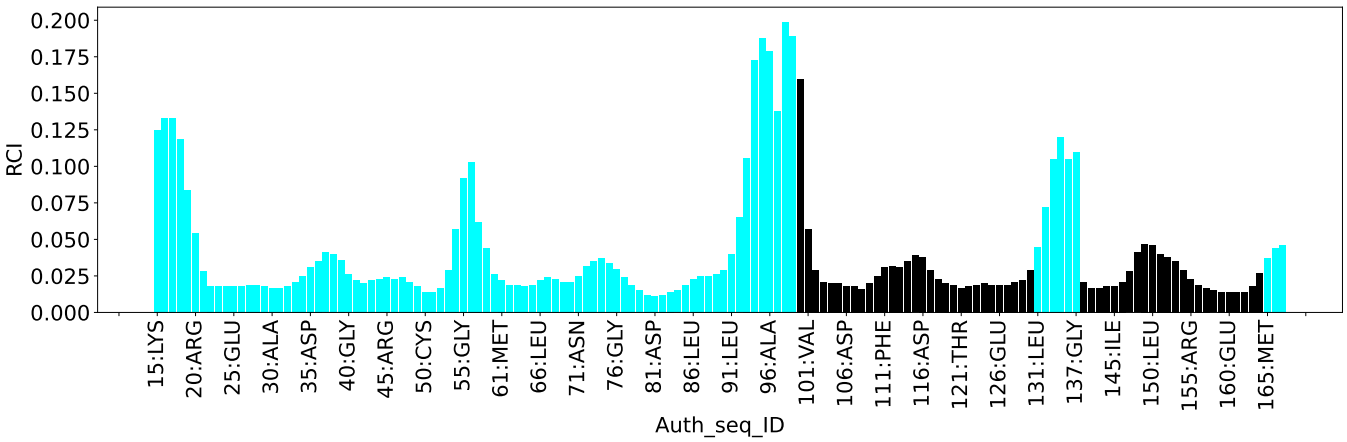
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
15:LYS
20:ARG
25:GLU
30:ALA
35:ASP
40:GLY
45:ARG
50:CYS
55:GLY
61:MET
66:LEU
71:ASN
76:GLY
81:ASP
86:LEU
91:LEU
96:ALA
101:VAL
106:ASP
111:PHE
116:ASP
121:THR
126:GLU
131:LEU
137:GLY
145:ILE
150:LEU
155:ARG
160:GLU
165:MET
Auth_seq_ID

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	596
Intra-residue (|i-j|=0)	179
Sequential (|i-j|=1)	122
Medium range (|i-j|>1 and |i-j|<5)	119
Long range (|i-j|≥5)	126
Inter-chain	0
Hydrogen bond restraints	50
Disulfide bond restraints	0
Total dihedral-angle restraints	82
Number of unmapped restraints	0
Number of restraints per residue	4.0
Number of long range restraints per residue[1]	0.8

[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)	11.7	0.2
0.2-0.5 (Medium)	11.5	0.5
>0.5 (Large)	13.1	5.39

8.2.2 Average number of dihedral-angle violations per model (i)

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.0	3.18
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

