wwPDB NMR Structure Validation Summary Report

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PDB ID	:	8PEK
BMRB ID	:	34826
Title	:	Structure of the dimeric, periplasmic domain of ExbD
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Deposited on	:	2023-06-14

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

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

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

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

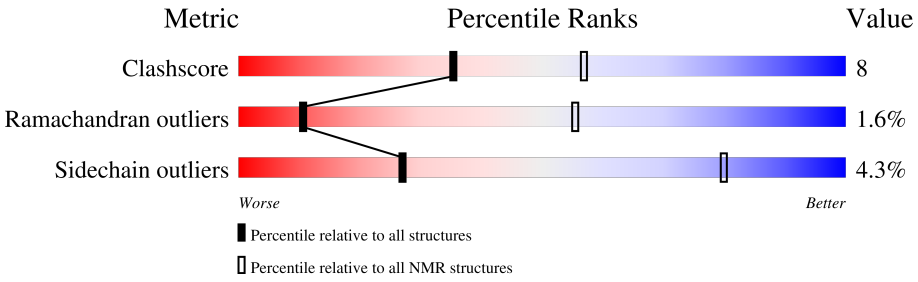
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 47%.

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	99	77% 18% • • •
1	B	99	75% 20% • • •

2 Ensemble composition and analysis

This entry contains 10 models. Model 7 is the overall representative, medoid model (most similar to other models).

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:43-A:137, B:43-B:137 (190)	0.46	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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3056 atoms, of which 1544 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Biopolymer transport protein ExbD.

Mol	Chain	Residues	Atoms						Trace
1	A	98	Total	C	H	N	O	S	0
			1528	476	772	128	149	3	
1	B	98	Total	C	H	N	O	S	0
			1528	476	772	128	149	3	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	SER	-	expression tag	UNP V5YUQ0
B	42	SER	-	expression tag	UNP V5YUQ0

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: Biopolymer transport protein ExbD

Chain A:

• Molecule 1: Biopolymer transport protein ExbD

Chain B:

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

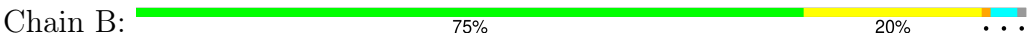
The representative model is number 7. Colouring as in section 4.1 above.

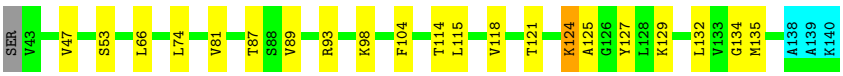
• Molecule 1: Biopolymer transport protein ExbD

Chain A:

• Molecule 1: Biopolymer transport protein ExbD

Chain B:





5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	structure calculation	1.2
ARIA	structure calculation	2.3.3

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	2468
Number of shifts mapped to atoms	2468
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	47%

6 Model quality

6.1 Standard geometry

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	736	749	748	14±2
1	B	736	749	748	14±2
All	All	14720	14980	14960	229

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 8.

5 of 67 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:LYS:HA	1:B:47:VAL:O	0.60	1.96	9	9
1:A:47:VAL:O	1:B:129:LYS:HA	0.60	1.96	9	9
1:B:74:LEU:HB2	1:B:81:VAL:O	0.58	1.99	7	9
1:A:74:LEU:HB2	1:A:81:VAL:O	0.57	1.99	7	9
1:A:66:LEU:O	1:A:104:PHE:HA	0.56	2.00	7	10

6.3 Torsion angles

6.3.1 Protein backbone

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	94/99 (95%)	88±1 (93±1%)	5±2 (5±2%)	2±1 (2±1%)	10 55
1	B	94/99 (95%)	88±1 (93±1%)	5±2 (5±2%)	2±1 (2±1%)	10 55
All	All	1880/1980 (95%)	1750 (93%)	100 (5%)	30 (2%)	10 55

5 of 8 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	134	GLY	7
1	B	134	GLY	7
1	A	53	SER	6
1	B	53	SER	6
1	A	52	SER	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	83/85 (98%)	79±1 (96±2%)	4±1 (4±2%)	27 80
1	B	83/85 (98%)	79±1 (96±2%)	4±1 (4±2%)	27 80
All	All	1660/1700 (98%)	1588 (96%)	72 (4%)	27 80

5 of 20 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	124	LYS	10
1	B	124	LYS	10
1	A	135	MET	7
1	B	135	MET	7
1	A	130	VAL	5

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

There are no ligands in this entry.

