wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2M28
BMRB ID	:	18877
Title	:	NMR structure of Ca2+ bound CaBP4 C-domain
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Deposited on	:	2012-12-17

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:

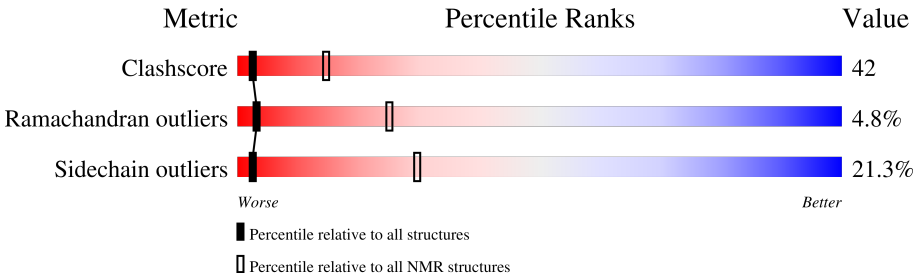
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 65%.

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	171	8% 19% 5% 10% 58%

2 Ensemble composition and analysis

This entry contains 14 models. Model 13 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:204-A:232, A:244-A:269 (55)	0.69	13

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	1, 6, 8, 9, 10, 11, 13
2	2, 7, 12
3	4, 5
Single-model clusters	3; 14

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1126 atoms, of which 555 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium-binding protein 4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	72	1124	352	555	98	114	5	0

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

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	2	2	2

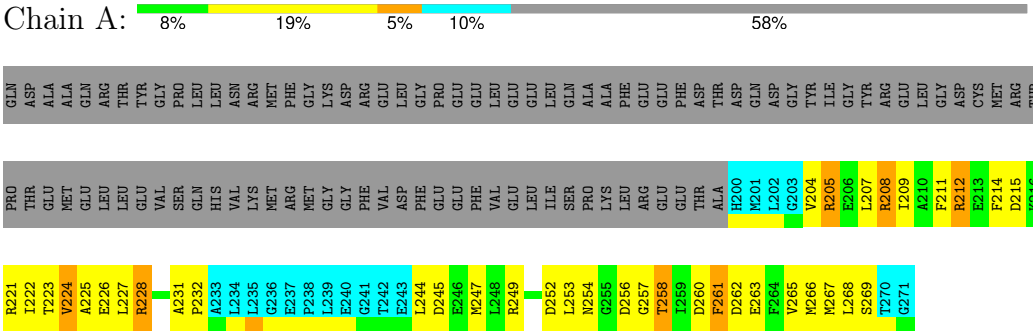
4 Residue-property plots

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: Calcium-binding protein 4

Chain A:

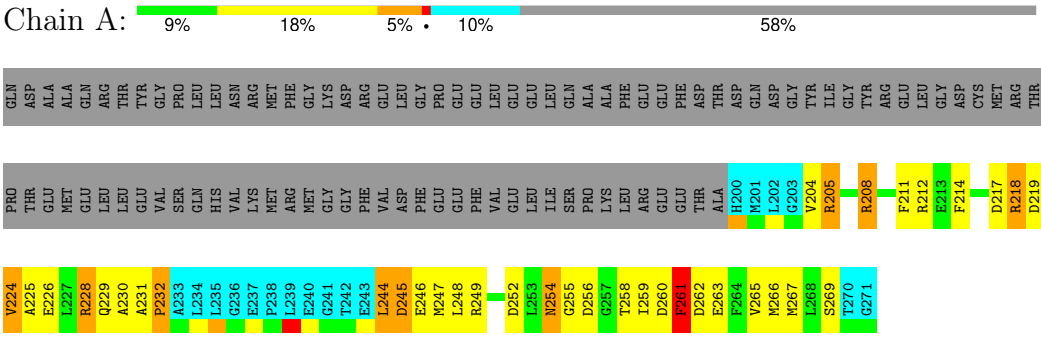


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 13. Colouring as in section 4.1 above.

• Molecule 1: Calcium-binding protein 4

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 70 calculated structures, 14 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	
X-PLOR NIH	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	1471
Number of shifts mapped to atoms	652
Number of unparsed shifts	0
Number of shifts with mapping errors	819
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	65%

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.

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	6.1±0.7
All	All	0	86

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	228	ARG	Sidechain	14
1	A	205	ARG	Sidechain	13
1	A	212	ARG	Sidechain	13
1	A	249	ARG	Sidechain	13
1	A	218	ARG	Sidechain	12

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	449	439	439	37±6
All	All	6314	6146	6146	522

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 42.

5 of 198 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:244:LEU:HD13	1:A:244:LEU:H	0.99	1.11	4	1
1:A:223:THR:HG22	1:A:258:THR:HG22	0.86	1.47	10	11
1:A:244:LEU:HD22	1:A:245:ASP:N	0.82	1.87	4	1
1:A:244:LEU:H	1:A:244:LEU:CD1	0.77	1.91	4	1
1:A:244:LEU:HD13	1:A:244:LEU:N	0.76	1.94	4	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	55/171 (32%)	43±2 (79±3%)	9±2 (17±3%)	3±1 (5±2%)	3	25
All	All	770/2394 (32%)	605 (79%)	128 (17%)	37 (5%)	3	25

5 of 10 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	224	VAL	12
1	A	269	SER	7
1	A	261	PHE	6
1	A	205	ARG	3
1	A	245	ASP	3

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	48/145 (33%)	38±2 (79±4%)	10±2 (21±4%)	2 30
All	All	672/2030 (33%)	529 (79%)	143 (21%)	2 30

5 of 37 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	261	PHE	12
1	A	217	ASP	11
1	A	258	THR	9
1	A	244	LEU	8
1	A	254	ASN	7