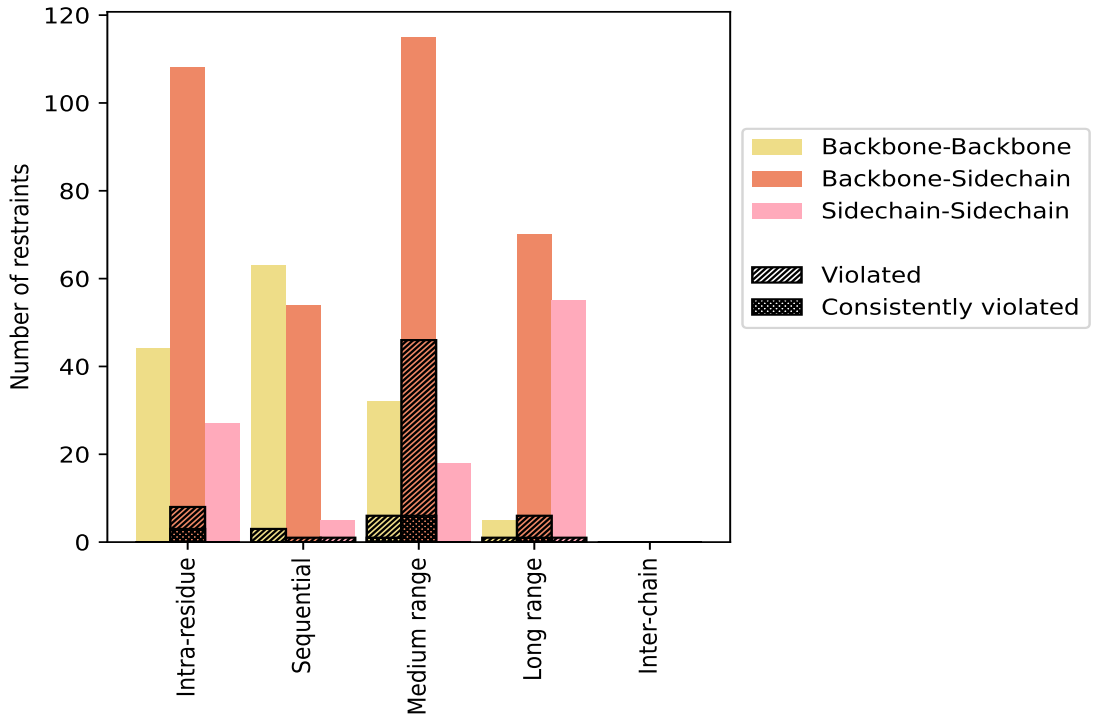
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	179	30.0	8	4.5	1.3	3	1.7	0.5
Backbone-Backbone	44	7.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	108	18.1	8	7.4	1.3	3	2.8	0.5
Sidechain-Sidechain	27	4.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	122	20.5	5	4.1	0.8	0	0.0	0.0
Backbone-Backbone	63	10.6	3	4.8	0.5	0	0.0	0.0
Backbone-Sidechain	54	9.1	1	1.9	0.2	0	0.0	0.0
Sidechain-Sidechain	5	0.8	1	20.0	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	119	20.0	11	9.2	1.8	1	0.8	0.2
Backbone-Backbone	32	5.4	6	18.8	1.0	1	3.1	0.2
Backbone-Sidechain	69	11.6	5	7.2	0.8	0	0.0	0.0
Sidechain-Sidechain	18	3.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	126	21.1	4	3.2	0.7	0	0.0	0.0
Backbone-Backbone	5	0.8	1	20.0	0.2	0	0.0	0.0
Backbone-Sidechain	66	11.1	2	3.0	0.3	0	0.0	0.0
Sidechain-Sidechain	55	9.2	1	1.8	0.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	50	8.4	45	90.0	7.6	7	14.0	1.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	596	100.0	73	12.2	12.2	11	1.8	1.8
Backbone-Backbone	144	24.2	10	6.9	1.7	1	0.7	0.2
Backbone-Sidechain	347	58.2	61	17.6	10.2	10	2.9	1.7
Sidechain-Sidechain	105	17.6	2	1.9	0.3	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	6	2	23	3	0	34	0.52	4.29	0.95	0.17
2	5	1	23	4	0	33	0.62	2.84	0.65	0.43
3	5	3	34	4	0	46	0.73	3.83	0.91	0.42
4	5	1	34	5	0	45	0.75	4.83	1.09	0.39
5	6	3	31	5	0	45	0.59	3.99	0.79	0.29
6	5	2	24	3	0	34	0.65	4.21	0.96	0.3
7	3	4	25	5	0	37	0.54	3.21	0.71	0.27
8	5	2	27	4	0	38	0.46	2.09	0.47	0.28
9	4	3	28	2	0	37	0.71	4.26	0.96	0.31
10	6	2	18	3	0	29	0.64	2.66	0.74	0.34