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 47% for the well-defined parts and 47% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	2468
Number of shifts mapped to atoms	2468
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	THR	C	172.565	.	1
1	A	100	THR	CA	64.001	.	1
1	A	100	THR	CB	70.784	.	1
1	A	100	THR	CG2	21.223	.	1
1	A	100	THR	H	7.315	.	1
1	A	100	THR	HA	3.917	.	1
1	A	100	THR	HB	4.093	.	1
1	A	100	THR	HG22	1.309	.	1
1	A	100	THR	HG23	1.309	.	1
1	A	100	THR	HG21	1.309	.	1
1	A	100	THR	N	117.620	.	1
1	A	101	THR	C	171.967	.	1
1	A	101	THR	CA	63.834	.	1
1	A	101	THR	CB	68.964	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	THR	CG2	21.041	.	1
1	A	101	THR	H	8.391	.	1
1	A	101	THR	HA	4.005	.	1
1	A	101	THR	HB	3.657	.	1
1	A	101	THR	HG22	0.025	.	1
1	A	101	THR	HG23	0.025	.	1
1	A	101	THR	HG21	0.025	.	1
1	A	101	THR	N	123.479	.	1
1	A	102	ILE	C	175.304	.	1
1	A	102	ILE	CA	57.564	.	1
1	A	102	ILE	CB	36.373	.	1
1	A	102	ILE	CD1	8.896	.	1
1	A	102	ILE	CG1	26.696	.	1
1	A	102	ILE	CG2	17.798	.	1
1	A	102	ILE	H	8.434	.	1
1	A	102	ILE	HA	4.241	.	1
1	A	102	ILE	HB	2.060	.	1
1	A	102	ILE	HD12	0.346	.	1
1	A	102	ILE	HD11	0.346	.	1
1	A	102	ILE	HD13	0.346	.	1
1	A	102	ILE	HG12	1.827	.	2
1	A	102	ILE	HG13	0.951	.	2
1	A	102	ILE	HG23	0.693	.	1
1	A	102	ILE	HG22	0.693	.	1
1	A	102	ILE	HG21	0.693	.	1
1	A	102	ILE	N	127.451	.	1
1	A	103	PHE	C	173.878	.	1
1	A	103	PHE	CA	58.786	.	1
1	A	103	PHE	CB	39.632	.	1
1	A	103	PHE	CD1	131.848	.	1
1	A	103	PHE	CD2	131.848	.	1
1	A	103	PHE	CE2	130.851	.	1
1	A	103	PHE	CE1	130.851	.	1
1	A	103	PHE	H	8.695	.	1
1	A	103	PHE	HA	4.845	.	1
1	A	103	PHE	HB2	2.410	.	1
1	A	103	PHE	HB3	2.410	.	1
1	A	103	PHE	HD2	6.919	.	1
1	A	103	PHE	HD1	6.919	.	1
1	A	103	PHE	HE2	7.219	.	1
1	A	103	PHE	HE1	7.219	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	PHE	N	127.132	.	1
1	A	104	PHE	C	173.153	.	1
1	A	104	PHE	CA	56.455	.	1
1	A	104	PHE	CB	42.464	.	1
1	A	104	PHE	CD1	131.212	.	1
1	A	104	PHE	CD2	131.212	.	1
1	A	104	PHE	H	9.472	.	1
1	A	104	PHE	HA	5.519	.	1
1	A	104	PHE	HB2	3.148	.	2
1	A	104	PHE	HB3	2.560	.	2
1	A	104	PHE	HD2	7.011	.	1
1	A	104	PHE	HD1	7.011	.	1
1	A	104	PHE	N	126.774	.	1
1	A	105	GLN	C	172.632	.	1
1	A	105	GLN	CA	53.874	.	1
1	A	105	GLN	CB	32.057	.	1
1	A	105	GLN	CG	34.044	.	1
1	A	105	GLN	H	8.557	.	1
1	A	105	GLN	HA	4.654	.	1
1	A	105	GLN	HB2	1.930	.	2
1	A	105	GLN	HB3	1.798	.	2
1	A	105	GLN	HE21	7.012	.	1
1	A	105	GLN	HE22	6.395	.	1
1	A	105	GLN	HG2	2.208	.	2
1	A	105	GLN	HG3	2.130	.	2
1	A	105	GLN	N	126.779	.	1
1	A	105	GLN	NE2	109.537	.	1
1	A	106	ALA	C	175.824	.	1
1	A	106	ALA	CA	49.691	.	1
1	A	106	ALA	CB	20.319	.	1
1	A	106	ALA	H	7.324	0.002	1
1	A	106	ALA	HA	4.815	.	1
1	A	106	ALA	HB2	0.425	0.003	1
1	A	106	ALA	HB3	0.425	0.003	1
1	A	106	ALA	HB1	0.425	0.003	1
1	A	106	ALA	N	122.986	0.003	1
1	A	107	ASP	C	176.365	.	1
1	A	107	ASP	CA	54.601	.	1
1	A	107	ASP	CB	42.773	.	1
1	A	107	ASP	H	7.289	.	1
1	A	107	ASP	HA	4.596	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	107	ASP	HB2	2.688	.	2
1	A	107	ASP	HB3	2.590	.	2
1	A	107	ASP	N	119.324	.	1
1	A	108	LYS	C	175.632	.	1
1	A	108	LYS	CA	59.918	.	1
1	A	108	LYS	CB	33.047	.	1
1	A	108	LYS	CD	29.527	.	1
1	A	108	LYS	CE	42.170	.	1
1	A	108	LYS	CG	24.603	.	1
1	A	108	LYS	H	8.535	.	1
1	A	108	LYS	HA	4.152	.	1
1	A	108	LYS	HB2	1.989	.	1
1	A	108	LYS	HB3	1.989	.	1
1	A	108	LYS	HD2	1.712	.	1
1	A	108	LYS	HD3	1.712	.	1
1	A	108	LYS	HE2	3.035	.	1
1	A	108	LYS	HE3	3.035	.	1
1	A	108	LYS	HG2	1.575	.	1
1	A	108	LYS	HG3	1.575	.	1
1	A	108	LYS	N	119.714	.	1
1	A	109	SER	C	175.514	.	1
1	A	109	SER	CA	58.984	.	1
1	A	109	SER	CB	64.568	.	1
1	A	109	SER	H	8.031	.	1
1	A	109	SER	HA	4.553	.	1
1	A	109	SER	HB2	4.152	.	2
1	A	109	SER	HB3	3.942	.	2
1	A	109	SER	N	109.540	.	1
1	A	110	VAL	C	175.354	.	1
1	A	110	VAL	CA	64.673	.	1
1	A	110	VAL	CB	31.683	.	1
1	A	110	VAL	CG1	24.522	.	1
1	A	110	VAL	CG2	20.673	.	1
1	A	110	VAL	H	7.888	.	1
1	A	110	VAL	HA	3.864	.	1
1	A	110	VAL	HB	2.060	.	1
1	A	110	VAL	HG13	0.960	.	1
1	A	110	VAL	HG12	0.960	.	1
1	A	110	VAL	HG11	0.960	.	1
1	A	110	VAL	HG22	1.030	.	1
1	A	110	VAL	HG21	1.030	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	110	VAL	HG23	1.030	.	1
1	A	110	VAL	N	125.909	.	1
1	A	111	ASP	C	176.431	.	1
1	A	111	ASP	CA	53.106	.	1
1	A	111	ASP	CB	42.842	.	1
1	A	111	ASP	H	8.323	0.001	1
1	A	111	ASP	HA	5.162	0.002	1
1	A	111	ASP	HB2	3.653	.	2
1	A	111	ASP	HB3	2.688	.	2
1	A	111	ASP	N	125.863	.	1
1	A	112	TYR	CA	62.038	.	1
1	A	112	TYR	CB	39.675	.	1
1	A	112	TYR	CD1	133.046	.	1
1	A	112	TYR	CD2	133.046	.	1
1	A	112	TYR	CE2	117.774	.	1
1	A	112	TYR	CE1	117.774	.	1
1	A	112	TYR	H	8.491	0.001	1
1	A	112	TYR	HA	4.234	.	1
1	A	112	TYR	HB2	3.169	.	2
1	A	112	TYR	HB3	3.073	.	2
1	A	112	TYR	HD2	6.960	0.019	1
1	A	112	TYR	HD1	6.960	0.019	1
1	A	112	TYR	HE2	6.856	0.018	1
1	A	112	TYR	HE1	6.856	0.018	1
1	A	112	TYR	N	123.014	0.006	1
1	A	113	GLU	C	179.386	.	1
1	A	113	GLU	CA	59.809	.	1
1	A	113	GLU	CB	29.750	.	1
1	A	113	GLU	CG	36.160	.	1
1	A	113	GLU	H	8.525	0.003	1
1	A	113	GLU	HA	3.991	0.002	1
1	A	113	GLU	HB2	2.177	0.004	2
1	A	113	GLU	HB3	2.123	.	2
1	A	113	GLU	HG2	2.256	.	1
1	A	113	GLU	HG3	2.256	.	1
1	A	113	GLU	N	118.049	0.017	1
1	A	114	THR	CA	67.344	.	1
1	A	114	THR	CB	67.389	.	1
1	A	114	THR	CG2	21.182	.	1
1	A	114	THR	H	8.666	0.002	1
1	A	114	THR	HA	3.912	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	114	THR	HB	4.451	.	1
1	A	114	THR	HG22	1.189	.	1
1	A	114	THR	HG23	1.189	.	1
1	A	114	THR	HG21	1.189	.	1
1	A	114	THR	N	120.083	0.007	1
1	A	115	LEU	C	178.397	.	1
1	A	115	LEU	CA	59.358	.	1
1	A	115	LEU	CB	42.099	.	1
1	A	115	LEU	CD1	25.664	.	2
1	A	115	LEU	CD2	25.515	.	2
1	A	115	LEU	CG	26.898	.	1
1	A	115	LEU	H	8.485	0.005	1
1	A	115	LEU	HA	3.746	.	1
1	A	115	LEU	HB2	1.514	.	2
1	A	115	LEU	HB3	1.927	.	2