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

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

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 65% for the well-defined parts and 66% 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	1471
Number of shifts mapped to atoms	652
Number of unparsed shifts	0
Number of shifts with mapping errors	819
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 819) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	GLN	H	8.389	0.02	1
1	A	101	GLN	HA	4.319	0.02	1
1	A	101	GLN	HB2	2.126	0.02	2
1	A	101	GLN	HB3	2.015	0.02	2
1	A	101	GLN	C	175.8	0.3	1
1	A	101	GLN	CA	56.25	0.3	1
1	A	101	GLN	CB	29.45	0.3	1
1	A	101	GLN	N	121.5	0.32	1
1	A	102	ASP	H	8.327	0.02	1
1	A	102	ASP	HA	4.57	0.02	1
1	A	102	ASP	HB2	2.69	0.02	2
1	A	102	ASP	HB3	2.7	0.02	2
1	A	102	ASP	C	176.3	0.3	1
1	A	102	ASP	CA	54.75	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	102	ASP	CB	41.11	0.3	1
1	A	102	ASP	N	121.2	0.3	1
1	A	103	ALA	H	8.17	0.02	1
1	A	103	ALA	HA	4.23	0.02	1
1	A	103	ALA	HB1	1.42	0.02	1
1	A	103	ALA	HB2	1.42	0.02	1
1	A	103	ALA	HB3	1.42	0.02	1
1	A	103	ALA	C	178.0	0.3	1
1	A	103	ALA	CA	53.29	0.3	1
1	A	103	ALA	CB	18.84	0.3	1
1	A	103	ALA	N	123.9	0.3	1
1	A	104	ALA	H	8.229	0.02	1
1	A	104	ALA	HA	4.229	0.02	1
1	A	104	ALA	HB1	1.429	0.02	1
1	A	104	ALA	HB2	1.429	0.02	1
1	A	104	ALA	HB3	1.429	0.02	1
1	A	104	ALA	C	178.0	0.3	1
1	A	104	ALA	CA	53.2	0.3	1
1	A	104	ALA	CB	18.65	0.3	1
1	A	104	ALA	N	122.1	0.3	1
1	A	105	GLN	H	8.144	0.02	1
1	A	105	GLN	HA	4.23	0.02	1
1	A	105	GLN	HB2	2.03	0.02	2
1	A	105	GLN	HB3	2.12	0.02	2
1	A	105	GLN	HG2	2.39	0.02	2
1	A	105	GLN	HE21	6.783	0.02	2
1	A	105	GLN	HE22	7.464	0.02	2
1	A	105	GLN	C	176.3	0.3	1
1	A	105	GLN	CA	56.33	0.3	1
1	A	105	GLN	CB	28.91	0.3	1
1	A	105	GLN	CG	34.02	0.3	1
1	A	105	GLN	N	118.6	0.3	1
1	A	105	GLN	NE2	112.3	0.3	1
1	A	106	ARG	H	8.195	0.02	1
1	A	106	ARG	HA	4.299	0.02	1
1	A	106	ARG	HB2	1.742	0.02	2
1	A	106	ARG	HB3	1.72	0.02	2
1	A	106	ARG	HG2	1.539	0.02	2
1	A	106	ARG	HG3	1.599	0.02	2
1	A	106	ARG	C	176.4	0.3	1
1	A	106	ARG	CA	56.31	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	ARG	CB	29.22	0.3	1
1	A	106	ARG	CG	27.45	0.3	1
1	A	106	ARG	N	121.5	0.3	1
1	A	107	THR	H	8.233	0.02	1
1	A	107	THR	HA	4.258	0.02	1
1	A	107	THR	HB	4.05	0.02	1
1	A	107	THR	HG21	1.009	0.02	1
1	A	107	THR	HG22	1.009	0.02	1
1	A	107	THR	HG23	1.009	0.02	1
1	A	107	THR	CA	62.61	0.3	1
1	A	107	THR	CB	69.72	0.3	1
1	A	107	THR	CG2	21.48	0.3	1
1	A	107	THR	N	115.7	0.3	1
1	A	108	TYR	H	8.59	0.02	1
1	A	108	TYR	HA	4.57	0.02	1
1	A	108	TYR	HB2	3.113	0.02	2
1	A	108	TYR	HB3	2.892	0.02	2
1	A	108	TYR	CA	58.8	0.3	1
1	A	108	TYR	CB	38.55	0.3	1
1	A	108	TYR	N	120.2	0.3	1
1	A	109	GLY	H	8.365	0.02	1
1	A	109	GLY	HA2	3.89	0.02	2
1	A	109	GLY	HA3	4.153	0.02	2
1	A	109	GLY	CA	47.55	0.3	1
1	A	109	GLY	N	109.4	0.3	1
1	A	110	PRO	C	178.6	0.3	1
1	A	110	PRO	CA	64.92	0.3	1
1	A	110	PRO	CB	31.6	0.3	1
1	A	111	LEU	H	7.666	0.02	1
1	A	111	LEU	HA	4.158	0.02	1
1	A	111	LEU	HB2	1.747	0.02	2
1	A	111	LEU	CA	57.67	0.3	1
1	A	111	LEU	CB	41.5	0.3	1
1	A	111	LEU	N	118.5	0.3	1
1	A	112	LEU	H	8.11	0.02	1
1	A	112	LEU	HA	4.143	0.02	1
1	A	112	LEU	C	178.5	0.3	1
1	A	112	LEU	CA	57.47	0.3	1
1	A	112	LEU	CB	41.19	0.3	1
1	A	112	LEU	N	118.7	0.3	1
1	A	113	ASN	H	8.226	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	113	ASN	HA	4.479	0.02	1
1	A	113	ASN	HB2	2.815	0.02	2
1	A	113	ASN	HB3	2.833	0.02	2
1	A	113	ASN	C	177.3	0.3	1
1	A	113	ASN	CA	56.02	0.3	1
1	A	113	ASN	CB	38.6	0.3	1
1	A	113	ASN	N	116.4	0.3	1
1	A	114	ARG	H	7.819	0.02	1
1	A	114	ARG	C	177.7	0.3	1
1	A	114	ARG	CA	57.96	0.3	1
1	A	114	ARG	CB	29.9	0.3	1
1	A	114	ARG	N	118.6	0.3	1
1	A	115	MET	H	7.9	0.02	1
1	A	115	MET	HA	4.184	0.02	1
1	A	115	MET	C	176.4	0.3	1
1	A	115	MET	CA	57.67	0.3	1
1	A	115	MET	CB	32.84	0.3	1
1	A	115	MET	N	117.2	0.3	1
1	A	116	PHE	H	7.789	0.02	1
1	A	116	PHE	HA	4.78	0.02	1
1	A	116	PHE	HB2	2.88	0.02	2
1	A	116	PHE	HB3	3.37	0.02	2
1	A	116	PHE	HD1	7.345	0.02	3
1	A	116	PHE	HE1	7.234	0.02	3
1	A	116	PHE	HZ	7.148	0.02	1
1	A	116	PHE	C	176.0	0.3	1
1	A	116	PHE	CA	57.7	0.3	1
1	A	116	PHE	CB	39.41	0.3	1
1	A	116	PHE	N	115.6	0.3	1
1	A	117	GLY	H	8.093	0.02	1
1	A	117	GLY	HA2	4.007	0.02	2
1	A	117	GLY	HA3	4.114	0.02	2
1	A	117	GLY	C	174.5	0.3	1
1	A	117	GLY	CA	45.74	0.3	1
1	A	117	GLY	N	108.4	0.3	1
1	A	118	LYS	H	8.087	0.02	1
1	A	118	LYS	HA	4.287	0.02	1
1	A	118	LYS	HB2	1.796	0.02	2
1	A	118	LYS	HB3	1.853	0.02	2
1	A	118	LYS	HG2	1.445	0.02	2
1	A	118	LYS	HD2	1.692	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	118	LYS	HE2	3.009	0.02	2
1	A	118	LYS	C	176.2	0.3	1
1	A	118	LYS	CA	56.86	0.3	1
1	A	118	LYS	CB	32.55	0.3	1
1	A	118	LYS	CG	24.61	0.3	1
1	A	118	LYS	CD	29.08	0.3	1
1	A	118	LYS	CE	42.04	0.3	1
1	A	118	LYS	N	120.0	0.3	1
1	A	119	ASP	H	8.344	0.02	1
1	A	119	ASP	HA	4.622	0.02	1
1	A	119	ASP	HB2	2.613	0.02	2
1	A	119	ASP	HB3	2.71	0.02	2
1	A	119	ASP	C	175.8	0.3	1
1	A	119	ASP	CA	54.46	0.3	1
1	A	119	ASP	CB	40.83	0.3	1
1	A	119	ASP	N	119.8	0.3	1
1	A	120	ARG	H	7.894	0.02	1
1	A	120	ARG	HA	4.33	0.02	1
1	A	120	ARG	HB2	1.794	0.02	2
1	A	120	ARG	C	175.7	0.3	1
1	A	120	ARG	CA	56.0	0.3	1
1	A	120	ARG	CB	30.46	0.3	1
1	A	120	ARG	N	120.2	0.3	1
1	A	121	GLU	H	8.364	0.02	1
1	A	121	GLU	HA	4.337	0.02	1
1	A	121	GLU	HB2	1.895	0.02	2
1	A	121	GLU	HB3	2.017	0.02	2
1	A	121	GLU	C	176.3	0.3	1
1	A	121	GLU	CA	55.9	0.3	1
1	A	121	GLU	CB	30.31	0.3	1
1	A	121	GLU	N	122.3	0.3	1
1	A	122	LEU	H	8.41	0.02	1
1	A	122	LEU	HA	4.332	0.02	1
1	A	122	LEU	HB2	1.456	0.02	2
1	A	122	LEU	HB3	1.68	0.02	2
1	A	122	LEU	HD11	0.805	0.02	1
1	A	122	LEU	HD12	0.805	0.02	1
1	A	122	LEU	HD13	0.805	0.02	1
1	A	122	LEU	HD21	0.774	0.02	1
1	A	122	LEU	HD22	0.774	0.02	1
1	A	122	LEU	HD23	0.774	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	122	LEU	C	177.3	0.3	1
1	A	122	LEU	CA	55.49	0.3	1
1	A	122	LEU	CB	41.62	0.3	1
1	A	122	LEU	CD1	25.74	0.3	1
1	A	122	LEU	CD2	23.97	0.3	1
1	A	122	LEU	N	123.8	0.3	1
1	A	123	GLY	H	8.894	0.02	1
1	A	123	GLY	HA2	4.0	0.02	2
1	A	123	GLY	HA3	4.472	0.02	2
1	A	123	GLY	CA	44.32	0.3	1
1	A	123	GLY	N	111.6	0.3	1
1	A	124	PRO	HA	4.28	0.02	1
1	A	124	PRO	HB2	2.029	0.02	2
1	A	124	PRO	HB3	2.399	0.02	2
1	A	124	PRO	C	179.4	0.3	1
1	A	124	PRO	CA	65.62	0.3	1
1	A	124	PRO	CB	31.46	0.3	1
1	A	125	GLU	H	9.069	0.02	1
1	A	125	GLU	HA	4.194	0.02	1
1	A	125	GLU	C	179.2	0.3	1
1	A	125	GLU	CA	59.58	0.3	1
1	A	125	GLU	CB	28.2	0.3	1
1	A	125	GLU	N	117.9	0.3	1
1	A	126	GLU	H	7.833	0.02	1
1	A	126	GLU	HA	4.223	0.02	1
1	A	126	GLU	HB2	2.062	0.02	2
1	A	126	GLU	HB3	2.326	0.02	2
1	A	126	GLU	HG2	2.383	0.02	2
1	A	126	GLU	C	179.2	0.3	1
1	A	126	GLU	CA	59.32	0.3	1
1	A	126	GLU	CB	29.76	0.3	1
1	A	126	GLU	CG	37.67	0.3	1
1	A	126	GLU	N	120.7	0.3	1
1	A	127	LEU	H	8.3	0.02	1
1	A	127	LEU	HA	4.172	0.02	1
1	A	127	LEU	HB2	1.814	0.02	2
1	A	127	LEU	HB3	1.724	0.02	2
1	A	127	LEU	HD11	0.94	0.02	1
1	A	127	LEU	HD12	0.94	0.02	1
1	A	127	LEU	HD13	0.94	0.02	1
1	A	127	LEU	HD21	0.973	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	LEU	HD22	0.973	0.02	1
1	A	127	LEU	HD23	0.973	0.02	1
1	A	127	LEU	C	179.2	0.3	1
1	A	127	LEU	CA	58.39	0.3	1
1	A	127	LEU	CB	41.19	0.3	1
1	A	127	LEU	CD1	24.88	0.3	1
1	A	127	LEU	CD2	24.4	0.3	1
1	A	127	LEU	N	119.9	0.3	1
1	A	128	GLU	H	8.085	0.02	1
1	A	128	GLU	HA	4.171	0.02	1
1	A	128	GLU	HB2	2.195	0.02	2
1	A	128	GLU	HB3	2.224	0.02	2
1	A	128	GLU	HG2	2.526	0.02	2
1	A	128	GLU	C	179.4	0.3	1
1	A	128	GLU	CA	59.69	0.3	1
1	A	128	GLU	CB	29.01	0.3	1
1	A	128	GLU	CG	36.43	0.3	1
1	A	128	GLU	N	119.2	0.3	1
1	A	129	GLU	H	7.712	0.02	1
1	A	129	GLU	HA	4.19	0.02	1
1	A	129	GLU	HB2	2.27	0.02	2
1	A	129	GLU	HG2	2.526	0.02	2
1	A	129	GLU	C	179.7	0.3	1
1	A	129	GLU	CA	59.45	0.3	1
1	A	129	GLU	CB	29.14	0.3	1
1	A	129	GLU	CG	36.35	0.3	1
1	A	129	GLU	N	120.2	0.3	1
1	A	130	LEU	H	8.161	0.02	1
1	A	130	LEU	HA	4.367	0.02	1
1	A	130	LEU	HB2	2.14	0.02	2
1	A	130	LEU	HB3	2.338	0.02	2
1	A	130	LEU	C	178.6	0.3	1
1	A	130	LEU	CA	58.5	0.3	1
1	A	130	LEU	CB	41.34	0.3	1
1	A	130	LEU	N	120.3	0.3	1
1	A	131	GLN	H	8.747	0.02	1
1	A	131	GLN	HA	3.711	0.02	1
1	A	131	GLN	HB2	2.009	0.02	2
1	A	131	GLN	HB3	1.807	0.02	2
1	A	131	GLN	HG2	1.88	0.02	2
1	A	131	GLN	HG3	1.797	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	131	GLN	HE21	6.364	0.02	2
1	A	131	GLN	HE22	7.039	0.02	2
1	A	131	GLN	C	177.8	0.3	1
1	A	131	GLN	CA	59.3	0.3	1
1	A	131	GLN	CB	27.66	0.3	1
1	A	131	GLN	CG	33.52	0.3	1