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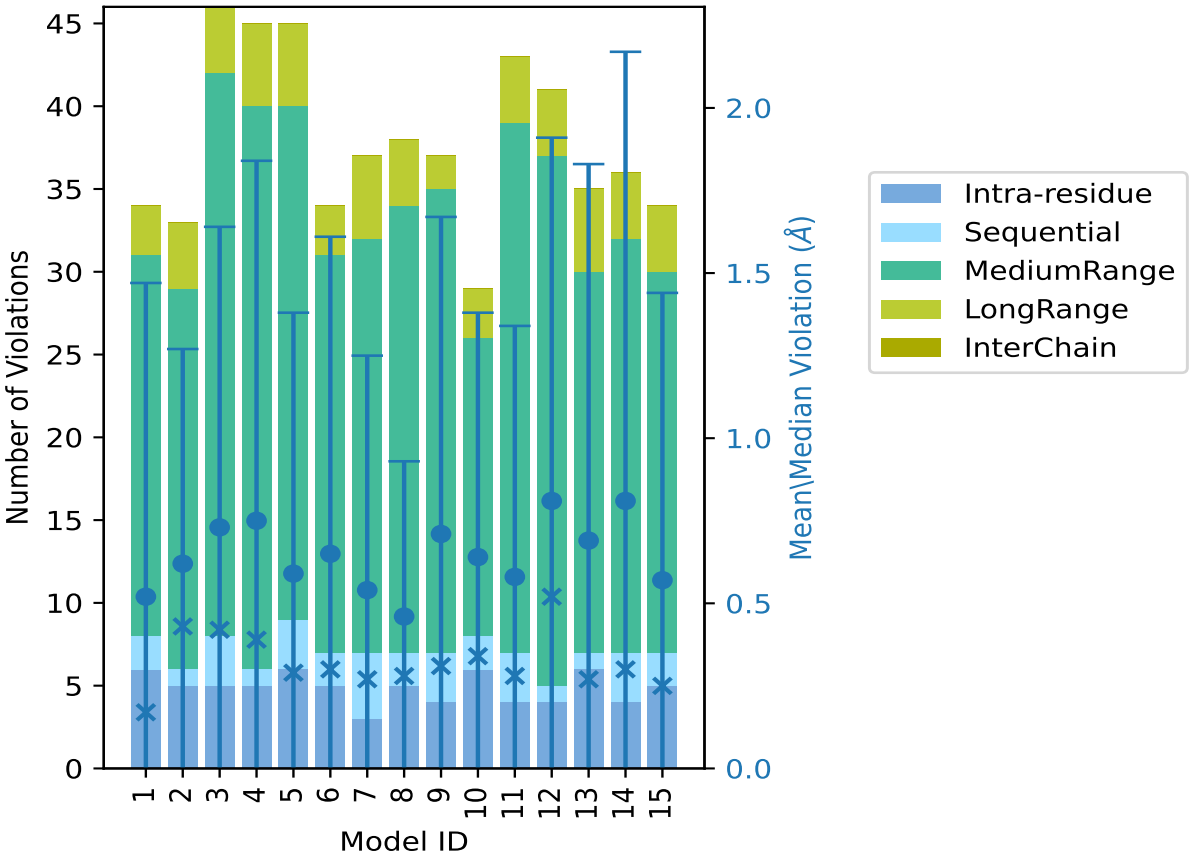
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	4	3	32	4	0	43	0.58	3.63	0.76	0.28
12	4	1	32	4	0	41	0.81	4.65	1.1	0.52
13	6	1	23	5	0	35	0.69	4.21	1.14	0.27
14	4	3	25	4	0	36	0.81	5.39	1.36	0.3
15	5	2	23	4	0	34	0.57	3.85	0.87	0.25

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

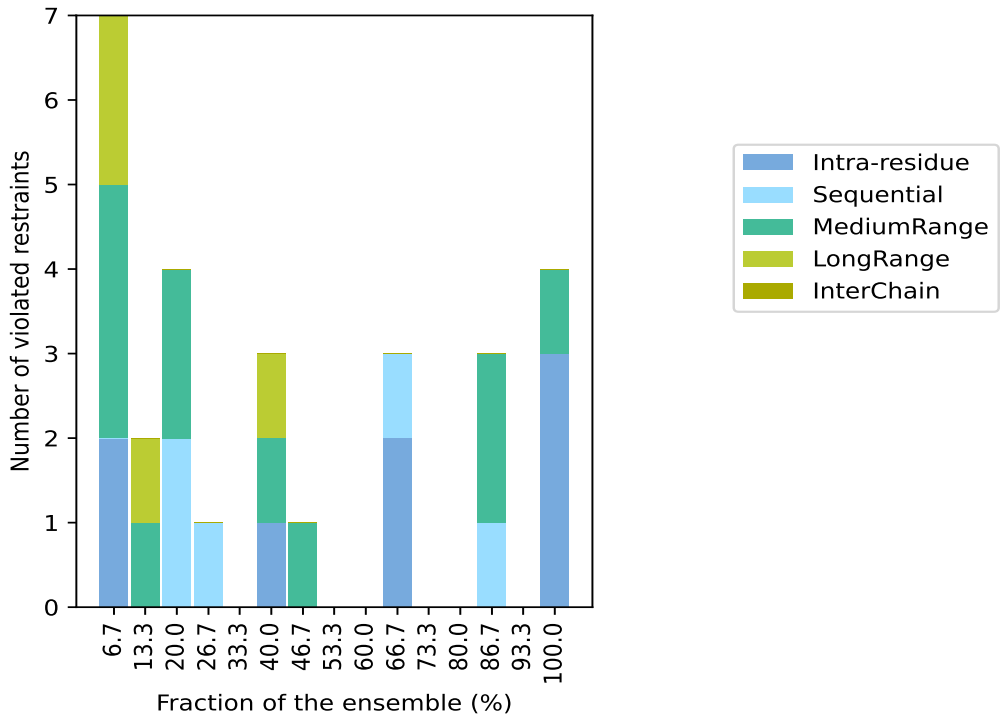
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 518(IR:171, SQ:117, MR:108, LR:122, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
2	0	3	2	0	7	1	6.7
0	0	1	1	0	2	2	13.3
0	2	2	0	0	4	3	20.0
0	1	0	0	0	1	4	26.7
0	0	0	0	0	0	5	33.3
1	0	1	1	0	3	6	40.0
0	0	1	0	0	1	7	46.7
0	0	0	0	0	0	8	53.3
0	0	0	0	0	0	9	60.0
2	1	0	0	0	3	10	66.7
0	0	0	0	0	0	11	73.3
0	0	0	0	0	0	12	80.0
0	1	2	0	0	3	13	86.7
0	0	0	0	0	0	14	93.3
3	0	1	0	0	4	15	100.0