1	A	115	LEU	HD11	0.766	.	2
1	A	115	LEU	HD12	0.766	.	2
1	A	115	LEU	HD13	0.766	.	2
1	A	115	LEU	HD21	0.648	.	2
1	A	115	LEU	HD22	0.648	.	2
1	A	115	LEU	HD23	0.648	.	2
1	A	115	LEU	HG	1.337	.	1
1	A	115	LEU	N	123.256	0.02	1
1	A	116	MET	C	179.002	.	1
1	A	116	MET	CA	56.812	.	1
1	A	116	MET	CB	32.258	.	1
1	A	116	MET	CE	18.656	.	1
1	A	116	MET	CG	33.620	.	1
1	A	116	MET	H	8.459	0.003	1
1	A	116	MET	HA	4.152	.	1
1	A	116	MET	HB2	2.060	.	2
1	A	116	MET	HB3	1.766	.	2
1	A	116	MET	HE3	1.719	.	1
1	A	116	MET	HE2	1.719	.	1
1	A	116	MET	HE1	1.719	.	1
1	A	116	MET	HG2	2.212	.	2
1	A	116	MET	HG3	1.803	.	2
1	A	116	MET	N	115.327	0.015	1
1	A	117	SER	CA	61.406	.	1
1	A	117	SER	CB	62.906	.	1
1	A	117	SER	H	8.156	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	117	SER	HA	4.333	.	1
1	A	117	SER	HB2	4.152	.	1
1	A	117	SER	HB3	4.152	.	1
1	A	117	SER	N	117.130	0.006	1
1	A	118	VAL	C	178.147	.	1
1	A	118	VAL	CA	67.028	.	1
1	A	118	VAL	CB	31.138	.	1
1	A	118	VAL	CG1	23.075	.	2
1	A	118	VAL	CG2	22.284	.	2
1	A	118	VAL	H	8.345	0.003	1
1	A	118	VAL	HA	3.632	.	1
1	A	118	VAL	HB	2.147	.	1
1	A	118	VAL	HG11	1.100	.	2
1	A	118	VAL	HG12	1.100	.	2
1	A	118	VAL	HG13	1.100	.	2
1	A	118	VAL	HG21	0.766	.	2
1	A	118	VAL	HG22	0.766	.	2
1	A	118	VAL	HG23	0.766	.	2
1	A	118	VAL	N	123.297	0.006	1
1	A	119	MET	C	178.096	.	1
1	A	119	MET	CA	58.366	.	1
1	A	119	MET	CB	32.318	.	1
1	A	119	MET	CE	18.576	.	1
1	A	119	MET	CG	33.619	.	1
1	A	119	MET	H	8.209	.	1
1	A	119	MET	HA	4.241	.	1
1	A	119	MET	HB2	2.293	.	2
1	A	119	MET	HB3	1.780	.	2
1	A	119	MET	HE3	1.393	.	1
1	A	119	MET	HE2	1.393	.	1
1	A	119	MET	HE1	1.393	.	1
1	A	119	MET	HG2	2.574	.	2
1	A	119	MET	HG3	2.477	.	2
1	A	119	MET	N	118.023	.	1
1	A	120	ASP	C	178.206	.	1
1	A	120	ASP	CA	57.883	.	1
1	A	120	ASP	CB	41.538	.	1
1	A	120	ASP	H	8.226	.	1
1	A	120	ASP	HA	4.429	.	1
1	A	120	ASP	HB2	2.848	.	2
1	A	120	ASP	HB3	2.778	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	120	ASP	N	119.274	.	1
1	A	121	THR	CA	67.278	.	1
1	A	121	THR	CB	68.353	.	1
1	A	121	THR	CG2	22.610	.	1
1	A	121	THR	H	8.103	.	1
1	A	121	THR	HA	3.845	.	1
1	A	121	THR	HB	4.394	.	1
1	A	121	THR	HG22	1.263	.	1
1	A	121	THR	HG23	1.263	.	1
1	A	121	THR	HG21	1.263	.	1
1	A	121	THR	N	117.744	.	1
1	A	122	LEU	C	178.532	.	1
1	A	122	LEU	CA	58.855	.	1
1	A	122	LEU	CB	40.188	.	1
1	A	122	LEU	CD1	25.648	.	2
1	A	122	LEU	CD2	23.571	.	2
1	A	122	LEU	CG	26.762	.	1
1	A	122	LEU	H	8.405	.	1
1	A	122	LEU	HA	3.929	.	1
1	A	122	LEU	HB2	1.990	.	2
1	A	122	LEU	HB3	1.858	.	2
1	A	122	LEU	HD11	0.766	.	2
1	A	122	LEU	HD12	0.766	.	2
1	A	122	LEU	HD13	0.766	.	2
1	A	122	LEU	HD21	0.652	.	2
1	A	122	LEU	HD22	0.652	.	2
1	A	122	LEU	HD23	0.652	.	2
1	A	122	LEU	HG	1.697	.	1
1	A	122	LEU	N	123.420	.	1
1	A	123	ARG	C	180.614	.	1
1	A	123	ARG	CA	59.127	.	1
1	A	123	ARG	CB	29.913	.	1
1	A	123	ARG	CD	44.137	.	1
1	A	123	ARG	CG	27.150	.	1
1	A	123	ARG	H	8.334	.	1
1	A	123	ARG	HA	3.858	.	1
1	A	123	ARG	HB2	1.896	.	1
1	A	123	ARG	HB3	1.896	.	1
1	A	123	ARG	HD2	3.208	.	1
1	A	123	ARG	HD3	3.208	.	1
1	A	123	ARG	HG2	1.791	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	123	ARG	HG3	1.743	.	2
1	A	123	ARG	N	119.080	.	1
1	A	124	LYS	C	178.074	.	1
1	A	124	LYS	CA	59.514	.	1
1	A	124	LYS	CB	32.344	.	1
1	A	124	LYS	CD	29.284	.	1
1	A	124	LYS	CE	42.077	.	1
1	A	124	LYS	CG	26.472	.	1
1	A	124	LYS	H	8.158	.	1
1	A	124	LYS	HA	4.005	.	1
1	A	124	LYS	HB2	1.928	.	1
1	A	124	LYS	HB3	1.928	.	1
1	A	124	LYS	HD2	1.675	.	2
1	A	124	LYS	HD3	1.622	.	2
1	A	124	LYS	HE2	2.955	.	1
1	A	124	LYS	HE3	2.955	.	1
1	A	124	LYS	HG2	1.622	.	2
1	A	124	LYS	HG3	1.436	.	2
1	A	124	LYS	N	121.385	.	1
1	A	125	ALA	C	176.286	.	1
1	A	125	ALA	CA	52.351	.	1
1	A	125	ALA	CB	20.277	.	1
1	A	125	ALA	H	7.731	.	1
1	A	125	ALA	HA	4.486	.	1
1	A	125	ALA	HB2	1.761	.	1
1	A	125	ALA	HB3	1.761	.	1
1	A	125	ALA	HB1	1.761	.	1
1	A	125	ALA	N	120.633	.	1
1	A	126	GLY	C	173.364	.	1
1	A	126	GLY	CA	45.059	.	1
1	A	126	GLY	H	7.791	.	1
1	A	126	GLY	HA2	4.051	.	2
1	A	126	GLY	HA3	3.449	.	2
1	A	126	GLY	N	105.162	.	1
1	A	127	TYR	C	172.832	.	1
1	A	127	TYR	CA	59.372	.	1
1	A	127	TYR	CB	38.282	.	1
1	A	127	TYR	CD1	133.724	.	1
1	A	127	TYR	CD2	133.724	.	1
1	A	127	TYR	CE2	118.051	.	1
1	A	127	TYR	CE1	118.051	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	TYR	H	7.780	.	1
1	A	127	TYR	HA	4.492	.	1
1	A	127	TYR	HB2	3.057	.	2
1	A	127	TYR	HB3	2.496	.	2
1	A	127	TYR	HD2	7.103	.	1
1	A	127	TYR	HD1	7.103	.	1
1	A	127	TYR	HE2	6.689	.	1
1	A	127	TYR	HE1	6.689	.	1
1	A	127	TYR	N	122.778	.	1
1	A	128	LEU	C	177.558	.	1
1	A	128	LEU	CA	54.002	.	1
1	A	128	LEU	CB	40.475	.	1
1	A	128	LEU	CD1	24.896	.	2
1	A	128	LEU	CD2	21.774	.	2
1	A	128	LEU	CG	26.997	.	1
1	A	128	LEU	H	7.360	.	1
1	A	128	LEU	HA	4.366	.	1
1	A	128	LEU	HB2	1.508	.	2
1	A	128	LEU	HB3	2.238	.	2
1	A	128	LEU	HD11	0.908	.	2
1	A	128	LEU	HD12	0.908	.	2
1	A	128	LEU	HD13	0.908	.	2
1	A	128	LEU	HD21	0.657	.	2
1	A	128	LEU	HD22	0.657	.	2
1	A	128	LEU	HD23	0.657	.	2
1	A	128	LEU	HG	1.488	.	1
1	A	128	LEU	N	115.000	.	1
1	A	129	LYS	C	174.339	.	1
1	A	129	LYS	CA	55.280	.	1
1	A	129	LYS	CB	32.348	.	1
1	A	129	LYS	CD	29.194	.	1
1	A	129	LYS	CE	42.282	.	1
1	A	129	LYS	CG	24.237	.	1
1	A	129	LYS	H	9.191	.	1
1	A	129	LYS	HB2	1.558	.	2
1	A	129	LYS	HB3	1.854	.	2
1	A	129	LYS	HD2	1.644	.	2
1	A	129	LYS	HD3	1.593	.	2
1	A	129	LYS	HE2	2.947	.	1
1	A	129	LYS	HE3	2.947	.	1
1	A	129	LYS	HG2	1.403	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	129	LYS	HG3	1.368	.	2
1	A	129	LYS	N	121.417	.	1
1	A	130	VAL	C	175.236	.	1
1	A	130	VAL	CA	59.184	.	1
1	A	130	VAL	CB	36.489	.	1
1	A	130	VAL	CG1	22.472	.	2
1	A	130	VAL	CG2	21.644	.	2
1	A	130	VAL	H	8.249	0.003	1
1	A	130	VAL	HA	5.054	.	1
1	A	130	VAL	HB	1.737	.	1
1	A	130	VAL	HG11	0.818	.	2
1	A	130	VAL	HG12	0.818	.	2
1	A	130	VAL	HG13	0.818	.	2
1	A	130	VAL	HG21	0.766	.	2
1	A	130	VAL	HG22	0.766	.	2