1	A	131	GLN	N	120.2	0.3	1
1	A	131	GLN	NE2	110.4	0.3	1
1	A	132	ALA	H	7.991	0.02	1
1	A	132	ALA	HA	4.168	0.02	1
1	A	132	ALA	HB1	1.555	0.02	1
1	A	132	ALA	HB2	1.555	0.02	1
1	A	132	ALA	HB3	1.555	0.02	1
1	A	132	ALA	C	180.6	0.3	1
1	A	132	ALA	CA	54.94	0.3	1
1	A	132	ALA	CB	17.61	0.3	1
1	A	132	ALA	N	120.6	0.3	1
1	A	133	ALA	H	7.766	0.02	1
1	A	133	ALA	HA	4.34	0.02	1
1	A	133	ALA	HB1	1.69	0.02	1
1	A	133	ALA	HB2	1.69	0.02	1
1	A	133	ALA	HB3	1.69	0.02	1
1	A	133	ALA	C	178.5	0.3	1
1	A	133	ALA	CA	55.05	0.3	1
1	A	133	ALA	CB	18.14	0.3	1
1	A	133	ALA	N	120.9	0.3	1
1	A	134	PHE	H	8.373	0.02	1
1	A	134	PHE	HA	3.69	0.02	1
1	A	134	PHE	HB2	2.89	0.02	2
1	A	134	PHE	HB3	3.27	0.02	2
1	A	134	PHE	HD1	6.584	0.02	3
1	A	134	PHE	HE1	6.961	0.02	3
1	A	134	PHE	HZ	7.417	0.02	1
1	A	134	PHE	C	177.4	0.3	1
1	A	134	PHE	CA	62.15	0.3	1
1	A	134	PHE	CB	39.88	0.3	1
1	A	134	PHE	N	119.2	0.3	1
1	A	135	GLU	H	8.527	0.02	1
1	A	135	GLU	HA	3.976	0.02	1
1	A	135	GLU	HB2	2.126	0.02	2
1	A	135	GLU	C	179.1	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	135	GLU	CA	59.3	0.3	1
1	A	135	GLU	CB	29.1	0.3	1
1	A	135	GLU	N	115.4	0.3	1
1	A	136	GLU	H	7.631	0.02	1
1	A	136	GLU	HA	3.892	0.02	1
1	A	136	GLU	HB2	2.093	0.02	2
1	A	136	GLU	HG2	2.085	0.02	2
1	A	136	GLU	HG3	1.865	0.02	2
1	A	136	GLU	C	177.7	0.3	1
1	A	136	GLU	CA	58.77	0.3	1
1	A	136	GLU	CB	28.77	0.3	1
1	A	136	GLU	CG	35.74	0.3	1
1	A	136	GLU	N	118.2	0.3	1
1	A	137	PHE	H	7.42	0.02	1
1	A	137	PHE	HA	4.29	0.02	1
1	A	137	PHE	HB2	2.66	0.02	2
1	A	137	PHE	HB3	3.04	0.02	2
1	A	137	PHE	HD1	7.552	0.02	3
1	A	137	PHE	HE1	7.377	0.02	3
1	A	137	PHE	HZ	7.204	0.02	1
1	A	137	PHE	C	175.8	0.3	1
1	A	137	PHE	CA	59.81	0.3	1
1	A	137	PHE	CB	39.34	0.3	1
1	A	137	PHE	N	114.7	0.3	1
1	A	138	ASP	H	7.735	0.02	1
1	A	138	ASP	HA	5.0	0.02	1
1	A	138	ASP	HB2	2.724	0.02	2
1	A	138	ASP	HB3	1.907	0.02	2
1	A	138	ASP	C	178.5	0.3	1
1	A	138	ASP	CA	52.52	0.3	1
1	A	138	ASP	CB	38.34	0.3	1
1	A	138	ASP	N	122.3	0.3	1
1	A	139	THR	H	7.86	0.02	1
1	A	139	THR	HA	3.99	0.02	1
1	A	139	THR	HB	4.285	0.02	1
1	A	139	THR	HG21	1.284	0.02	1
1	A	139	THR	HG22	1.284	0.02	1
1	A	139	THR	HG23	1.284	0.02	1
1	A	139	THR	C	175.6	0.3	1
1	A	139	THR	CA	65.16	0.3	1
1	A	139	THR	CB	68.54	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	139	THR	CG2	22.32	0.3	1
1	A	139	THR	N	114.9	0.3	1
1	A	140	ASP	H	8.193	0.02	1
1	A	140	ASP	HA	4.603	0.02	1
1	A	140	ASP	HB2	3.01	0.02	2
1	A	140	ASP	C	175.3	0.3	1
1	A	140	ASP	CA	52.99	0.3	1
1	A	140	ASP	CB	39.1	0.3	1
1	A	140	ASP	N	116.9	0.3	1
1	A	141	GLN	H	7.733	0.02	1
1	A	141	GLN	HA	3.949	0.02	1
1	A	141	GLN	HB2	2.17	0.02	2
1	A	141	GLN	HB3	2.374	0.02	2
1	A	141	GLN	HG2	2.25	0.02	2
1	A	141	GLN	HG3	2.34	0.02	2
1	A	141	GLN	HE21	7.547	0.02	2
1	A	141	GLN	HE22	6.718	0.02	2
1	A	141	GLN	C	175.2	0.3	1
1	A	141	GLN	CA	57.25	0.3	1
1	A	141	GLN	CB	26.14	0.3	1
1	A	141	GLN	CG	34.53	0.3	1
1	A	141	GLN	N	114.6	0.3	1
1	A	141	GLN	NE2	113.0	0.3	1
1	A	142	ASP	H	8.364	0.02	1
1	A	142	ASP	HA	4.762	0.02	1
1	A	142	ASP	HB2	3.124	0.02	2
1	A	142	ASP	HB3	2.552	0.02	2
1	A	142	ASP	C	177.2	0.3	1
1	A	142	ASP	CA	53.33	0.3	1
1	A	142	ASP	CB	41.0	0.3	1
1	A	142	ASP	N	118.3	0.3	1
1	A	143	GLY	H	10.31	0.02	1
1	A	143	GLY	HA2	3.581	0.02	2
1	A	143	GLY	HA3	4.158	0.02	2
1	A	143	GLY	C	173.3	0.3	1
1	A	143	GLY	CA	45.04	0.3	1
1	A	143	GLY	N	112.1	0.3	1
1	A	144	TYR	H	7.987	0.02	1
1	A	144	TYR	HA	5.69	0.02	1
1	A	144	TYR	HB2	2.842	0.02	2
1	A	144	TYR	HD1	6.84	0.02	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	144	TYR	HE1	6.929	0.02	3
1	A	144	TYR	C	176.6	0.3	1
1	A	144	TYR	CA	56.76	0.3	1
1	A	144	TYR	CB	42.22	0.3	1
1	A	144	TYR	N	116.2	0.3	1
1	A	145	ILE	H	9.43	0.02	1
1	A	145	ILE	HA	4.913	0.02	1
1	A	145	ILE	HB	1.834	0.02	1
1	A	145	ILE	HG12	0.933	0.02	2
1	A	145	ILE	HG13	1.235	0.02	2
1	A	145	ILE	HG21	0.383	0.02	1
1	A	145	ILE	HG22	0.383	0.02	1
1	A	145	ILE	HG23	0.383	0.02	1
1	A	145	ILE	HD11	0.363	0.02	1
1	A	145	ILE	HD12	0.363	0.02	1
1	A	145	ILE	HD13	0.363	0.02	1
1	A	145	ILE	C	175.1	0.3	1
1	A	145	ILE	CA	60.2	0.3	1
1	A	145	ILE	CB	40.42	0.3	1
1	A	145	ILE	CG1	25.65	0.3	1
1	A	145	ILE	CG2	16.61	0.3	1
1	A	145	ILE	CD1	13.62	0.3	1
1	A	145	ILE	N	119.0	0.3	1
1	A	146	GLY	H	8.643	0.02	1
1	A	146	GLY	C	175.2	0.3	1
1	A	146	GLY	CA	44.58	0.3	1
1	A	146	GLY	N	109.9	0.3	1
1	A	147	TYR	H	7.689	0.02	1
1	A	147	TYR	HA	4.128	0.02	1
1	A	147	TYR	HB2	2.753	0.02	2
1	A	147	TYR	HB3	3.168	0.02	2
1	A	147	TYR	HD1	7.083	0.02	3
1	A	147	TYR	HE1	6.843	0.02	3
1	A	147	TYR	C	177.2	0.3	1
1	A	147	TYR	CA	60.5	0.3	1
1	A	147	TYR	CB	37.13	0.3	1
1	A	147	TYR	N	116.9	0.3	1
1	A	148	ARG	H	8.048	0.02	1
1	A	148	ARG	HA	3.944	0.02	1
1	A	148	ARG	C	173.7	0.3	1
1	A	148	ARG	CA	58.8	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	148	ARG	CB	28.9	0.3	1
1	A	148	ARG	N	121.2	0.3	1
1	A	149	GLU	H	8.062	0.02	1
1	A	149	GLU	HA	4.317	0.02	1
1	A	149	GLU	HG2	2.395	0.02	2
1	A	149	GLU	C	177.1	0.3	1
1	A	149	GLU	CA	58.5	0.3	1
1	A	149	GLU	CB	29.44	0.3	1
1	A	149	GLU	CG	37.57	0.3	1
1	A	149	GLU	N	118.5	0.3	1
1	A	150	LEU	H	7.716	0.02	1
1	A	150	LEU	HA	3.78	0.02	1
1	A	150	LEU	HB2	1.706	0.02	2
1	A	150	LEU	HD21	0.943	0.02	1
1	A	150	LEU	HD11	0.943	0.02	1
1	A	150	LEU	HD12	0.943	0.02	1
1	A	150	LEU	HD13	0.943	0.02	1
1	A	150	LEU	HD22	0.943	0.02	1
1	A	150	LEU	HD23	0.943	0.02	1
1	A	150	LEU	CA	58.55	0.3	1
1	A	150	LEU	CB	41.43	0.3	1
1	A	150	LEU	CD2	25.6	0.3	1
1	A	150	LEU	N	119.3	0.3	1
1	A	151	GLY	H	8.231	0.02	1
1	A	151	GLY	HA2	3.62	0.02	2
1	A	151	GLY	HA3	3.893	0.02	2
1	A	151	GLY	C	175.4	0.3	1
1	A	151	GLY	CA	47.93	0.3	1
1	A	151	GLY	N	106.3	0.3	1
1	A	152	ASP	H	7.754	0.02	1
1	A	152	ASP	HA	4.384	0.02	1
1	A	152	ASP	HB2	2.57	0.02	2
1	A	152	ASP	C	178.3	0.3	1
1	A	152	ASP	CA	57.43	0.3	1
1	A	152	ASP	CB	40.19	0.3	1
1	A	152	ASP	N	121.7	0.3	1
1	A	153	CYS	H	7.962	0.02	1
1	A	153	CYS	HA	3.374	0.02	1
1	A	153	CYS	HB2	2.226	0.02	2
1	A	153	CYS	HB3	2.599	0.02	2
1	A	153	CYS	C	176.8	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	153	CYS	CA	62.81	0.3	1
1	A	153	CYS	CB	26.22	0.3	1
1	A	153	CYS	N	121.8	0.3	1
1	A	154	MET	H	8.409	0.02	1
1	A	154	MET	HA	3.99	0.02	1
1	A	154	MET	HB2	2.34	0.02	2
1	A	154	MET	C	178.1	0.3	1
1	A	154	MET	CA	60.52	0.3	1
1	A	154	MET	CB	32.28	0.3	1
1	A	154	MET	N	116.8	0.3	1
1	A	155	ARG	H	8.109	0.02	1
1	A	155	ARG	HA	4.384	0.02	1
1	A	155	ARG	C	180.7	0.3	1
1	A	155	ARG	CA	59.59	0.3	1
1	A	155	ARG	CB	29.7	0.3	1
1	A	155	ARG	N	118.2	0.3	1
1	A	156	THR	H	8.056	0.02	1
1	A	156	THR	HA	4.181	0.02	1
1	A	156	THR	HB	4.533	0.02	1
1	A	156	THR	HG21	1.55	0.02	1
1	A	156	THR	HG22	1.55	0.02	1
1	A	156	THR	HG23	1.55	0.02	1
1	A	156	THR	C	175.6	0.3	1
1	A	156	THR	CA	66.17	0.3	1
1	A	156	THR	CB	69.1	0.3	1
1	A	156	THR	CG2	21.76	0.3	1
1	A	156	THR	N	116.6	0.3	1
1	A	157	LEU	H	7.533	0.02	1
1	A	157	LEU	HA	4.393	0.02	1
1	A	157	LEU	HB2	1.75	0.02	2
1	A	157	LEU	HB3	1.984	0.02	2
1	A	157	LEU	HD11	0.017	0.02	1
1	A	157	LEU	HD12	0.017	0.02	1
1	A	157	LEU	HD13	0.017	0.02	1
1	A	157	LEU	HD21	1.055	0.02	1
1	A	157	LEU	HD22	1.055	0.02	1
1	A	157	LEU	HD23	1.055	0.02	1
1	A	157	LEU	C	176.6	0.3	1
1	A	157	LEU	CA	55.49	0.3	1
1	A	157	LEU	CB	42.25	0.3	1
1	A	157	LEU	CD1	26.74	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	157	LEU	CD2	23.52	0.3	1
1	A	157	LEU	N	120.2	0.3	1
1	A	158	GLY	H	7.794	0.02	1
1	A	158	GLY	HA2	3.69	0.02	2
1	A	158	GLY	HA3	4.186	0.02	2
1	A	158	GLY	C	173.8	0.3	1
1	A	158	GLY	CA	45.33	0.3	1
1	A	158	GLY	N	105.5	0.3	1
1	A	159	TYR	H	7.759	0.02	1
1	A	159	TYR	HA	4.64	0.02	1
1	A	159	TYR	HB2	2.668	0.02	2
1	A	159	TYR	HB3	2.893	0.02	2
1	A	159	TYR	C	120.7	0.3	1
1	A	159	TYR	CA	57.32	0.3	1
1	A	159	TYR	CB	39.08	0.3	1
1	A	159	TYR	N	120.7	0.3	1
1	A	161	PRO	C	177.5	0.3	1
1	A	161	PRO	CA	62.62	0.3	1
1	A	161	PRO	CB	31.52	0.3	1
1	A	162	THR	H	8.474	0.02	1
1	A	162	THR	HA	4.46	0.02	1
1	A	162	THR	HB	4.67	0.02	1
1	A	162	THR	HG21	1.374	0.02	1
1	A	162	THR	HG22	1.374	0.02	1
1	A	162	THR	HG23	1.374	0.02	1
1	A	162	THR	C	175.2	0.3	1
1	A	162	THR	CA	61.18	0.3	1
1	A	162	THR	CB	70.83	0.3	1
1	A	162	THR	CG2	22.0	0.3	1
1	A	162	THR	N	112.1	0.3	1
1	A	163	GLU	H	8.82	0.02	1
1	A	163	GLU	C	179.2	0.3	1
1	A	163	GLU	CA	59.78	0.3	1
1	A	163	GLU	CB	29.0	0.3	1
1	A	163	GLU	N	120.9	0.3	1
1	A	164	MET	H	8.347	0.02	1
1	A	164	MET	HA	4.3	0.02	1
1	A	164	MET	HB2	2.082	0.02	2
1	A	164	MET	CA	58.27	0.3	1
1	A	164	MET	CB	31.65	0.3	1
1	A	164	MET	N	117.3	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	166	LEU	H	8.145	0.02	1