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

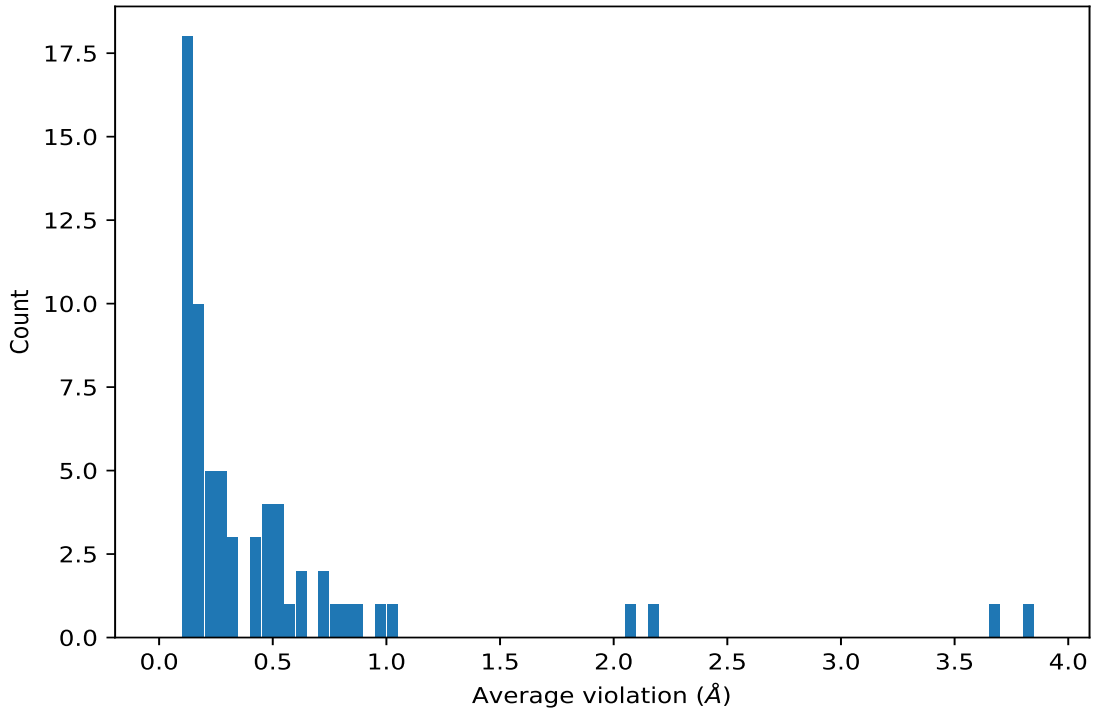
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of 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.