1	A	130	VAL	HG23	0.766	.	2
1	A	130	VAL	N	123.286	0.02	1
1	A	131	GLY	C	172.115	.	1
1	A	131	GLY	CA	43.952	.	1
1	A	131	GLY	H	8.722	.	1
1	A	131	GLY	HA2	2.797	.	1
1	A	131	GLY	HA3	2.797	.	1
1	A	131	GLY	N	114.174	.	1
1	A	132	LEU	C	176.624	.	1
1	A	132	LEU	CA	54.850	.	1
1	A	132	LEU	CB	41.331	.	1
1	A	132	LEU	CD1	24.596	.	2
1	A	132	LEU	CD2	23.231	.	2
1	A	132	LEU	CG	26.553	.	1
1	A	132	LEU	H	9.434	0.002	1
1	A	132	LEU	HB2	1.868	.	1
1	A	132	LEU	HB3	1.868	.	1
1	A	132	LEU	HD11	0.723	.	2
1	A	132	LEU	HD12	0.723	.	2
1	A	132	LEU	HD13	0.723	.	2
1	A	132	LEU	HD21	0.766	.	2
1	A	132	LEU	HD22	0.766	.	2
1	A	132	LEU	HD23	0.766	.	2
1	A	132	LEU	HG	1.699	.	1
1	A	132	LEU	N	125.833	0.017	1
1	A	133	VAL	C	177.750	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	133	VAL	CA	62.544	.	1
1	A	133	VAL	CB	32.933	.	1
1	A	133	VAL	CG1	21.613	.	2
1	A	133	VAL	CG2	21.588	.	2
1	A	133	VAL	H	8.874	.	1
1	A	133	VAL	HA	4.502	.	1
1	A	133	VAL	HB	2.296	.	1
1	A	133	VAL	HG11	1.139	.	1
1	A	133	VAL	HG12	1.139	.	1
1	A	133	VAL	HG13	1.139	.	1
1	A	133	VAL	HG21	1.139	.	1
1	A	133	VAL	HG22	1.139	.	1
1	A	133	VAL	HG23	1.139	.	1
1	A	133	VAL	N	125.288	.	1
1	A	134	GLY	C	173.951	.	1
1	A	134	GLY	CA	45.280	.	1
1	A	134	GLY	H	9.035	0.0	1
1	A	134	GLY	HA2	4.241	.	2
1	A	134	GLY	HA3	4.152	.	2
1	A	134	GLY	N	115.921	.	1
1	A	135	MET	C	176.546	.	1
1	A	135	MET	CA	56.250	.	1
1	A	135	MET	CB	33.008	.	1
1	A	135	MET	CE	17.351	.	1
1	A	135	MET	CG	32.964	.	1
1	A	135	MET	H	8.808	.	1
1	A	135	MET	HA	4.451	.	1
1	A	135	MET	HB2	2.142	.	1
1	A	135	MET	HB3	2.142	.	1
1	A	135	MET	HE3	2.042	.	1
1	A	135	MET	HE2	2.042	.	1
1	A	135	MET	HE1	2.042	.	1
1	A	135	MET	HG2	2.053	.	1
1	A	135	MET	HG3	2.053	.	1
1	A	135	MET	N	120.539	.	1
1	A	136	GLU	C	176.889	.	1
1	A	136	GLU	CA	56.759	.	1
1	A	136	GLU	CB	30.272	.	1
1	A	136	GLU	CG	36.273	.	1
1	A	136	GLU	H	8.695	.	1
1	A	136	GLU	HA	4.241	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	136	GLU	HB2	2.060	.	2
1	A	136	GLU	HB3	1.936	.	2
1	A	136	GLU	HG2	2.249	.	1
1	A	136	GLU	HG3	2.249	.	1
1	A	136	GLU	N	122.370	.	1
1	A	137	GLY	C	173.707	.	1
1	A	137	GLY	CA	45.208	.	1
1	A	137	GLY	H	8.463	.	1
1	A	137	GLY	HA2	3.946	.	2
1	A	137	GLY	HA3	3.897	.	2
1	A	137	GLY	N	110.159	.	1
1	A	138	ALA	C	177.354	.	1
1	A	138	ALA	CA	52.295	.	1
1	A	138	ALA	CB	19.519	.	1
1	A	138	ALA	H	8.189	.	1
1	A	138	ALA	HA	4.295	.	1
1	A	138	ALA	HB2	1.362	.	1
1	A	138	ALA	HB3	1.362	.	1
1	A	138	ALA	HB1	1.362	.	1
1	A	138	ALA	N	123.821	.	1
1	A	139	ALA	C	176.716	.	1
1	A	139	ALA	CA	52.427	.	1
1	A	139	ALA	CB	19.254	.	1
1	A	139	ALA	H	8.305	.	1
1	A	139	ALA	HA	4.241	.	1
1	A	139	ALA	HB2	1.356	.	1
1	A	139	ALA	HB3	1.356	.	1
1	A	139	ALA	HB1	1.356	.	1
1	A	139	ALA	N	124.091	.	1
1	A	140	LYS	C	181.323	.	1
1	A	140	LYS	CA	57.563	.	1
1	A	140	LYS	CB	33.727	.	1
1	A	140	LYS	CD	29.125	.	1
1	A	140	LYS	CE	42.188	.	1
1	A	140	LYS	CG	24.628	.	1
1	A	140	LYS	H	7.894	.	1
1	A	140	LYS	HA	4.101	.	1
1	A	140	LYS	HB2	1.783	.	2
1	A	140	LYS	HB3	1.672	.	2
1	A	140	LYS	HD2	1.638	.	1
1	A	140	LYS	HD3	1.638	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	140	LYS	HE2	2.962	.	1
1	A	140	LYS	HE3	2.962	.	1
1	A	140	LYS	HG2	1.361	.	1
1	A	140	LYS	HG3	1.361	.	1
1	A	140	LYS	N	125.860	.	1
1	A	43	VAL	C	174.334	.	1
1	A	43	VAL	CA	61.164	.	1
1	A	43	VAL	CB	33.485	.	1
1	A	43	VAL	CG1	21.237	.	2
1	A	43	VAL	CG2	20.223	.	2
1	A	43	VAL	HA	4.333	.	1
1	A	43	VAL	HB	2.060	.	1
1	A	43	VAL	HG11	0.847	.	1
1	A	43	VAL	HG12	0.847	.	1
1	A	43	VAL	HG13	0.847	.	1
1	A	43	VAL	HG21	0.847	.	1
1	A	43	VAL	HG22	0.847	.	1
1	A	43	VAL	HG23	0.847	.	1
1	A	44	ASP	C	175.693	.	1
1	A	44	ASP	CA	53.911	.	1
1	A	44	ASP	CB	41.534	.	1
1	A	44	ASP	H	8.361	0.001	1
1	A	44	ASP	HA	5.031	.	1
1	A	44	ASP	HB2	2.606	.	2
1	A	44	ASP	HB3	2.408	.	2
1	A	44	ASP	N	124.606	.	1
1	A	45	ILE	C	175.617	.	1
1	A	45	ILE	CA	61.127	.	1
1	A	45	ILE	CB	39.927	.	1
1	A	45	ILE	CD1	13.501	.	1
1	A	45	ILE	CG1	27.953	.	1
1	A	45	ILE	CG2	18.186	.	1
1	A	45	ILE	H	8.577	0.001	1
1	A	45	ILE	HA	4.141	.	1
1	A	45	ILE	HB	1.863	.	1
1	A	45	ILE	HD12	0.766	.	1
1	A	45	ILE	HD11	0.766	.	1
1	A	45	ILE	HD13	0.766	.	1
1	A	45	ILE	HG12	1.759	.	2
1	A	45	ILE	HG13	0.873	.	2
1	A	45	ILE	HG23	0.766	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	ILE	HG22	0.766	.	1
1	A	45	ILE	HG21	0.766	.	1
1	A	45	ILE	N	122.437	0.018	1
1	A	46	ARG	C	174.965	.	1
1	A	46	ARG	CA	55.862	.	1
1	A	46	ARG	CB	30.249	.	1
1	A	46	ARG	CD	42.573	.	1
1	A	46	ARG	CG	27.822	.	1
1	A	46	ARG	H	8.188	0.004	1
1	A	46	ARG	HA	4.767	.	1
1	A	46	ARG	HB2	1.917	.	1
1	A	46	ARG	HB3	1.917	.	1
1	A	46	ARG	HD2	3.114	.	1
1	A	46	ARG	HD3	3.114	.	1
1	A	46	ARG	HG2	1.734	.	2
1	A	46	ARG	HG3	1.517	.	2
1	A	46	ARG	N	128.265	0.011	1
1	A	47	VAL	C	173.664	.	1
1	A	47	VAL	CA	61.019	.	1
1	A	47	VAL	CB	34.853	.	1
1	A	47	VAL	CG1	21.683	.	2
1	A	47	VAL	CG2	21.705	.	2
1	A	47	VAL	H	9.058	0.004	1
1	A	47	VAL	HA	4.466	.	1
1	A	47	VAL	HB	1.834	.	1
1	A	47	VAL	HG11	0.767	.	2
1	A	47	VAL	HG12	0.767	.	2
1	A	47	VAL	HG13	0.767	.	2
1	A	47	VAL	HG21	0.713	.	2
1	A	47	VAL	HG22	0.713	.	2
1	A	47	VAL	HG23	0.713	.	2
1	A	47	VAL	N	125.118	0.005	1
1	A	48	ASP	C	175.696	.	1
1	A	48	ASP	CA	52.501	.	1
1	A	48	ASP	CB	41.898	.	1
1	A	48	ASP	H	8.907	0.003	1
1	A	48	ASP	HA	5.485	.	1
1	A	48	ASP	HB2	2.566	.	2
1	A	48	ASP	HB3	2.534	.	2
1	A	48	ASP	N	127.985	0.016	1
1	A	49	LEU	C	173.972	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	LEU	CA	52.489	.	1
1	A	49	LEU	CB	41.910	.	1
1	A	49	LEU	CD1	26.497	.	2
1	A	49	LEU	CD2	24.606	.	2
1	A	49	LEU	CG	26.965	.	1
1	A	49	LEU	H	9.663	0.002	1
1	A	49	LEU	HA	4.451	.	1
1	A	49	LEU	HB2	1.896	.	2
1	A	49	LEU	HB3	1.060	.	2
1	A	49	LEU	HD11	1.060	.	2
1	A	49	LEU	HD12	1.060	.	2
1	A	49	LEU	HD13	1.060	.	2
1	A	49	LEU	HD21	0.818	.	2
1	A	49	LEU	HD22	0.818	.	2
1	A	49	LEU	HD23	0.818	.	2
1	A	49	LEU	HG	1.638	.	1