1	A	166	LEU	HA	4.12	0.02	1
1	A	166	LEU	HB2	1.745	0.02	2
1	A	166	LEU	HD11	0.912	0.02	2
1	A	166	LEU	HD12	0.912	0.02	2
1	A	166	LEU	HD13	0.912	0.02	2
1	A	166	LEU	HD21	0.943	0.02	2
1	A	166	LEU	HD22	0.943	0.02	2
1	A	166	LEU	HD23	0.943	0.02	2
1	A	166	LEU	C	179.5	0.3	1
1	A	166	LEU	CA	57.46	0.3	1
1	A	166	LEU	CB	40.97	0.3	1
1	A	166	LEU	CD1	24.47	0.3	1
1	A	166	LEU	CD2	24.78	0.3	1
1	A	166	LEU	N	119.3	0.3	1
1	A	167	LEU	H	8.096	0.02	1
1	A	167	LEU	HA	4.144	0.02	1
1	A	167	LEU	HB2	1.757	0.02	2
1	A	167	LEU	HB3	1.858	0.02	2
1	A	167	LEU	HD11	0.929	0.02	1
1	A	167	LEU	HD12	0.929	0.02	1
1	A	167	LEU	HD13	0.929	0.02	1
1	A	167	LEU	HD21	0.905	0.02	1
1	A	167	LEU	HD22	0.905	0.02	1
1	A	167	LEU	HD23	0.905	0.02	1
1	A	167	LEU	C	179.1	0.3	1
1	A	167	LEU	CA	57.99	0.3	1
1	A	167	LEU	CB	41.08	0.3	1
1	A	167	LEU	CD1	25.0	0.3	1
1	A	167	LEU	CD2	24.12	0.3	1
1	A	167	LEU	N	122.1	0.3	1
1	A	168	GLU	H	7.936	0.02	1
1	A	168	GLU	HA	4.074	0.02	1
1	A	168	GLU	HG2	2.259	0.02	2
1	A	168	GLU	HG3	2.42	0.02	2
1	A	168	GLU	C	179.5	0.3	1
1	A	168	GLU	CA	59.5	0.3	1
1	A	168	GLU	CB	29.21	0.3	1
1	A	168	GLU	CG	36.55	0.3	1
1	A	168	GLU	N	119.3	0.3	1
1	A	169	VAL	H	8.17	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	169	VAL	HA	3.94	0.02	1
1	A	169	VAL	HB	2.231	0.02	1
1	A	169	VAL	HG11	1.036	0.02	1
1	A	169	VAL	HG12	1.036	0.02	1
1	A	169	VAL	HG13	1.036	0.02	1
1	A	169	VAL	HG21	1.11	0.02	1
1	A	169	VAL	HG22	1.11	0.02	1
1	A	169	VAL	HG23	1.11	0.02	1
1	A	169	VAL	C	177.5	0.3	1
1	A	169	VAL	CA	65.76	0.3	1
1	A	169	VAL	CB	31.37	0.3	1
1	A	169	VAL	CG1	21.89	0.3	1
1	A	169	VAL	CG2	22.88	0.3	1
1	A	169	VAL	N	118.9	0.3	1
1	A	170	SER	H	8.314	0.02	1
1	A	170	SER	C	176.0	0.3	1
1	A	170	SER	CA	62.48	0.3	1
1	A	170	SER	N	116.1	0.3	1
1	A	171	GLN	H	8.143	0.02	1
1	A	171	GLN	C	177.6	0.3	1
1	A	171	GLN	CA	58.53	0.3	1
1	A	171	GLN	CB	28.19	0.3	1
1	A	171	GLN	N	120.3	0.3	1
1	A	172	HIS	H	7.955	0.02	1
1	A	172	HIS	C	177.6	0.3	1
1	A	172	HIS	CA	59.86	0.3	1
1	A	172	HIS	CB	30.77	0.3	1
1	A	172	HIS	N	120.0	0.3	1
1	A	173	VAL	H	8.261	0.02	1
1	A	173	VAL	HA	3.585	0.02	1
1	A	173	VAL	HB	2.139	0.02	1
1	A	173	VAL	HG11	0.831	0.02	1
1	A	173	VAL	HG12	0.831	0.02	1
1	A	173	VAL	HG13	0.831	0.02	1
1	A	173	VAL	HG21	1.15	0.02	1
1	A	173	VAL	HG22	1.15	0.02	1
1	A	173	VAL	HG23	1.15	0.02	1
1	A	173	VAL	CA	65.62	0.3	1
1	A	173	VAL	CB	31.15	0.3	1
1	A	173	VAL	CG1	22.22	0.3	1
1	A	173	VAL	CG2	23.31	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	173	VAL	N	118.7	0.3	1
1	A	174	LYS	H	8.274	0.02	1
1	A	174	LYS	CA	59.88	0.3	1
1	A	174	LYS	CB	32.41	0.3	1
1	A	174	LYS	N	120.3	0.3	1
1	A	175	MET	H	8.275	0.02	1
1	A	175	MET	HA	4.4	0.02	1
1	A	175	MET	HB2	2.121	0.02	2
1	A	175	MET	CA	56.93	0.3	1
1	A	175	MET	CB	30.1	0.3	1
1	A	175	MET	N	114.6	0.3	1
1	A	176	ARG	H	8.378	0.02	1
1	A	176	ARG	CA	56.5	0.3	1
1	A	176	ARG	CB	30.1	0.3	1
1	A	176	ARG	N	116.9	0.3	1
1	A	179	GLY	H	8.12	0.02	1
1	A	179	GLY	HA2	3.272	0.02	2
1	A	179	GLY	C	172.3	0.3	1
1	A	179	GLY	CA	45.57	0.3	1
1	A	179	GLY	N	105.5	0.3	1
1	A	180	PHE	H	7.383	0.02	1
1	A	180	PHE	HA	5.34	0.02	1
1	A	180	PHE	HB2	2.705	0.02	2
1	A	180	PHE	HB3	2.951	0.02	2
1	A	180	PHE	HD1	7.005	0.02	3
1	A	180	PHE	HE1	7.303	0.02	3
1	A	180	PHE	HZ	6.838	0.02	1
1	A	180	PHE	C	174.1	0.3	1
1	A	180	PHE	CA	56.94	0.3	1
1	A	180	PHE	CB	43.09	0.3	1
1	A	180	PHE	N	118.0	0.3	1
1	A	181	VAL	H	9.27	0.02	1
1	A	181	VAL	HA	5.238	0.02	1
1	A	181	VAL	HB	2.58	0.02	1
1	A	181	VAL	HG11	1.168	0.02	1
1	A	181	VAL	HG12	1.168	0.02	1
1	A	181	VAL	HG13	1.168	0.02	1
1	A	181	VAL	HG21	1.108	0.02	1
1	A	181	VAL	HG22	1.108	0.02	1
1	A	181	VAL	HG23	1.108	0.02	1
1	A	181	VAL	C	175.5	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	181	VAL	CA	60.09	0.3	1
1	A	181	VAL	CB	34.45	0.3	1
1	A	181	VAL	CG1	23.54	0.3	1
1	A	181	VAL	CG2	21.1	0.3	1
1	A	181	VAL	N	115.4	0.3	1
1	A	182	ASP	H	8.983	0.02	1
1	A	182	ASP	HA	5.49	0.02	1
1	A	182	ASP	HB2	2.563	0.02	2
1	A	182	ASP	HB3	3.042	0.02	2
1	A	182	ASP	C	176.3	0.3	1
1	A	182	ASP	CA	51.97	0.3	1
1	A	182	ASP	CB	41.04	0.3	1
1	A	182	ASP	N	124.6	0.3	1
1	A	183	PHE	H	8.432	0.02	1
1	A	183	PHE	HA	3.39	0.02	1
1	A	183	PHE	HB2	2.183	0.02	2
1	A	183	PHE	HB3	2.467	0.02	2
1	A	183	PHE	HD1	6.687	0.02	3
1	A	183	PHE	HE1	7.091	0.02	3
1	A	183	PHE	HZ	7.311	0.02	1
1	A	183	PHE	C	176.3	0.3	1
1	A	183	PHE	CA	62.09	0.3	1
1	A	183	PHE	CB	38.28	0.3	1
1	A	183	PHE	N	118.5	0.3	1
1	A	184	GLU	H	7.871	0.02	1
1	A	184	GLU	HA	3.58	0.02	1
1	A	184	GLU	HB2	2.015	0.02	2
1	A	184	GLU	HB3	2.124	0.02	2
1	A	184	GLU	HG2	2.298	0.02	2
1	A	184	GLU	HG3	2.339	0.02	2
1	A	184	GLU	C	180.2	0.3	1
1	A	184	GLU	CA	60.15	0.3	1
1	A	184	GLU	CB	28.63	0.3	1
1	A	184	GLU	CG	37.14	0.3	1
1	A	184	GLU	N	117.7	0.3	1
1	A	185	GLU	H	8.646	0.02	1
1	A	185	GLU	HA	4.024	0.02	1
1	A	185	GLU	HB2	2.063	0.02	2
1	A	185	GLU	HG2	2.34	0.02	2
1	A	185	GLU	HG3	2.73	0.02	2
1	A	185	GLU	C	178.7	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	185	GLU	CA	58.85	0.3	1
1	A	185	GLU	CB	29.5	0.3	1
1	A	185	GLU	CG	36.93	0.3	1
1	A	185	GLU	N	120.7	0.3	1
1	A	186	PHE	H	8.765	0.02	1
1	A	186	PHE	HA	4.08	0.02	1
1	A	186	PHE	HB2	3.256	0.02	2
1	A	186	PHE	HB3	3.493	0.02	2
1	A	186	PHE	HD1	7.107	0.02	3
1	A	186	PHE	HE1	7.323	0.02	3
1	A	186	PHE	HZ	7.168	0.02	1
1	A	186	PHE	C	176.3	0.3	1
1	A	186	PHE	CA	61.24	0.3	1
1	A	186	PHE	CB	39.05	0.3	1
1	A	186	PHE	N	121.7	0.3	1
1	A	187	VAL	H	8.198	0.02	1
1	A	187	VAL	HA	2.97	0.02	1
1	A	187	VAL	HB	1.78	0.02	1
1	A	187	VAL	HG11	0.65	0.02	1
1	A	187	VAL	HG12	0.65	0.02	1
1	A	187	VAL	HG13	0.65	0.02	1
1	A	187	VAL	HG21	0.308	0.02	1
1	A	187	VAL	HG22	0.308	0.02	1
1	A	187	VAL	HG23	0.308	0.02	1
1	A	187	VAL	C	178.7	0.3	1
1	A	187	VAL	CA	66.97	0.3	1
1	A	187	VAL	CB	30.84	0.3	1
1	A	187	VAL	CG1	21.65	0.3	1
1	A	187	VAL	CG2	23.9	0.3	1
1	A	187	VAL	N	118.4	0.3	1
1	A	188	GLU	H	7.561	0.02	1
1	A	188	GLU	HA	3.881	0.02	1
1	A	188	GLU	HB2	2.105	0.02	2
1	A	188	GLU	HG2	2.22	0.02	2
1	A	188	GLU	HG3	2.36	0.02	2
1	A	188	GLU	C	178.3	0.3	1
1	A	188	GLU	CA	59.15	0.3	1
1	A	188	GLU	CB	28.99	0.3	1
1	A	188	GLU	CG	36.03	0.3	1
1	A	188	GLU	N	119.7	0.3	1
1	A	189	LEU	H	7.795	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	189	LEU	HA	4.049	0.02	1
1	A	189	LEU	HB2	1.824	0.02	2
1	A	189	LEU	HB3	1.385	0.02	2
1	A	189	LEU	HD11	0.853	0.02	1
1	A	189	LEU	HD12	0.853	0.02	1
1	A	189	LEU	HD13	0.853	0.02	1
1	A	189	LEU	HD21	0.81	0.02	1
1	A	189	LEU	HD22	0.81	0.02	1
1	A	189	LEU	HD23	0.81	0.02	1
1	A	189	LEU	C	178.3	0.3	1
1	A	189	LEU	CA	57.1	0.3	1
1	A	189	LEU	CB	42.36	0.3	1
1	A	189	LEU	CD1	25.94	0.3	1
1	A	189	LEU	CD2	24.28	0.3	1
1	A	189	LEU	N	117.4	0.3	1
1	A	190	ILE	H	7.724	0.02	1
1	A	190	ILE	HA	3.98	0.02	1
1	A	190	ILE	HB	1.383	0.02	1
1	A	190	ILE	HG12	0.961	0.02	2
1	A	190	ILE	HG13	0.905	0.02	2
1	A	190	ILE	HG21	0.495	0.02	1
1	A	190	ILE	HG22	0.495	0.02	1
1	A	190	ILE	HG23	0.495	0.02	1
1	A	190	ILE	HD11	0.427	0.02	1
1	A	190	ILE	HD12	0.427	0.02	1
1	A	190	ILE	HD13	0.427	0.02	1
1	A	190	ILE	C	176.5	0.3	1
1	A	190	ILE	CA	60.82	0.3	1
1	A	190	ILE	CB	38.0	0.3	1
1	A	190	ILE	CG1	27.86	0.3	1
1	A	190	ILE	CG2	18.22	0.3	1
1	A	190	ILE	CD1	13.29	0.3	1
1	A	190	ILE	N	114.2	0.3	1
1	A	191	SER	H	8.067	0.02	1
1	A	191	SER	CA	60.81	0.3	1
1	A	191	SER	N	117.7	0.3	1
1	A	196	GLU	H	8.015	0.02	1
1	A	196	GLU	C	177.2	0.3	1
1	A	196	GLU	CA	57.65	0.3	1
1	A	196	GLU	CB	29.9	0.3	1
1	A	196	GLU	N	120.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	197	GLU	H	8.356	0.02	1
1	A	197	GLU	HA	4.32	0.02	1
1	A	197	GLU	C	177.1	0.3	1
1	A	197	GLU	CA	57.49	0.3	1
1	A	197	GLU	CB	29.77	0.3	1
1	A	197	GLU	N	120.3	0.3	1
1	A	198	THR	H	7.933	0.02	1
1	A	198	THR	HA	4.35	0.02	1
1	A	198	THR	HB	4.25	0.02	1
1	A	198	THR	HG21	1.2	0.02	1
1	A	198	THR	HG22	1.2	0.02	1
1	A	198	THR	HG23	1.2	0.02	1
1	A	198	THR	C	174.6	0.3	1
1	A	198	THR	CA	62.19	0.3	1
1	A	198	THR	CB	69.71	0.3	1
1	A	198	THR	CG2	21.67	0.3	1
1	A	198	THR	N	112.8	0.3	1
1	A	199	ALA	H	8.098	0.02	1
1	A	199	ALA	HA	4.237	0.02	1
1	A	199	ALA	HB1	1.385	0.02	1
1	A	199	ALA	HB2	1.385	0.02	1
1	A	199	ALA	HB3	1.385	0.02	1
1	A	199	ALA	C	177.5	0.3	1
1	A	199	ALA	CA	53.3	0.3	1
1	A	199	ALA	CB	19.2	0.3	1
1	A	199	ALA	N	124.8	0.3	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	162	-0.26 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	145	0.54 ± 0.12	Should be checked
$^{13}C'$	150	-0.36 ± 0.18	None needed (< 0.5 ppm)
^{15}N	156	0.92 ± 0.20	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 65%, i.e. 510 atoms were assigned a chemical