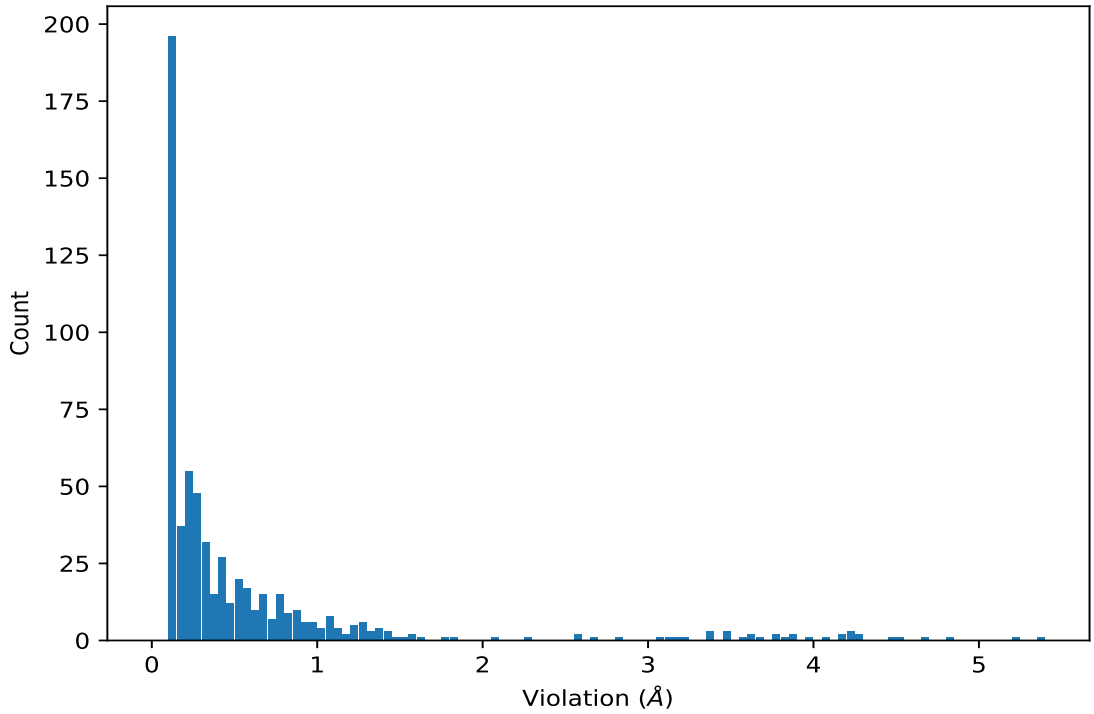
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,28)	1:139:A:ARG:O	1:143:A:GLU:H	15	3.84	0.88	3.99
(1,27)	1:139:A:ARG:O	1:143:A:GLU:N	15	3.66	0.94	3.8
(1,34)	1:142:A:GLU:O	1:146:A:ARG:H	15	1.02	0.34	0.99
(1,33)	1:142:A:GLU:O	1:146:A:ARG:N	15	0.85	0.33	0.85
(1,16)	1:122:A:SER:O	1:126:A:GLU:H	15	0.82	0.25	0.87
(1,15)	1:122:A:SER:O	1:126:A:GLU:N	15	0.7	0.24	0.73
(1,48)	1:119:A:ILE:O	1:156:A:VAL:H	15	0.43	0.26	0.37
(2,336)	1:121:A:THR:H	1:123:A:GLU:H	15	0.2	0.04	0.21
(2,174)	1:162:A:VAL:HA	1:162:A:VAL:HB	15	0.11	0.01	0.11
(2,105)	1:113:A:THR:HA	1:113:A:THR:HB	15	0.11	0.01	0.11

[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)
(1,28)	1:139:A:ARG:O	1:143:A:GLU:H	14	5.39
(1,27)	1:139:A:ARG:O	1:143:A:GLU:N	14	5.22
(1,28)	1:139:A:ARG:O	1:143:A:GLU:H	4	4.83
(1,28)	1:139:A:ARG:O	1:143:A:GLU:H	12	4.65
(1,27)	1:139:A:ARG:O	1:143:A:GLU:N	4	4.5
(1,27)	1:139:A:ARG:O	1:143:A:GLU:N	12	4.47
(1,28)	1:139:A:ARG:O	1:143:A:GLU:H	1	4.29
(1,28)	1:139:A:ARG:O	1:143:A:GLU:H	9	4.26
(1,27)	1:139:A:ARG:O	1:143:A:GLU:N	9	4.24
(1,28)	1:139:A:ARG:O	1:143:A:GLU:H	6	4.21