1	A	49	LEU	N	125.984	0.014	1
1	A	50	PRO	CA	61.996	.	1
1	A	50	PRO	CB	31.494	.	1
1	A	50	PRO	CD	50.341	.	1
1	A	50	PRO	CG	27.586	.	1
1	A	50	PRO	HA	4.451	.	1
1	A	50	PRO	HB2	2.281	.	2
1	A	50	PRO	HB3	1.809	.	2
1	A	50	PRO	HD2	4.005	.	2
1	A	50	PRO	HD3	3.309	.	2
1	A	50	PRO	HG2	2.104	.	2
1	A	50	PRO	HG3	1.954	.	2
1	A	51	ALA	C	180.038	.	1
1	A	51	ALA	CA	52.064	.	1
1	A	51	ALA	CB	19.037	.	1
1	A	51	ALA	H	8.664	0.002	1
1	A	51	ALA	HA	4.241	.	1
1	A	51	ALA	HB2	1.436	.	1
1	A	51	ALA	HB3	1.436	.	1
1	A	51	ALA	HB1	1.436	.	1
1	A	51	ALA	N	124.515	0.011	1
1	A	52	SER	H	9.349	.	1
1	A	52	SER	N	118.420	.	1
1	A	53	SER	CA	57.553	.	1
1	A	53	SER	CB	63.527	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	SER	HA	4.451	.	1
1	A	53	SER	HB2	4.064	.	2
1	A	53	SER	HB3	3.801	.	2
1	A	54	ALA	C	177.512	.	1
1	A	54	ALA	CA	52.528	.	1
1	A	54	ALA	CB	19.814	.	1
1	A	54	ALA	H	7.530	.	1
1	A	54	ALA	HA	4.241	.	1
1	A	54	ALA	HB2	1.445	.	1
1	A	54	ALA	HB3	1.445	.	1
1	A	54	ALA	HB1	1.445	.	1
1	A	54	ALA	N	125.057	.	1
1	A	55	LYS	C	174.782	.	1
1	A	55	LYS	CA	53.929	.	1
1	A	55	LYS	CB	32.105	.	1
1	A	55	LYS	CD	29.124	.	1
1	A	55	LYS	CE	42.189	.	1
1	A	55	LYS	CG	24.714	.	1
1	A	55	LYS	H	8.535	.	1
1	A	55	LYS	HA	4.580	.	1
1	A	55	LYS	HB2	1.836	.	2
1	A	55	LYS	HB3	1.702	.	2
1	A	55	LYS	HD2	1.696	.	1
1	A	55	LYS	HE2	3.015	.	1
1	A	55	LYS	HE3	3.015	.	1
1	A	55	LYS	HG2	1.560	.	2
1	A	55	LYS	HG3	1.499	.	2
1	A	55	LYS	N	122.746	.	1
1	A	56	PRO	CA	63.063	.	1
1	A	56	PRO	CB	32.171	.	1
1	A	56	PRO	CD	50.643	.	1
1	A	56	PRO	CG	27.468	.	1
1	A	56	PRO	HA	4.451	.	1
1	A	56	PRO	HB2	2.351	.	2
1	A	56	PRO	HB3	1.896	.	2
1	A	56	PRO	HD2	3.849	.	2
1	A	56	PRO	HD3	3.627	.	2
1	A	56	PRO	HG2	2.060	.	1
1	A	56	PRO	HG3	2.060	.	1
1	A	57	GLN	C	174.331	.	1
1	A	57	GLN	CA	53.380	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	GLN	CB	29.016	.	1
1	A	57	GLN	CG	33.649	.	1
1	A	57	GLN	H	8.748	.	1
1	A	57	GLN	HA	4.630	.	1
1	A	57	GLN	HB2	2.119	.	2
1	A	57	GLN	HB3	1.972	.	2
1	A	57	GLN	HE21	6.958	.	1
1	A	57	GLN	HE22	7.636	.	1
1	A	57	GLN	HG2	2.490	.	1
1	A	57	GLN	HG3	2.490	.	1
1	A	57	GLN	N	123.646	.	1
1	A	57	GLN	NE2	112.826	.	1
1	A	58	PRO	CA	63.025	.	1
1	A	58	PRO	CB	32.123	.	1
1	A	58	PRO	CD	50.636	.	1
1	A	58	PRO	CG	27.434	.	1
1	A	58	PRO	HA	4.429	.	1
1	A	58	PRO	HB2	2.302	.	2
1	A	58	PRO	HB3	1.856	.	2
1	A	58	PRO	HD2	3.816	.	2
1	A	58	PRO	HD3	3.628	.	2
1	A	58	PRO	HG2	2.003	.	1
1	A	58	PRO	HG3	2.003	.	1
1	A	59	ARG	C	174.049	.	1
1	A	59	ARG	CA	54.654	.	1
1	A	59	ARG	CB	29.889	.	1
1	A	59	ARG	CD	43.282	.	1
1	A	59	ARG	CG	27.876	.	1
1	A	59	ARG	H	8.599	.	1
1	A	59	ARG	HA	4.502	.	1
1	A	59	ARG	HB2	1.557	.	2
1	A	59	ARG	HB3	1.348	.	2
1	A	59	ARG	HD2	2.805	.	2
1	A	59	ARG	HD3	2.093	.	2
1	A	59	ARG	HG2	1.390	.	2
1	A	59	ARG	HG3	1.675	.	2
1	A	59	ARG	N	123.052	.	1
1	A	60	PRO	CA	62.425	.	1
1	A	60	PRO	CB	32.450	.	1
1	A	60	PRO	CD	50.656	.	1
1	A	60	PRO	CG	27.547	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	PRO	HA	4.451	.	1
1	A	60	PRO	HB2	2.422	.	2
1	A	60	PRO	HB3	1.682	.	2
1	A	60	PRO	HD2	3.326	.	2
1	A	60	PRO	HD3	4.005	.	2
1	A	60	PRO	HG2	2.228	.	2
1	A	60	PRO	HG3	2.060	.	2
1	A	61	GLU	C	176.828	.	1
1	A	61	GLU	CA	58.683	.	1
1	A	61	GLU	CB	29.957	.	1
1	A	61	GLU	CG	36.416	.	1
1	A	61	GLU	H	8.477	.	1
1	A	61	GLU	HA	3.946	.	1
1	A	61	GLU	HB2	1.987	.	1
1	A	61	GLU	HB3	1.987	.	1
1	A	61	GLU	HG2	2.344	.	2
1	A	61	GLU	HG3	2.279	.	2
1	A	61	GLU	N	120.162	.	1
1	A	62	LYS	C	173.168	.	1
1	A	62	LYS	CA	53.789	.	1
1	A	62	LYS	CB	32.028	.	1
1	A	62	LYS	CD	29.220	.	1
1	A	62	LYS	CE	42.179	.	1
1	A	62	LYS	CG	24.726	.	1
1	A	62	LYS	H	8.391	.	1
1	A	62	LYS	HA	4.520	.	1
1	A	62	LYS	HB2	1.754	.	1
1	A	62	LYS	HB3	1.754	.	1
1	A	62	LYS	HD2	1.679	.	1
1	A	62	LYS	HG2	1.360	.	2
1	A	62	LYS	HG3	1.338	.	2
1	A	62	LYS	N	117.543	.	1
1	A	63	PRO	CA	62.152	.	1
1	A	63	PRO	CB	32.051	.	1
1	A	63	PRO	CD	50.392	.	1
1	A	63	PRO	CG	27.207	.	1
1	A	63	PRO	HA	4.371	.	1
1	A	63	PRO	HB2	1.571	.	2
1	A	63	PRO	HB3	0.991	.	2
1	A	63	PRO	HD2	3.689	.	2
1	A	63	PRO	HD3	3.425	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	63	PRO	HG2	1.765	.	2
1	A	63	PRO	HG3	1.669	.	2
1	A	64	VAL	C	173.496	.	1
1	A	64	VAL	CA	62.691	.	1
1	A	64	VAL	CB	31.659	.	1
1	A	64	VAL	CG1	21.637	.	2
1	A	64	VAL	CG2	21.651	.	2
1	A	64	VAL	H	9.281	0.004	1
1	A	64	VAL	HA	3.873	.	1
1	A	64	VAL	HB	2.112	.	1
1	A	64	VAL	HG11	0.879	.	2
1	A	64	VAL	HG12	0.879	.	2
1	A	64	VAL	HG13	0.879	.	2
1	A	64	VAL	HG21	0.675	.	2
1	A	64	VAL	HG22	0.675	.	2
1	A	64	VAL	HG23	0.675	.	2
1	A	64	VAL	N	124.374	0.011	1
1	A	65	PHE	C	174.968	.	1
1	A	65	PHE	CA	56.843	.	1
1	A	65	PHE	CB	41.696	.	1
1	A	65	PHE	CD1	131.914	.	1
1	A	65	PHE	CD2	131.914	.	1
1	A	65	PHE	CE2	130.684	.	1
1	A	65	PHE	CE1	130.684	.	1
1	A	65	PHE	H	8.369	0.001	1
1	A	65	PHE	HA	5.450	.	1
1	A	65	PHE	HB2	2.852	.	2
1	A	65	PHE	HB3	2.779	.	2
1	A	65	PHE	HD2	7.090	.	1
1	A	65	PHE	HD1	7.090	.	1
1	A	65	PHE	HE2	6.960	.	1
1	A	65	PHE	HE1	6.960	.	1
1	A	65	PHE	N	125.755	.	1
1	A	66	LEU	C	174.855	.	1
1	A	66	LEU	CA	53.271	.	1
1	A	66	LEU	CB	45.786	.	1
1	A	66	LEU	CD1	26.712	.	2
1	A	66	LEU	CD2	25.881	.	2
1	A	66	LEU	CG	27.894	.	1
1	A	66	LEU	H	9.458	.	1
1	A	66	LEU	HA	5.377	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	66	LEU	HB2	1.784	.	2
1	A	66	LEU	HB3	1.202	.	2
1	A	66	LEU	HD11	0.766	.	2
1	A	66	LEU	HD12	0.766	.	2
1	A	66	LEU	HD13	0.766	.	2
1	A	66	LEU	HD21	0.818	.	2
1	A	66	LEU	HD22	0.818	.	2
1	A	66	LEU	HD23	0.818	.	2
1	A	66	LEU	HG	1.579	.	1
1	A	66	LEU	N	128.254	.	1
1	A	67	SER	C	173.004	.	1
1	A	67	SER	CA	56.365	.	1
1	A	67	SER	CB	65.714	.	1
1	A	67	SER	H	9.229	.	1
1	A	67	SER	HA	5.557	.	1
1	A	67	SER	HB2	3.609	.	2
1	A	67	SER	HB3	3.552	.	2
1	A	67	SER	N	118.676	.	1
1	A	68	VAL	C	175.830	.	1
1	A	68	VAL	CA	60.556	.	1
1	A	68	VAL	CB	33.644	.	1
1	A	68	VAL	CG1	21.664	.	2
1	A	68	VAL	CG2	21.775	.	2
1	A	68	VAL	H	8.031	.	1
1	A	68	VAL	HA	4.952	.	1