shift out of a possible 785. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	274/276 (99%)	110/112 (98%)	110/110 (100%)	54/54 (100%)
Sidechain	227/469 (48%)	145/301 (48%)	82/144 (57%)	0/24 (0%)
Aromatic	9/40 (22%)	9/20 (45%)	0/20 (0%)	0/0 (—%)
Overall	510/785 (65%)	264/433 (61%)	192/274 (70%)	54/78 (69%)

7.1.4 Statistically unusual chemical shifts (i)

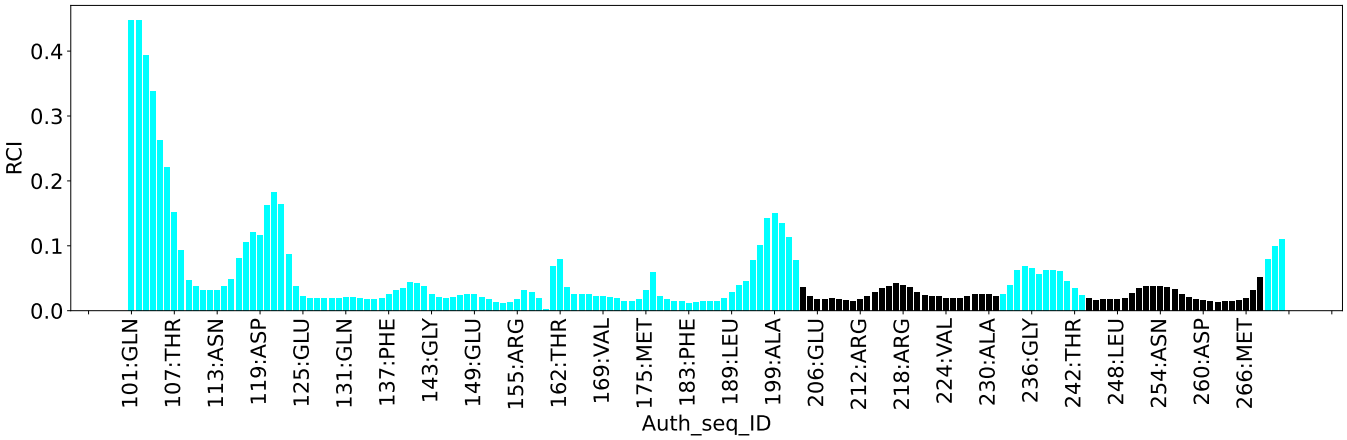
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	159	TYR	C	120.70	165.86 – 185.23	-28.3

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	775
Intra-residue (|i-j|=0)	254
Sequential (|i-j|=1)	217
Medium range (|i-j|>1 and |i-j|<5)	126
Long range (|i-j|≥5)	138
Inter-chain	0
Hydrogen bond restraints	40
Disulfide bond restraints	0
Total dihedral-angle restraints	92
Number of unmapped restraints	0
Number of restraints per residue	5.0
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)	13.9	0.2
0.2-0.5 (Medium)	7.5	0.46
>0.5 (Large)	2.6	1.57

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.0	2.83
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

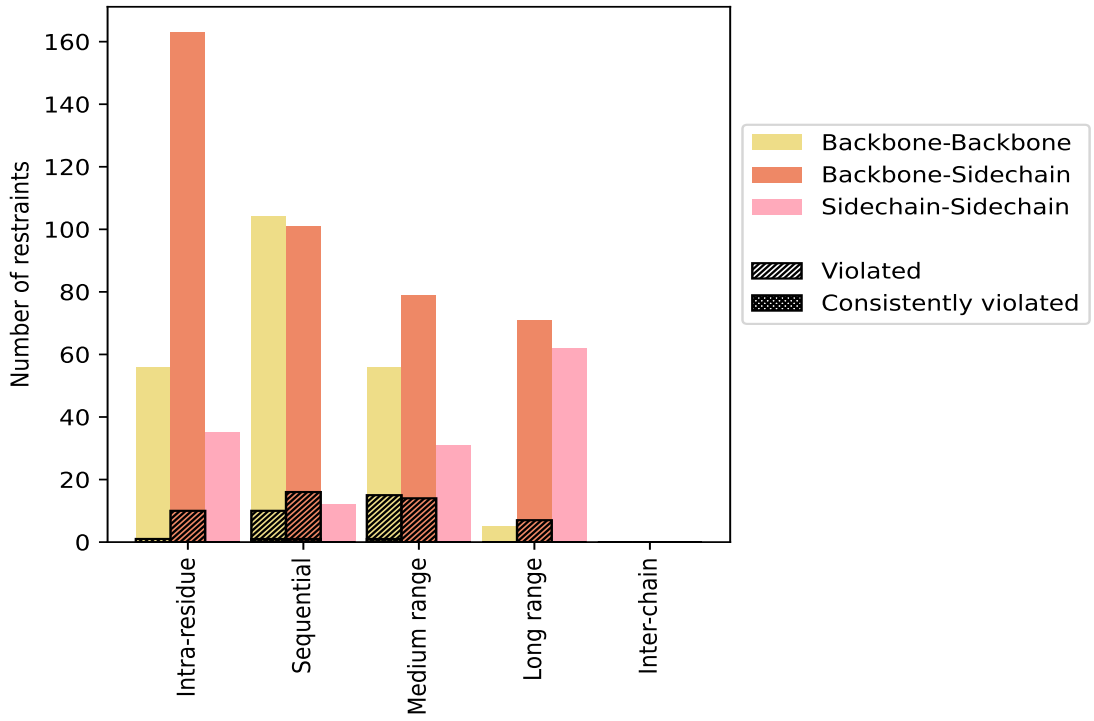
9.1 Summary of distance violations (i)