10 Dihedral-angle violation analysis

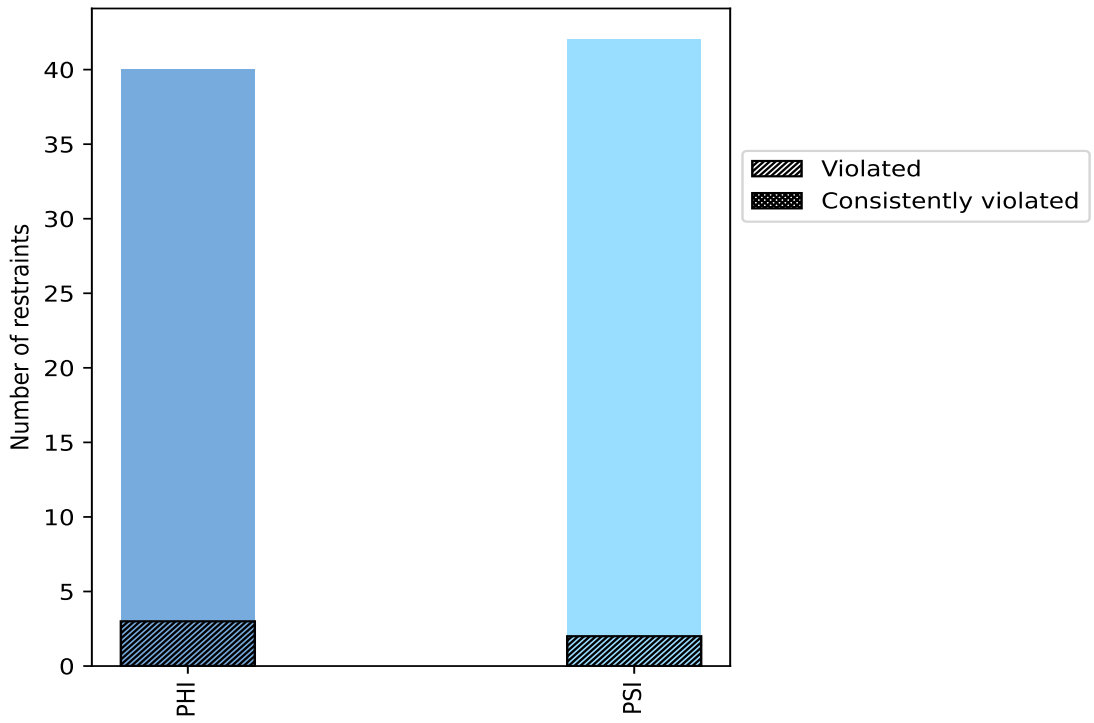
10.1 Summary of dihedral-angle violations

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]
PHI	40	48.8	3	7.5	3.7	0	0.0	0.0
PSI	42	51.2	2	4.8	2.4	0	0.0	0.0
Total	82	100.0	5	6.1	6.1	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



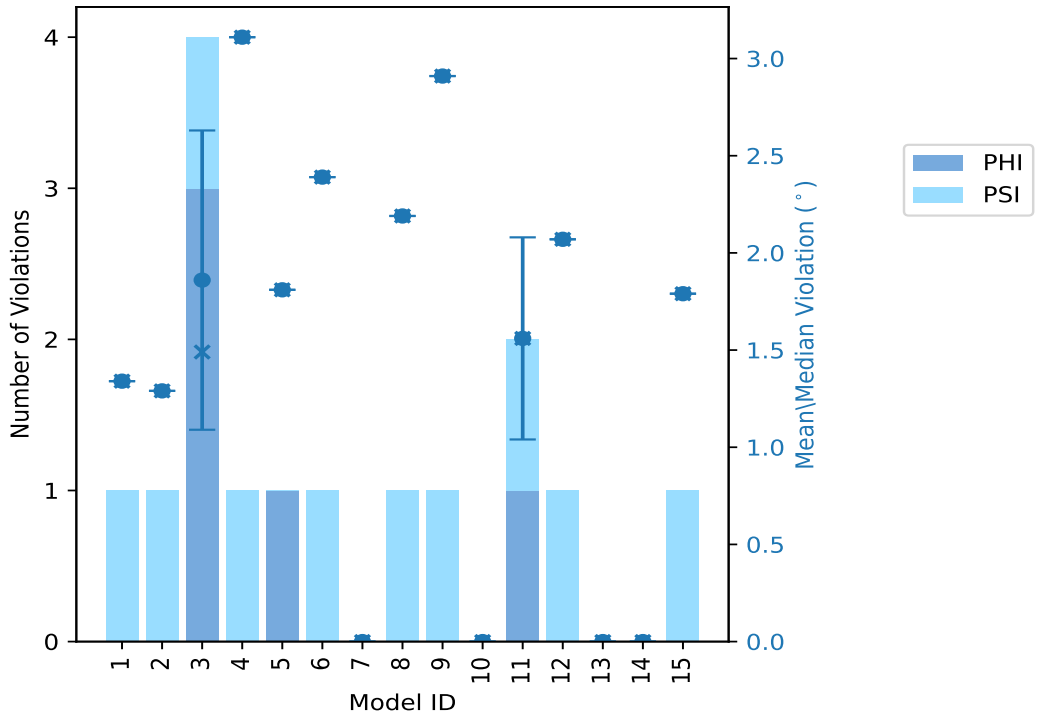
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	1	1	1.34	1.34	0.0	1.34
2	0	1	1	1.29	1.29	0.0	1.29
3	3	1	4	1.86	3.18	0.77	1.49
4	0	1	1	3.11	3.11	0.0	3.11
5	1	0	1	1.81	1.81	0.0	1.81
6	0	1	1	2.39	2.39	0.0	2.39
7	0	0	0	0.0	0.0	0.0	0.0
8	0	1	1	2.19	2.19	0.0	2.19
9	0	1	1	2.91	2.91	0.0	2.91
10	0	0	0	0.0	0.0	0.0	0.0
11	1	1	2	1.56	2.08	0.52	1.56
12	0	1	1	2.07	2.07	0.0	2.07
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	1	1	1.79	1.79	0.0	1.79