1	A	68	VAL	HB	1.841	.	1
1	A	68	VAL	HG11	0.956	.	2
1	A	68	VAL	HG12	0.956	.	2
1	A	68	VAL	HG13	0.956	.	2
1	A	68	VAL	HG21	0.818	.	2
1	A	68	VAL	HG22	0.818	.	2
1	A	68	VAL	HG23	0.818	.	2
1	A	68	VAL	N	121.110	.	1
1	A	69	LYS	C	177.483	.	1
1	A	69	LYS	CA	54.605	.	1
1	A	69	LYS	CB	33.266	.	1
1	A	69	LYS	CD	27.849	.	1
1	A	69	LYS	CE	41.663	.	1
1	A	69	LYS	CG	25.634	.	1
1	A	69	LYS	H	8.141	.	1
1	A	69	LYS	HA	4.529	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	69	LYS	HB2	2.189	.	2
1	A	69	LYS	HB3	2.060	.	2
1	A	69	LYS	HD2	1.426	.	2
1	A	69	LYS	HD3	1.291	.	2
1	A	69	LYS	HE2	2.348	.	1
1	A	69	LYS	HE3	2.348	.	1
1	A	69	LYS	HG2	1.389	.	2
1	A	69	LYS	HG3	1.297	.	2
1	A	69	LYS	N	125.123	.	1
1	A	70	ALA	C	177.674	.	1
1	A	70	ALA	CA	54.874	.	1
1	A	70	ALA	CB	18.497	.	1
1	A	70	ALA	H	8.818	.	1
1	A	70	ALA	HA	3.908	.	1
1	A	70	ALA	HB2	1.441	.	1
1	A	70	ALA	HB3	1.441	.	1
1	A	70	ALA	HB1	1.441	.	1
1	A	70	ALA	N	121.611	.	1
1	A	71	ASP	C	176.228	.	1
1	A	71	ASP	CA	53.511	.	1
1	A	71	ASP	CB	39.293	.	1
1	A	71	ASP	H	7.934	.	1
1	A	71	ASP	HA	4.451	.	1
1	A	71	ASP	HB2	3.028	.	2
1	A	71	ASP	HB3	2.601	.	2
1	A	71	ASP	N	115.356	.	1
1	A	72	LYS	C	174.712	.	1
1	A	72	LYS	CA	58.410	.	1
1	A	72	LYS	CB	29.309	.	1
1	A	72	LYS	CD	29.400	.	1
1	A	72	LYS	CE	42.310	.	1
1	A	72	LYS	CG	26.091	.	1
1	A	72	LYS	H	8.535	.	1
1	A	72	LYS	HA	3.593	.	1
1	A	72	LYS	HB2	2.253	.	2
1	A	72	LYS	HB3	2.024	.	2
1	A	72	LYS	HD2	1.768	.	2
1	A	72	LYS	HD3	1.679	.	2
1	A	72	LYS	HE2	3.055	.	1
1	A	72	LYS	HE3	3.055	.	1
1	A	72	LYS	HG2	1.409	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	LYS	HG3	1.349	.	2
1	A	72	LYS	N	112.877	.	1
1	A	73	GLN	C	174.526	.	1
1	A	73	GLN	CA	56.141	.	1
1	A	73	GLN	CB	30.181	.	1
1	A	73	GLN	CG	34.449	.	1
1	A	73	GLN	H	7.801	.	1
1	A	73	GLN	HA	4.152	.	1
1	A	73	GLN	HB2	2.099	.	2
1	A	73	GLN	HB3	2.060	.	2
1	A	73	GLN	HE21	6.888	.	1
1	A	73	GLN	HE22	7.975	.	1
1	A	73	GLN	HG2	2.113	.	1
1	A	73	GLN	N	119.276	.	1
1	A	73	GLN	NE2	116.887	.	1
1	A	74	LEU	C	177.090	.	1
1	A	74	LEU	CA	54.150	.	1
1	A	74	LEU	CB	44.086	.	1
1	A	74	LEU	CD1	25.192	.	2
1	A	74	LEU	CD2	25.326	.	2
1	A	74	LEU	CG	27.179	.	1
1	A	74	LEU	H	8.247	.	1
1	A	74	LEU	HA	5.204	.	1
1	A	74	LEU	HB2	1.984	.	2
1	A	74	LEU	HB3	1.235	.	2
1	A	74	LEU	HD11	0.818	.	2
1	A	74	LEU	HD12	0.818	.	2
1	A	74	LEU	HD13	0.818	.	2
1	A	74	LEU	HD21	0.876	.	2
1	A	74	LEU	HD22	0.876	.	2
1	A	74	LEU	HD23	0.876	.	2
1	A	74	LEU	HG	1.807	.	1
1	A	74	LEU	N	124.250	.	1
1	A	75	TYR	C	175.991	.	1
1	A	75	TYR	CA	56.869	.	1
1	A	75	TYR	CB	42.409	.	1
1	A	104	PHE	CE2	130.826	.	1
1	A	104	PHE	CE1	130.826	.	1
1	A	75	TYR	CE2	118.160	.	1
1	A	75	TYR	CE1	118.160	.	1
1	A	75	TYR	H	9.139	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	75	TYR	HA	5.155	.	1
1	A	75	TYR	HB2	2.742	.	2
1	A	75	TYR	HB3	2.669	.	2
1	A	104	PHE	HE2	6.888	.	1
1	A	104	PHE	HE1	6.888	.	1
1	A	75	TYR	HE2	6.689	.	1
1	A	75	TYR	HE1	6.689	.	1
1	A	75	TYR	N	120.549	.	1
1	A	76	VAL	C	177.773	.	1
1	A	76	VAL	CA	61.394	.	1
1	A	76	VAL	CB	32.060	.	1
1	A	76	VAL	CG1	21.489	.	1
1	A	76	VAL	CG2	21.489	.	1
1	A	76	VAL	H	8.677	.	1
1	A	76	VAL	HB	1.847	.	1
1	A	76	VAL	HG11	0.766	.	1
1	A	76	VAL	HG12	0.766	.	1
1	A	76	VAL	HG13	0.766	.	1
1	A	76	VAL	HG21	0.766	.	1
1	A	76	VAL	HG22	0.766	.	1
1	A	76	VAL	HG23	0.766	.	1
1	A	76	VAL	N	120.815	.	1
1	A	77	GLY	C	174.798	.	1
1	A	77	GLY	CA	47.583	.	1
1	A	77	GLY	H	9.129	.	1
1	A	77	GLY	HA2	4.152	.	2
1	A	77	GLY	HA3	3.778	.	2
1	A	77	GLY	N	118.822	.	1
1	A	78	ASP	CA	54.043	.	1
1	A	78	ASP	CB	40.946	.	1
1	A	78	ASP	HA	4.652	.	1
1	A	78	ASP	HB2	2.773	.	1
1	A	78	ASP	HB3	2.773	.	1
1	A	79	GLN	C	172.750	.	1
1	A	79	GLN	CA	52.753	.	1
1	A	79	GLN	CB	30.598	.	1
1	A	79	GLN	CG	32.827	.	1
1	A	79	GLN	H	8.237	.	1
1	A	79	GLN	HA	4.891	.	1
1	A	79	GLN	HB2	2.259	.	2
1	A	79	GLN	HB3	2.060	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	GLN	HE21	7.621	.	1
1	A	79	GLN	HE22	6.958	.	1
1	A	79	GLN	HG2	2.380	.	2
1	A	79	GLN	HG3	2.332	.	2
1	A	79	GLN	N	122.566	.	1
1	A	79	GLN	NE2	112.273	.	1
1	A	80	PRO	CA	62.190	.	1
1	A	80	PRO	CB	31.362	.	1
1	A	80	PRO	CD	50.766	.	1
1	A	80	PRO	CG	26.992	.	1
1	A	80	PRO	HA	4.152	.	1
1	A	80	PRO	HB2	1.659	.	2
1	A	80	PRO	HB3	1.575	.	2
1	A	80	PRO	HD2	4.005	.	2
1	A	80	PRO	HD3	3.863	.	2
1	A	80	PRO	HG2	2.060	.	2
1	A	80	PRO	HG3	1.967	.	2
1	A	81	VAL	C	173.945	.	1
1	A	81	VAL	CA	59.460	.	1
1	A	81	VAL	CB	35.794	.	1
1	A	81	VAL	CG1	21.834	.	2
1	A	81	VAL	CG2	20.843	.	2
1	A	81	VAL	H	8.236	.	1
1	A	81	VAL	HA	4.488	.	1
1	A	81	VAL	HB	1.896	.	1
1	A	81	VAL	HG11	0.766	.	2
1	A	81	VAL	HG12	0.766	.	2
1	A	81	VAL	HG13	0.766	.	2
1	A	81	VAL	HG21	0.711	.	2
1	A	81	VAL	HG22	0.711	.	2
1	A	81	VAL	HG23	0.711	.	2
1	A	81	VAL	N	118.688	.	1
1	A	82	ASN	C	177.000	.	1
1	A	82	ASN	CA	51.880	.	1
1	A	82	ASN	CB	39.405	.	1
1	A	82	ASN	H	8.304	.	1
1	A	82	ASN	HB2	2.886	.	2
1	A	82	ASN	HB3	2.822	.	2
1	A	82	ASN	HD21	6.958	.	1
1	A	82	ASN	HD22	7.750	.	1
1	A	82	ASN	N	121.026	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	82	ASN	ND2	113.279	.	1
1	A	83	ALA	C	179.138	.	1
1	A	83	ALA	CA	56.179	.	1
1	A	83	ALA	CB	18.114	.	1
1	A	83	ALA	H	9.030	.	1
1	A	83	ALA	HA	3.827	.	1
1	A	83	ALA	HB2	1.487	.	1
1	A	83	ALA	HB3	1.487	.	1
1	A	83	ALA	HB1	1.487	.	1
1	A	83	ALA	N	123.974	.	1
1	A	84	ASP	C	177.197	.	1
1	A	84	ASP	CA	55.797	.	1
1	A	84	ASP	CB	39.981	.	1
1	A	84	ASP	H	8.391	.	1
1	A	84	ASP	HA	4.451	.	1
1	A	84	ASP	HB2	2.777	.	2
1	A	84	ASP	HB3	2.669	.	2
1	A	84	ASP	N	114.506	.	1
1	A	85	GLN	C	176.086	.	1
1	A	85	GLN	CA	55.275	.	1
1	A	85	GLN	CB	30.455	.	1
1	A	85	GLN	CG	34.032	.	1
1	A	85	GLN	H	7.805	.	1
1	A	85	GLN	HA	4.555	.	1
1	A	85	GLN	HB2	2.291	.	2
1	A	85	GLN	HB3	2.060	.	2
1	A	85	GLN	HE21	7.544	.	1
1	A	85	GLN	HE22	6.888	.	1
1	A	85	GLN	HG2	2.426	.	1
1	A	85	GLN	HG3	2.426	.	1
1	A	85	GLN	N	117.725	.	1
1	A	85	GLN	NE2	112.594	.	1
1	A	86	LEU	C	177.366	.	1