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)	254	32.8	11	4.3	1.4	0	0.0	0.0
Backbone-Backbone	56	7.2	1	1.8	0.1	0	0.0	0.0
Backbone-Sidechain	163	21.0	10	6.1	1.3	0	0.0	0.0
Sidechain-Sidechain	35	4.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	217	28.0	26	12.0	3.4	2	0.9	0.3
Backbone-Backbone	104	13.4	10	9.6	1.3	1	1.0	0.1
Backbone-Sidechain	101	13.0	16	15.8	2.1	1	1.0	0.1
Sidechain-Sidechain	12	1.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	126	16.3	17	13.5	2.2	1	0.8	0.1
Backbone-Backbone	56	7.2	15	26.8	1.9	1	1.8	0.1
Backbone-Sidechain	39	5.0	2	5.1	0.3	0	0.0	0.0
Sidechain-Sidechain	31	4.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	138	17.8	7	5.1	0.9	0	0.0	0.0
Backbone-Backbone	5	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	71	9.2	7	9.9	0.9	0	0.0	0.0
Sidechain-Sidechain	62	8.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	40	5.2	12	30.0	1.5	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	775	100.0	73	9.4	9.4	3	0.4	0.4
Backbone-Backbone	221	28.5	26	11.8	3.4	2	0.9	0.3
Backbone-Sidechain	414	53.4	47	11.4	6.1	1	0.2	0.1
Sidechain-Sidechain	140	18.1	0	0.0	0.0	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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	3	6	9	4	0	22	0.3	1.24	0.26	0.25
2	5	9	7	4	0	25	0.29	1.28	0.27	0.22
3	4	6	15	5	0	30	0.27	0.98	0.24	0.18
4	2	8	6	2	0	18	0.21	0.38	0.08	0.21
5	6	9	8	5	0	28	0.26	1.11	0.25	0.16
6	1	9	10	6	0	26	0.27	1.49	0.3	0.17
7	3	9	11	6	0	29	0.3	1.52	0.31	0.19
8	4	6	8	6	0	24	0.3	1.44	0.37	0.16
9	4	6	9	4	0	23	0.21	1.03	0.18	0.16
10	3	8	9	4	0	24	0.24	1.01	0.21	0.18

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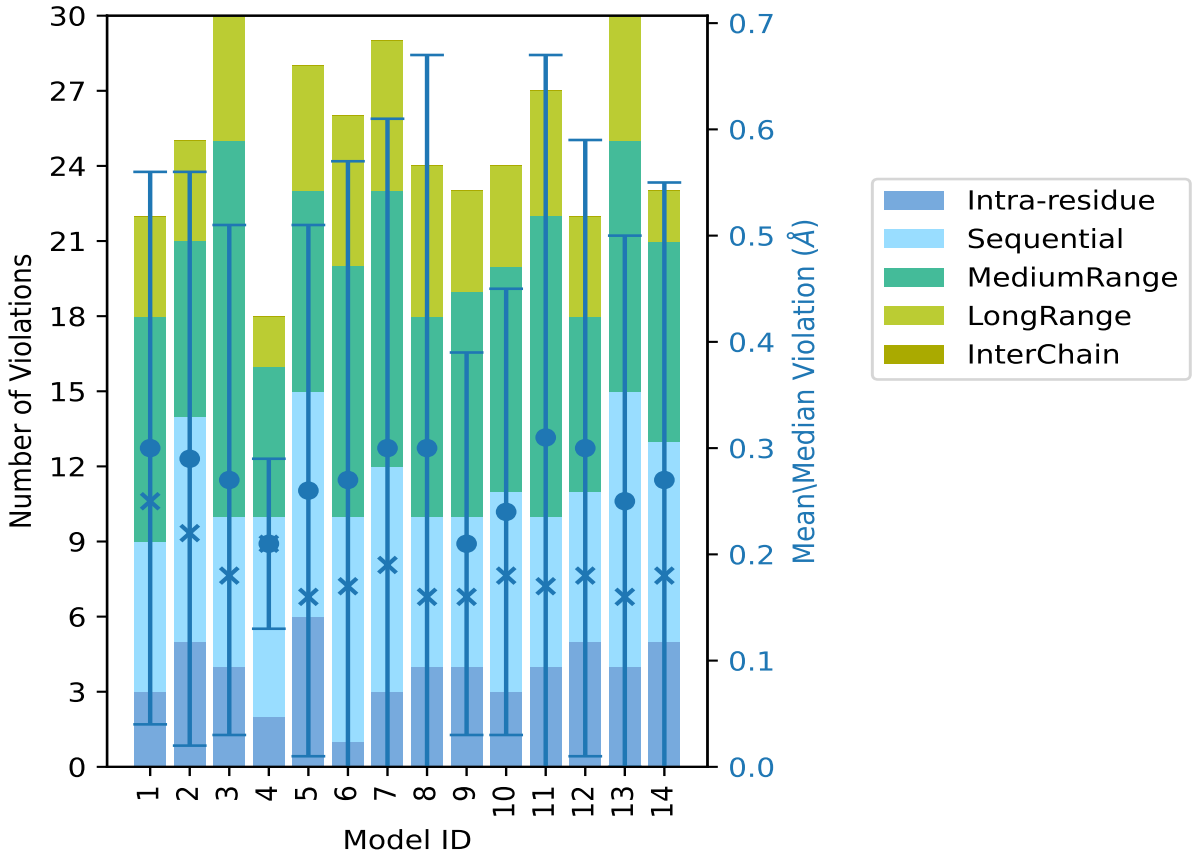
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	4	6	12	5	0	27	0.31	1.57	0.36	0.17
12	5	6	7	4	0	22	0.3	1.34	0.29	0.18
13	4	11	10	5	0	30	0.25	1.1	0.25	0.16
14	5	8	8	2	0	23	0.27	1.48	0.28	0.18

[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

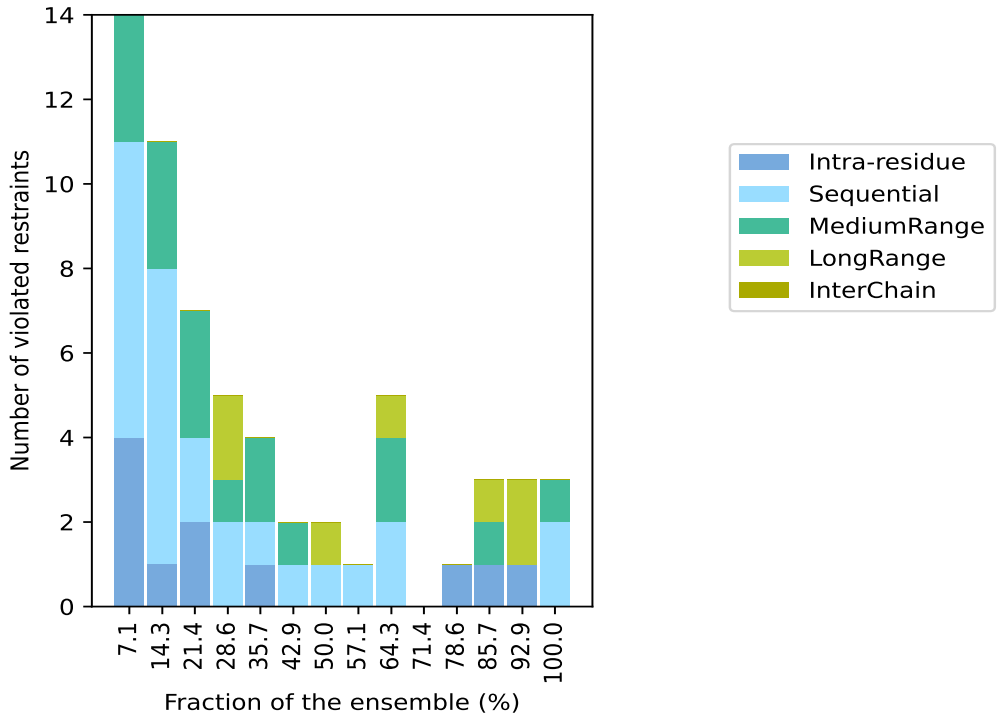
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for

a given fraction of the ensemble. In total, 674(IR:243, SQ:191, MR:109, LR:131, 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]	%
4	7	3	0	0	14	1	7.1
1	7	3	0	0	11	2	14.3
2	2	3	0	0	7	3	21.4
0	2	1	2	0	5	4	28.6
1	1	2	0	0	4	5	35.7
0	1	1	0	0	2	6	42.9
0	1	0	1	0	2	7	50.0
0	1	0	0	0	1	8	57.1
0	2	2	1	0	5	9	64.3
0	0	0	0	0	0	10	71.4
1	0	0	0	0	1	11	78.6
1	0	1	1	0	3	12	85.7
1	0	0	2	0	3	13	92.9
0	2	1	0	0	3	14	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

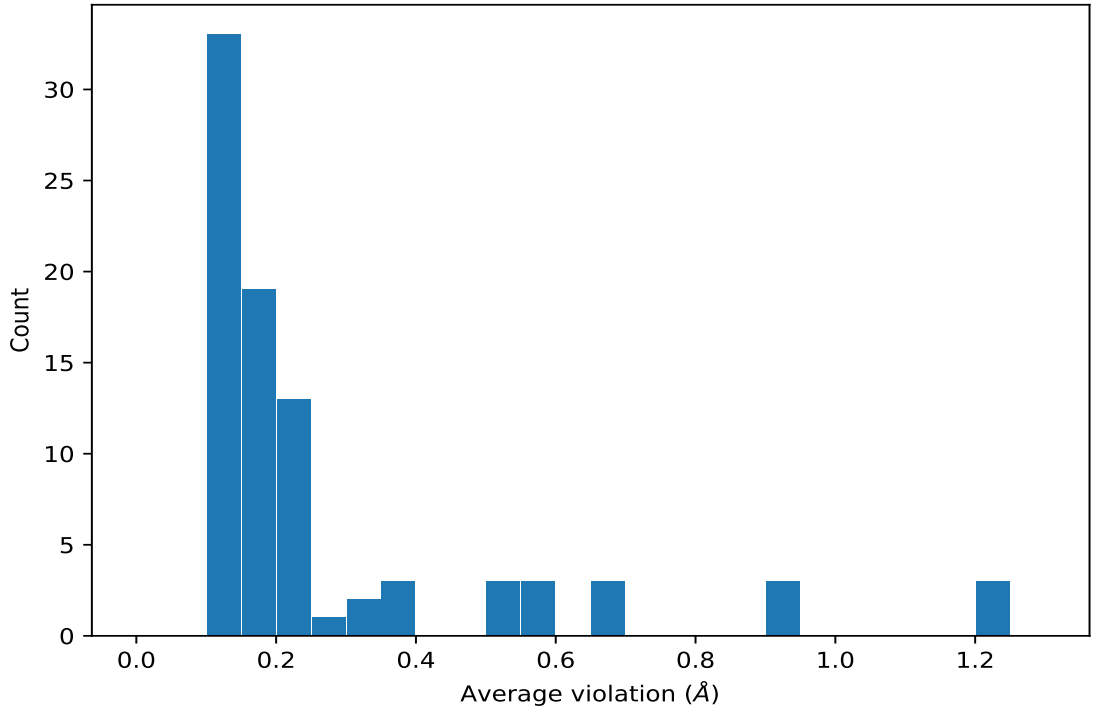
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(2,506)	1:224:A:VAL:HB	1:225:A:ALA:H	14	0.32	0.03	0.32
(2,338)	1:242:A:THR:HA	1:243:A:GLU:H	14	0.32	0.07	0.3
(2,311)	1:223:A:THR:HA	1:225:A:ALA:H	14	0.27	0.02	0.26
(2,657)	1:227:A:LEU:HD21	1:248:A:LEU:HA	13	1.21	0.19	1.24
(2,657)	1:227:A:LEU:HD22	1:248:A:LEU:HA	13	1.21	0.19	1.24
(2,657)	1:227:A:LEU:HD23	1:248:A:LEU:HA	13	1.21	0.19	1.24
(2,716)	1:253:A:LEU:HD11	1:266:A:MET:H	13	0.92	0.4	0.86
(2,716)	1:253:A:LEU:HD12	1:266:A:MET:H	13	0.92	0.4	0.86
(2,716)	1:253:A:LEU:HD13	1:266:A:MET:H	13	0.92	0.4	0.86