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

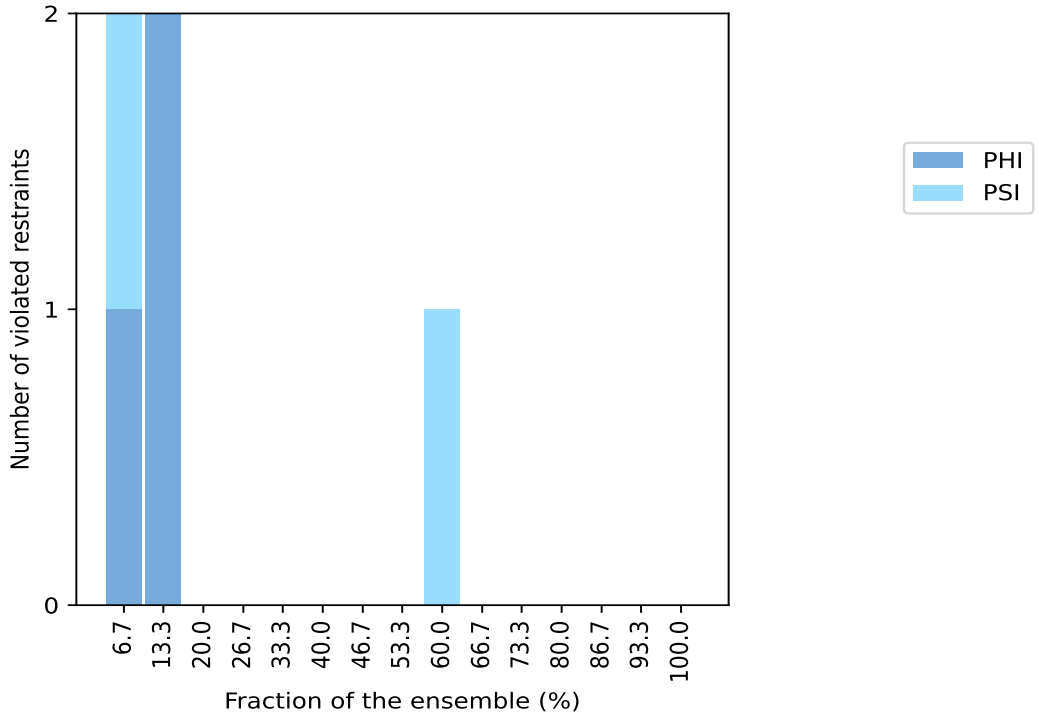
10.3 Dihedral-angle violation statistics for the ensemble (i)

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]	%
1	1	2	1	6.7
2	0	2	2	13.3
0	0	0	3	20.0
0	0	0	4	26.7
0	0	0	5	33.3
0	0	0	6	40.0
0	0	0	7	46.7
0	0	0	8	53.3
0	1	1	9	60.0
0	0	0	10	66.7
0	0	0	11	73.3
0	0	0	12	80.0
0	0	0	13	86.7
0	0	0	14	93.3
0	0	0	15	100.0