1	A	86	LEU	CA	59.366	.	1
1	A	86	LEU	CB	42.104	.	1
1	A	86	LEU	CD1	24.465	.	2
1	A	86	LEU	CD2	25.468	.	2
1	A	86	LEU	CG	27.113	.	1
1	A	86	LEU	H	7.325	.	1
1	A	86	LEU	HA	3.762	.	1
1	A	86	LEU	HB2	1.821	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	LEU	HB3	1.491	.	2
1	A	86	LEU	HD11	0.766	.	1
1	A	86	LEU	HD12	0.766	.	1
1	A	86	LEU	HD13	0.766	.	1
1	A	86	LEU	HD21	0.766	.	1
1	A	86	LEU	HD22	0.766	.	1
1	A	86	LEU	HD23	0.766	.	1
1	A	86	LEU	HG	1.439	.	1
1	A	86	LEU	N	120.579	.	1
1	A	87	THR	C	175.469	.	1
1	A	87	THR	CA	67.482	.	1
1	A	87	THR	CB	67.746	.	1
1	A	87	THR	CG2	22.464	.	1
1	A	87	THR	H	8.609	.	1
1	A	87	THR	HA	3.707	.	1
1	A	87	THR	HB	4.241	.	1
1	A	87	THR	HG22	1.299	.	1
1	A	87	THR	HG23	1.299	.	1
1	A	87	THR	HG21	1.299	.	1
1	A	87	THR	N	112.006	.	1
1	A	88	SER	C	177.595	.	1
1	A	88	SER	CA	61.462	.	1
1	A	88	SER	CB	62.818	.	1
1	A	88	SER	H	7.938	.	1
1	A	88	SER	HA	4.241	.	1
1	A	88	SER	HB2	4.005	.	1
1	A	88	SER	HB3	4.005	.	1
1	A	88	SER	N	116.080	.	1
1	A	89	VAL	C	178.917	.	1
1	A	89	VAL	CA	66.698	.	1
1	A	89	VAL	CB	31.867	.	1
1	A	89	VAL	CG1	23.078	.	2
1	A	89	VAL	CG2	21.184	.	2
1	A	89	VAL	H	8.071	.	1
1	A	89	VAL	HA	3.793	.	1
1	A	89	VAL	HB	1.967	.	1
1	A	89	VAL	HG11	1.053	.	2
1	A	89	VAL	HG12	1.053	.	2
1	A	89	VAL	HG13	1.053	.	2
1	A	89	VAL	HG21	0.876	.	2
1	A	89	VAL	HG22	0.876	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	89	VAL	HG23	0.876	.	2
1	A	89	VAL	N	122.927	.	1
1	A	90	LEU	C	179.053	.	1
1	A	90	LEU	CA	58.768	.	1
1	A	90	LEU	CB	41.510	.	1
1	A	90	LEU	CD1	23.119	.	1
1	A	90	LEU	CD2	23.119	.	1
1	A	90	LEU	CG	25.922	.	1
1	A	90	LEU	H	8.677	.	1
1	A	90	LEU	HA	3.824	.	1
1	A	90	LEU	HB2	1.736	.	2
1	A	90	LEU	HB3	0.766	.	2
1	A	90	LEU	HD11	0.433	.	1
1	A	90	LEU	HD12	0.433	.	1
1	A	90	LEU	HD13	0.433	.	1
1	A	90	LEU	HD21	0.433	.	1
1	A	90	LEU	HD22	0.433	.	1
1	A	90	LEU	HD23	0.433	.	1
1	A	90	LEU	HG	0.258	.	1
1	A	90	LEU	N	120.132	.	1
1	A	91	ASP	C	179.673	.	1
1	A	91	ASP	CA	57.613	.	1
1	A	91	ASP	CB	39.580	.	1
1	A	91	ASP	H	8.758	.	1
1	A	91	ASP	HA	4.241	.	1
1	A	91	ASP	HB2	3.019	.	2
1	A	91	ASP	HB3	2.604	.	2
1	A	91	ASP	N	117.637	.	1
1	A	92	GLN	C	178.964	.	1
1	A	92	GLN	CA	59.249	.	1
1	A	92	GLN	CB	28.390	.	1
1	A	92	GLN	CG	34.032	.	1
1	A	92	GLN	H	7.965	.	1
1	A	92	GLN	HA	4.152	.	1
1	A	92	GLN	HB2	2.334	.	1
1	A	92	GLN	HB3	2.334	.	1
1	A	92	GLN	HE21	7.446	.	1
1	A	92	GLN	HE22	6.841	.	1
1	A	92	GLN	HG2	2.636	.	2
1	A	92	GLN	HG3	2.448	.	2
1	A	92	GLN	N	119.797	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	92	GLN	NE2	111.736	.	1
1	A	93	ARG	C	178.572	.	1
1	A	93	ARG	CA	57.002	.	1
1	A	93	ARG	CB	30.184	.	1
1	A	93	ARG	CD	41.899	.	1
1	A	93	ARG	CG	26.914	.	1
1	A	93	ARG	H	8.140	.	1
1	A	93	ARG	HA	4.241	.	1
1	A	93	ARG	HB2	2.060	.	2
1	A	93	ARG	HB3	2.009	.	2
1	A	93	ARG	HD2	3.280	.	2
1	A	93	ARG	HD3	3.244	.	2
1	A	93	ARG	HG2	1.937	.	2
1	A	93	ARG	HG3	1.611	.	2
1	A	93	ARG	N	117.746	.	1
1	A	94	THR	C	176.433	.	1
1	A	94	THR	CA	61.487	.	1
1	A	94	THR	CB	71.206	.	1
1	A	94	THR	CG2	21.131	.	1
1	A	94	THR	H	8.677	.	1
1	A	94	THR	HA	4.451	.	1
1	A	94	THR	HG22	1.350	.	1
1	A	94	THR	HG23	1.350	.	1
1	A	94	THR	HG21	1.350	.	1
1	A	94	THR	N	107.695	.	1
1	A	95	GLN	C	175.246	.	1
1	A	95	GLN	CA	57.791	.	1
1	A	95	GLN	CB	26.089	.	1
1	A	95	GLN	CG	34.590	.	1
1	A	95	GLN	H	7.772	.	1
1	A	95	GLN	HA	4.005	.	1
1	A	95	GLN	HB2	2.387	.	2
1	A	95	GLN	HB3	2.250	.	2
1	A	95	GLN	HE21	6.841	.	1
1	A	95	GLN	HE22	7.574	.	1
1	A	95	GLN	HG2	2.348	.	1
1	A	95	GLN	HG3	2.348	.	1
1	A	95	GLN	N	118.867	.	1
1	A	95	GLN	NE2	112.662	.	1
1	A	96	ALA	C	174.789	.	1
1	A	96	ALA	CA	52.566	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	96	ALA	CB	16.973	.	1
1	A	96	ALA	H	9.104	.	1
1	A	96	ALA	HA	3.660	.	1
1	A	96	ALA	HB2	1.355	.	1
1	A	96	ALA	HB3	1.355	.	1
1	A	96	ALA	HB1	1.355	.	1
1	A	96	ALA	N	119.732	.	1
1	A	97	ASN	C	176.595	.	1
1	A	97	ASN	CA	51.758	.	1
1	A	97	ASN	CB	37.695	.	1
1	A	97	ASN	H	7.629	.	1
1	A	97	ASN	HA	4.899	.	1
1	A	97	ASN	HB2	3.156	.	2
1	A	97	ASN	HB3	2.836	.	2
1	A	97	ASN	HD21	7.459	.	1
1	A	97	ASN	HD22	6.998	.	1
1	A	97	ASN	N	116.577	.	1
1	A	97	ASN	ND2	110.314	.	1
1	A	98	LYS	C	177.382	.	1
1	A	98	LYS	CA	56.345	.	1
1	A	98	LYS	CB	30.060	.	1
1	A	98	LYS	CD	27.101	.	1
1	A	98	LYS	CE	42.864	.	1
1	A	98	LYS	CG	24.835	.	1
1	A	98	LYS	H	8.677	.	1
1	A	98	LYS	HA	3.839	.	1
1	A	98	LYS	HB2	1.959	.	2
1	A	98	LYS	HB3	1.565	.	2
1	A	98	LYS	HD2	0.818	.	2
1	A	98	LYS	HD3	0.681	.	2
1	A	98	LYS	HE2	2.796	.	1
1	A	98	LYS	HE3	2.796	.	1
1	A	98	LYS	HG2	1.086	.	1
1	A	98	LYS	HG3	1.086	.	1
1	A	98	LYS	N	124.026	.	1
1	A	99	GLU	C	175.587	.	1
1	A	99	GLU	CA	56.225	.	1
1	A	99	GLU	CB	28.889	.	1
1	A	99	GLU	CG	36.623	.	1
1	A	99	GLU	H	8.057	.	1
1	A	99	GLU	HA	4.241	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	GLU	HB2	2.247	.	2
1	A	99	GLU	HB3	2.060	.	2
1	A	99	GLU	HG2	2.320	.	2
1	A	99	GLU	HG3	2.205	.	2
1	A	99	GLU	N	117.598	.	1
1	A	75	TYR	CD1	132.703	.	1
1	A	75	TYR	CD2	132.703	.	1
1	A	75	TYR	HD2	6.706	.	1
1	A	75	TYR	HD1	6.706	.	1
1	A	103	PHE	CZ	128.780	.	1
1	A	103	PHE	HZ	7.216	.	1
1	A	65	PHE	CZ	128.950	.	1
1	A	65	PHE	HZ	6.979	.	1
1	A	104	PHE	CZ	128.280	.	1
1	A	104	PHE	HZ	6.745	.	1
1	A	58	PRO	C	177.057	.	1
1	A	60	PRO	C	175.117	.	1
1	A	53	SER	C	174.191	.	1
1	A	63	PRO	C	176.208	.	1
1	A	50	PRO	C	176.789	.	1
1	A	56	PRO	C	176.752	.	1
1	A	78	ASP	C	175.453	.	1
1	A	121	THR	C	177.171	.	1
1	A	114	THR	C	176.366	.	1
1	A	112	TYR	C	177.587	.	1
1	A	117	SER	C	177.737	.	1
1	A	80	PRO	C	177.079	.	1
1	A	82	ASN	HA	4.844	.	1
1	A	129	LYS	HA	4.852	.	1
1	A	78	ASP	H	8.863	.	1
1	A	78	ASP	N	125.980	.	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
$^{13}C_{\alpha}$	97	-0.18 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	92	0.53 ± 0.12	Should be checked
$^{13}C'$	97	-0.02 ± 0.15	None needed (< 0.5 ppm)
^{15}N	90	-0.91 ± 0.48	None needed (imprecise)