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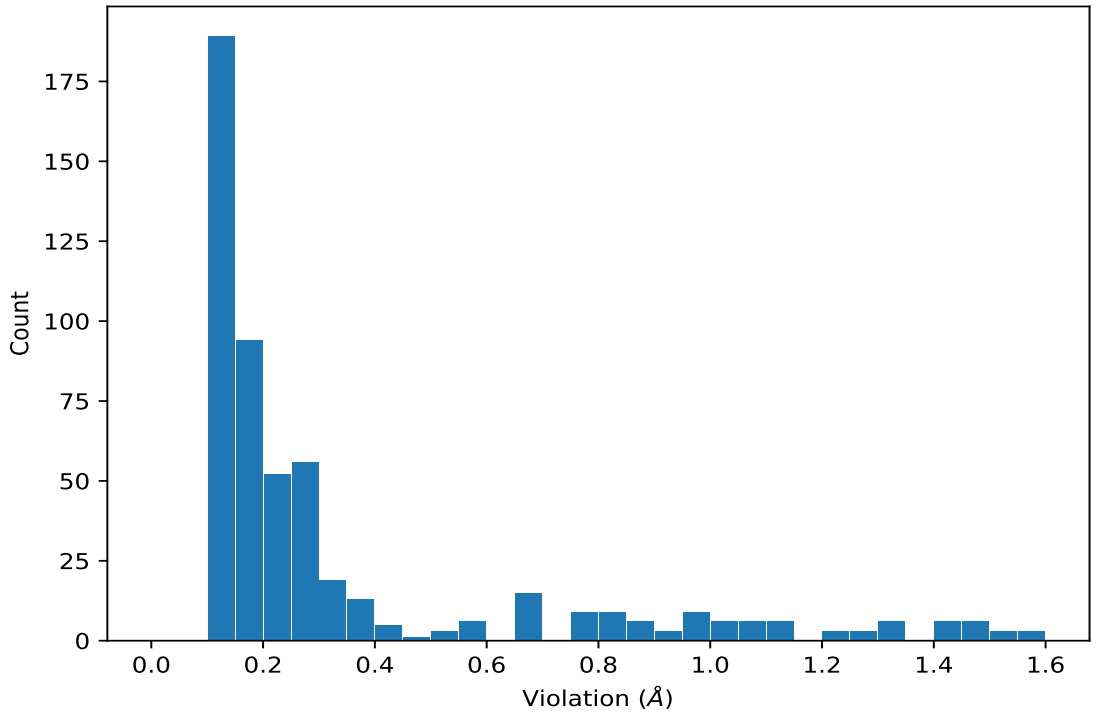
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,241)	1:259:A:ILE:HA	1:259:A:ILE:HD11	13	0.2	0.05	0.2
(2,241)	1:259:A:ILE:HA	1:259:A:ILE:HD12	13	0.2	0.05	0.2
(2,241)	1:259:A:ILE:HA	1:259:A:ILE:HD13	13	0.2	0.05	0.2
(2,128)	1:258:A:THR:HB	1:258:A:THR:H	12	0.22	0.04	0.22
(2,695)	1:212:A:ARG:H	1:261:A:PHE:HZ	12	0.22	0.06	0.21
(2,367)	1:254:A:ASN:H	1:256:A:ASP:H	12	0.19	0.05	0.18
(1,26)	1:242:A:THR:O	1:246:A:GLU:H	11	0.13	0.03	0.13

[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)
(2,716)	1:253:A:LEU:HD11	1:266:A:MET:H	11	1.57
(2,716)	1:253:A:LEU:HD12	1:266:A:MET:H	11	1.57
(2,716)	1:253:A:LEU:HD13	1:266:A:MET:H	11	1.57
(2,716)	1:253:A:LEU:HD11	1:266:A:MET:H	7	1.52
(2,716)	1:253:A:LEU:HD12	1:266:A:MET:H	7	1.52
(2,716)	1:253:A:LEU:HD13	1:266:A:MET:H	7	1.52
(2,657)	1:227:A:LEU:HD21	1:248:A:LEU:HA	6	1.49
(2,657)	1:227:A:LEU:HD22	1:248:A:LEU:HA	6	1.49
(2,657)	1:227:A:LEU:HD23	1:248:A:LEU:HA	6	1.49
(2,657)	1:227:A:LEU:HD21	1:248:A:LEU:HA	14	1.48
(2,657)	1:227:A:LEU:HD22	1:248:A:LEU:HA	14	1.48
(2,657)	1:227:A:LEU:HD23	1:248:A:LEU:HA	14	1.48
(2,716)	1:253:A:LEU:HD11	1:266:A:MET:H	8	1.44
(2,716)	1:253:A:LEU:HD12	1:266:A:MET:H	8	1.44
(2,716)	1:253:A:LEU:HD13	1:266:A:MET:H	8	1.44
(2,657)	1:227:A:LEU:HD21	1:248:A:LEU:HA	8	1.42
(2,657)	1:227:A:LEU:HD22	1:248:A:LEU:HA	8	1.42
(2,657)	1:227:A:LEU:HD23	1:248:A:LEU:HA	8	1.42
(2,657)	1:227:A:LEU:HD21	1:248:A:LEU:HA	12	1.34
(2,657)	1:227:A:LEU:HD22	1:248:A:LEU:HA	12	1.34
(2,657)	1:227:A:LEU:HD23	1:248:A:LEU:HA	12	1.34
(2,657)	1:227:A:LEU:HD21	1:248:A:LEU:HA	11	1.33
(2,657)	1:227:A:LEU:HD22	1:248:A:LEU:HA	11	1.33
(2,657)	1:227:A:LEU:HD23	1:248:A:LEU:HA	11	1.33
(2,657)	1:227:A:LEU:HD21	1:248:A:LEU:HA	2	1.28
(2,657)	1:227:A:LEU:HD22	1:248:A:LEU:HA	2	1.28
(2,657)	1:227:A:LEU:HD23	1:248:A:LEU:HA	2	1.28
(2,657)	1:227:A:LEU:HD21	1:248:A:LEU:HA	1	1.24

10 Dihedral-angle violation analysis

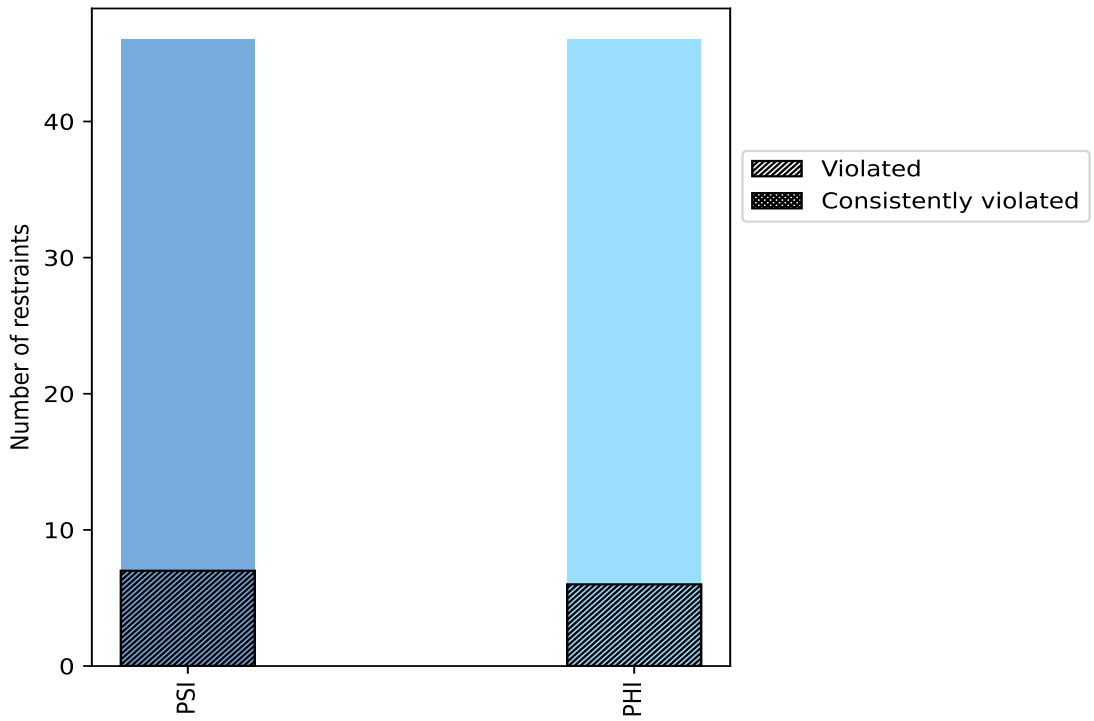
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	46	50.0	7	15.2	7.6	0	0.0	0.0
PHI	46	50.0	6	13.0	6.5	0	0.0	0.0
Total	92	100.0	13	14.1	14.1	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



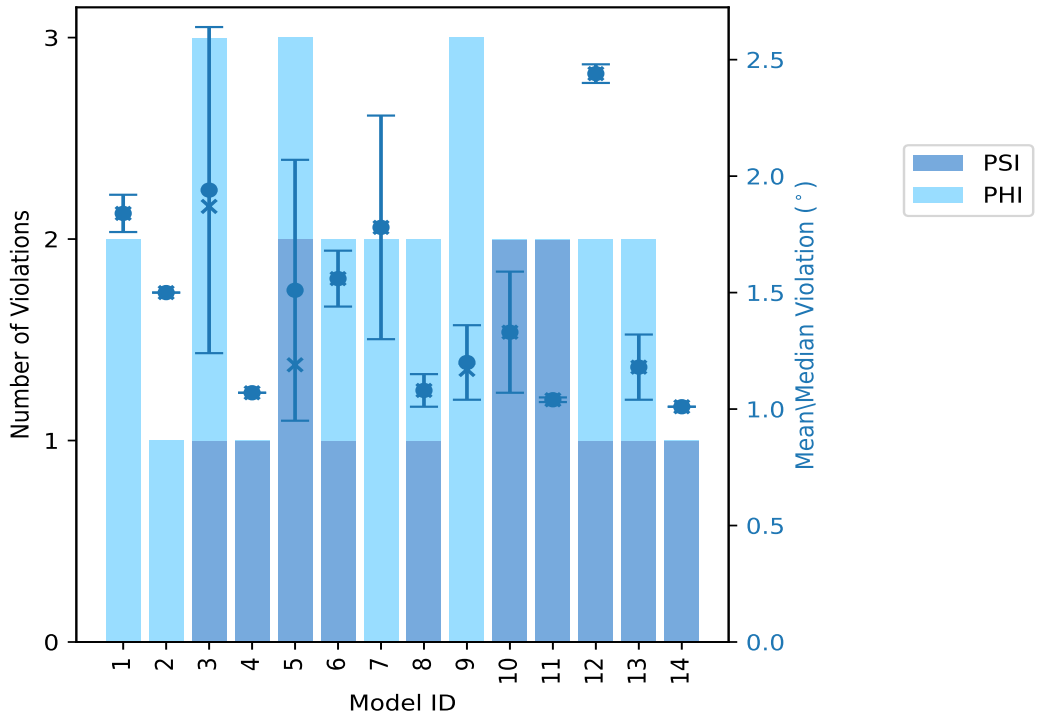
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	0	2	2	1.84	1.93	0.08	1.84
2	0	1	1	1.5	1.5	0.0	1.5
3	1	2	3	1.94	2.83	0.7	1.87
4	1	0	1	1.07	1.07	0.0	1.07
5	2	1	3	1.51	2.3	0.56	1.19
6	1	1	2	1.56	1.68	0.12	1.56
7	0	2	2	1.78	2.26	0.48	1.78
8	1	1	2	1.08	1.16	0.07	1.08
9	0	3	3	1.2	1.41	0.16	1.17
10	2	0	2	1.33	1.58	0.26	1.33
11	2	0	2	1.04	1.05	0.01	1.04
12	1	1	2	2.44	2.48	0.04	2.44
13	1	1	2	1.18	1.32	0.14	1.18
14	1	0	1	1.01	1.01	0.0	1.01