[1] Number of models with violations

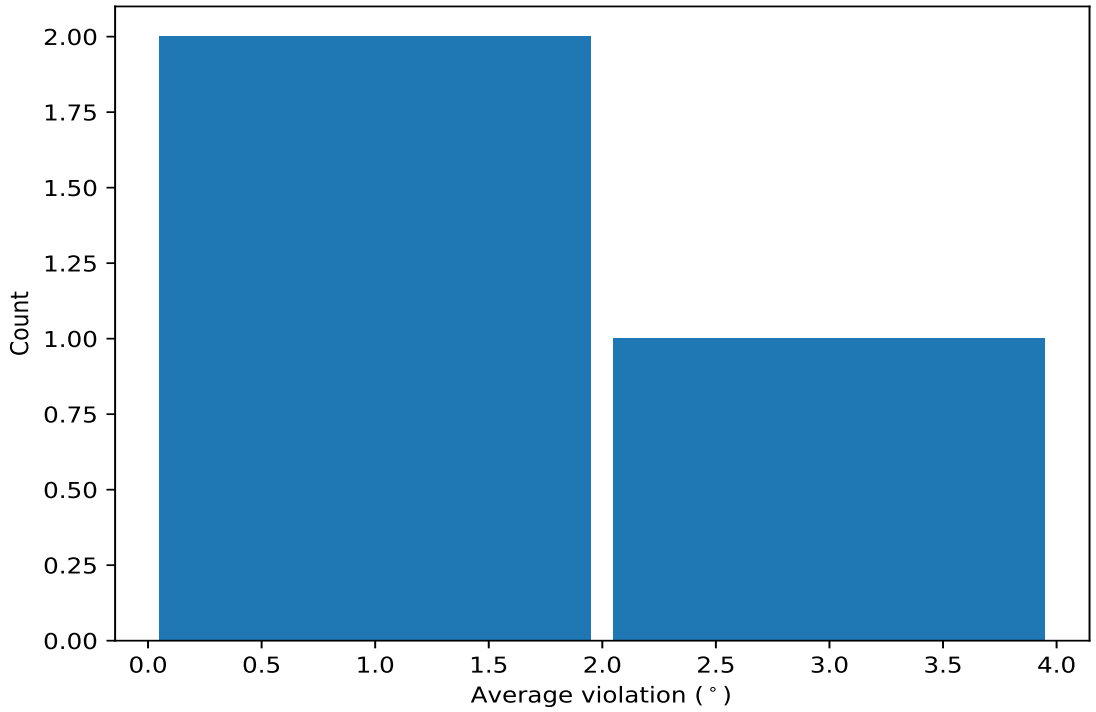
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



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

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

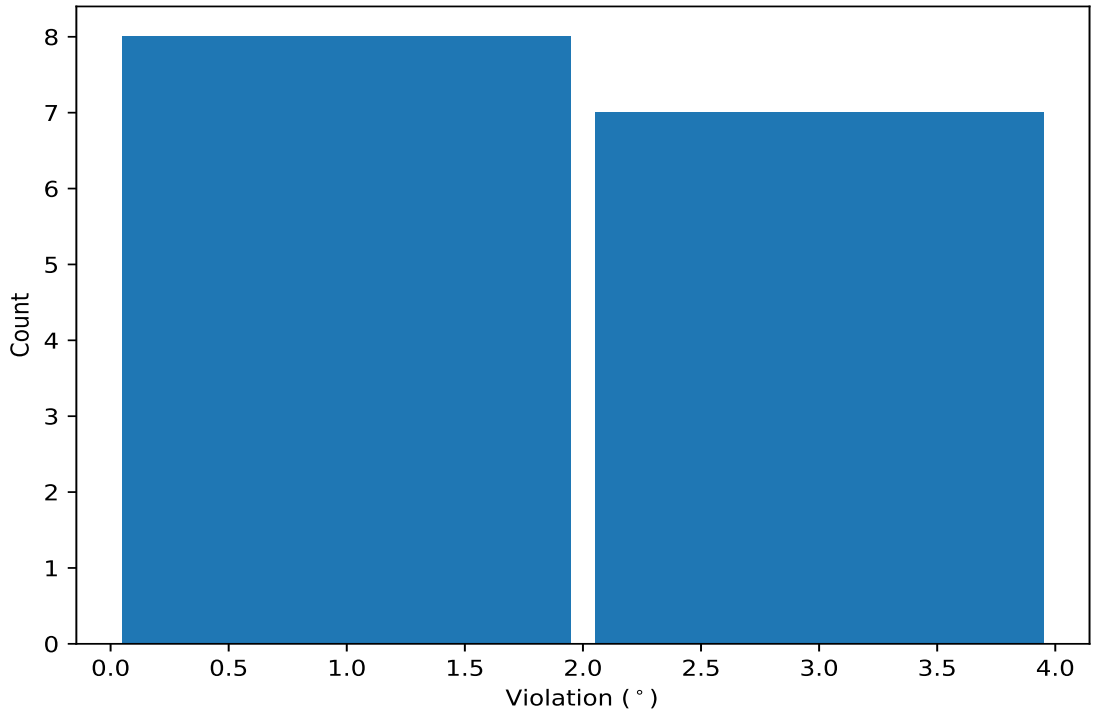
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,65)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	9	2.22	0.72	2.19
(1,25)	1:142:A:GLU:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	2	1.84	0.24	1.84
(1,4)	1:103:A:GLU:C	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	2	1.54	0.26	1.54

[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 (°)
(1,65)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	3	3.18
(1,65)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	4	3.11
(1,65)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	9	2.91
(1,65)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	6	2.39
(1,65)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	8	2.19
(1,25)	1:142:A:GLU:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	11	2.08
(1,65)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	12	2.07
(1,4)	1:103:A:GLU:C	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	5	1.81
(1,65)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	15	1.79
(1,25)	1:142:A:GLU:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	3	1.6