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

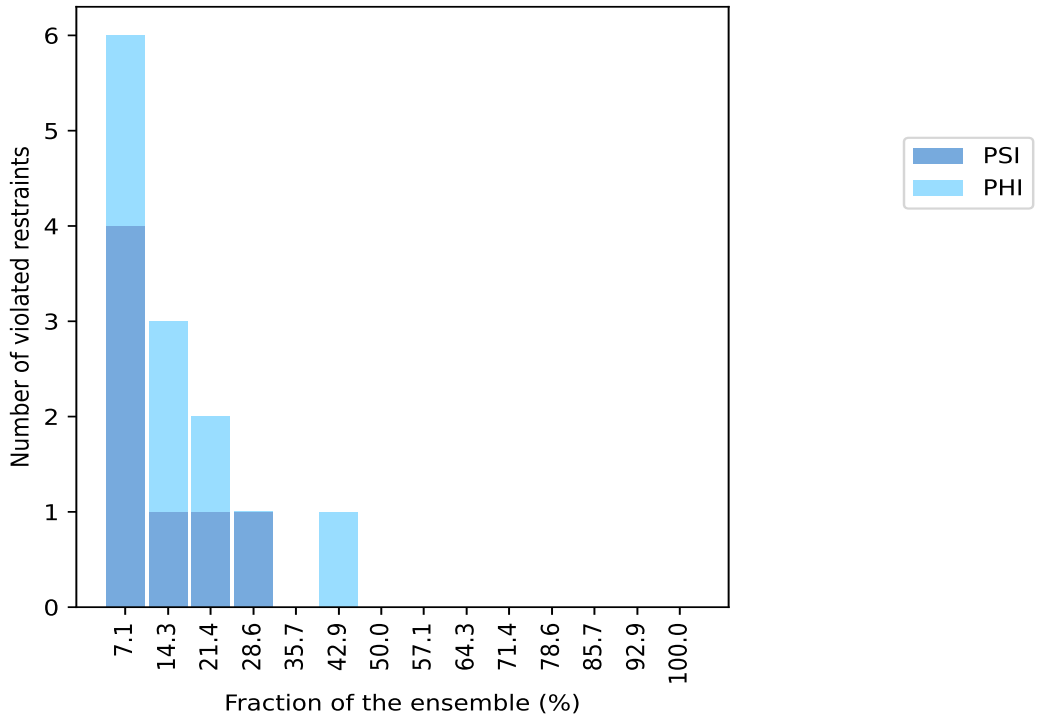
10.3 Dihedral-angle violation statistics for the ensemble

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	
PSI	PHI	Total	Count[1]	%
4	2	6	1	7.1
1	2	3	2	14.3
1	1	2	3	21.4
1	0	1	4	28.6
0	0	0	5	35.7
0	1	1	6	42.9
0	0	0	7	50.0
0	0	0	8	57.1
0	0	0	9	64.3
0	0	0	10	71.4
0	0	0	11	78.6
0	0	0	12	85.7
0	0	0	13	92.9
0	0	0	14	100.0

[1] Number of models with violations

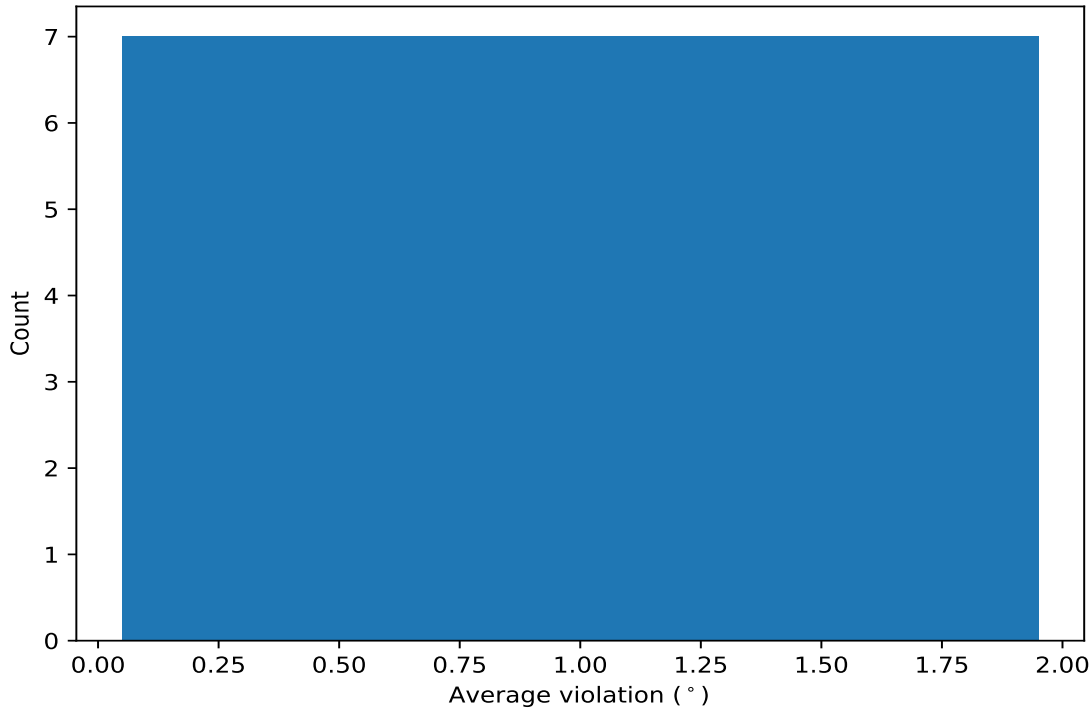
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



10.4.2 Table: Most violated dihedral-angle restraints

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

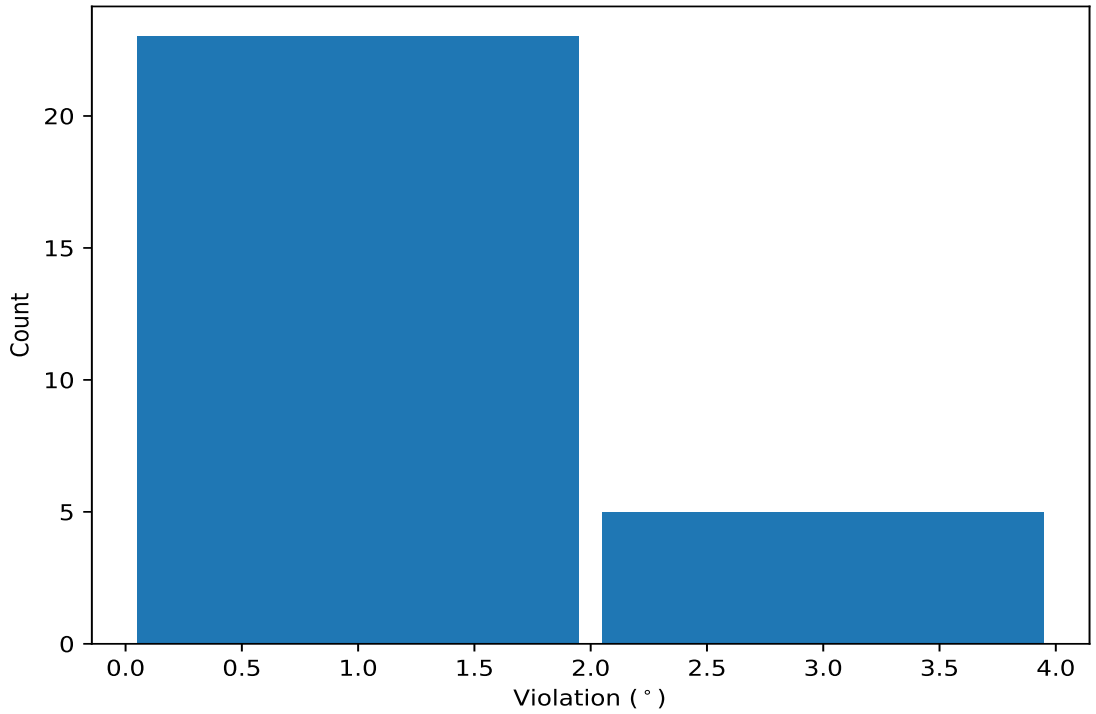
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,46)	1:268:A:LEU:C	1:269:A:SER:N	1:269:A:SER:CA	1:269:A:SER:C	6	1.89	0.51	2.01
(1,58)	1:221:A:ARG:N	1:221:A:ARG:CA	1:221:A:ARG:C	1:222:A:ILE:N	4	1.07	0.05	1.06
(1,42)	1:264:A:PHE:C	1:265:A:VAL:N	1:265:A:VAL:CA	1:265:A:VAL:C	3	1.76	0.78	1.43
(1,66)	1:229:A:GLN:N	1:229:A:GLN:CA	1:229:A:GLN:C	1:230:A:ALA:N	3	1.4	0.21	1.32
(1,21)	1:229:A:GLN:C	1:230:A:ALA:N	1:230:A:ALA:CA	1:230:A:ALA:C	2	1.9	0.03	1.9
(1,71)	1:234:A:LEU:N	1:234:A:LEU:CA	1:234:A:LEU:C	1:235:A:LEU:N	2	1.76	0.64	1.76
(1,22)	1:230:A:ALA:C	1:231:A:ALA:N	1:231:A:ALA:CA	1:231:A:ALA:C	2	1.35	0.06	1.35

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

The following table 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 (°)
(1,42)	1:264:A:PHE:C	1:265:A:VAL:N	1:265:A:VAL:CA	1:265:A:VAL:C	3	2.83
(1,46)	1:268:A:LEU:C	1:269:A:SER:N	1:269:A:SER:CA	1:269:A:SER:C	12	2.48
(1,71)	1:234:A:LEU:N	1:234:A:LEU:CA	1:234:A:LEU:C	1:235:A:LEU:N	12	2.4
(1,46)	1:268:A:LEU:C	1:269:A:SER:N	1:269:A:SER:CA	1:269:A:SER:C	5	2.3
(1,46)	1:268:A:LEU:C	1:269:A:SER:N	1:269:A:SER:CA	1:269:A:SER:C	7	2.26
(1,21)	1:229:A:GLN:C	1:230:A:ALA:N	1:230:A:ALA:CA	1:230:A:ALA:C	1	1.93
(1,21)	1:229:A:GLN:C	1:230:A:ALA:N	1:230:A:ALA:CA	1:230:A:ALA:C	3	1.87
(1,46)	1:268:A:LEU:C	1:269:A:SER:N	1:269:A:SER:CA	1:269:A:SER:C	1	1.76
(1,66)	1:229:A:GLN:N	1:229:A:GLN:CA	1:229:A:GLN:C	1:230:A:ALA:N	6	1.68
(1,91)	1:268:A:LEU:N	1:268:A:LEU:CA	1:268:A:LEU:C	1:269:A:SER:N	10	1.58