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 47%, i.e. 1199 atoms were assigned a chemical shift out of a possible 2572. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	459/936 (49%)	184/378 (49%)	188/380 (49%)	87/178 (49%)
Sidechain	686/1522 (45%)	466/988 (47%)	211/476 (44%)	9/58 (16%)
Aromatic	54/114 (47%)	27/54 (50%)	27/60 (45%)	0/0 (—%)
Overall	1199/2572 (47%)	677/1420 (48%)	426/916 (47%)	96/236 (41%)

7.1.4 Statistically unusual chemical shifts

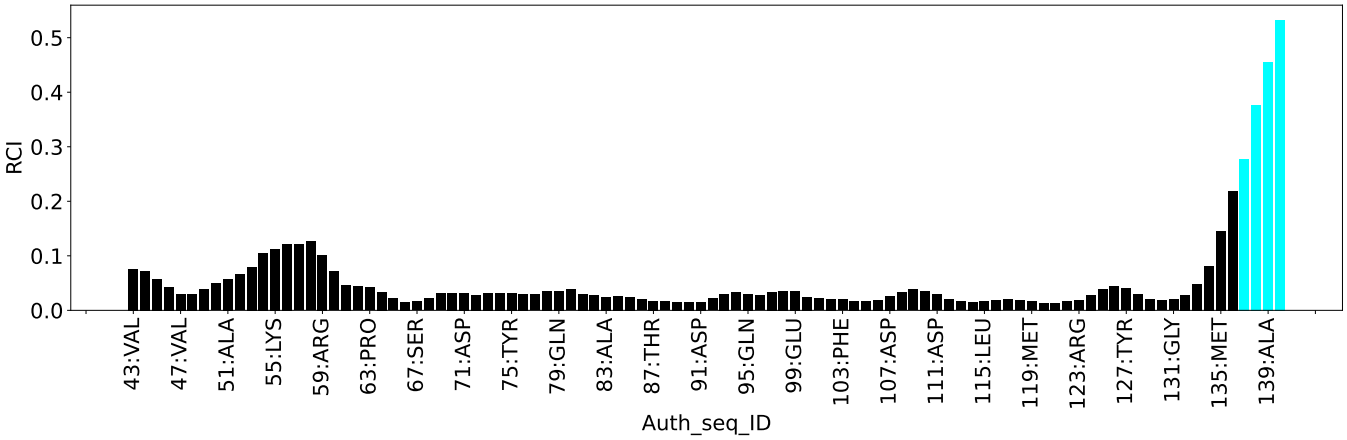
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	101	THR	HG22	0.01	0.08 – 2.19	-5.3
1	A	101	THR	HG23	0.01	0.08 – 2.19	-5.3
1	A	101	THR	HG21	0.01	0.08 – 2.19	-5.3

7.1.5 Random Coil Index (RCI) plots

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

Random coil index (RCI) for chain A:


RCI
0.5
0.4
0.3
0.2
0.1
0.0
43:VAL
47:VAL
51:ALA
55:LYS
59:ARG
63:PRO
67:SER
71:ASP
75:TYR
79:GLN
83:ALA
87:THR
91:ASP
95:GLN
99:GLU
103:PHE
107:ASP
111:ASP
115:LEU
119:MET
123:ARG
127:TYR
131:GLY
135:MET
139:ALA
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	9092
Intra-residue (|i-j|=0)	1774
Sequential (|i-j|=1)	1764
Medium range (|i-j|>1 and |i-j|<5)	1888
Long range (|i-j|≥5)	2772
Inter-chain	892
Hydrogen bond restraints	2
Disulfide bond restraints	0
Total dihedral-angle restraints	320
Number of unmapped restraints	0
Number of restraints per residue	48.0
Number of long range restraints per residue[1]	14.2

[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)	121.9	0.2
0.2-0.5 (Medium)	251.0	0.5
>0.5 (Large)	477.5	3.69

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)	13.1	3.54
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

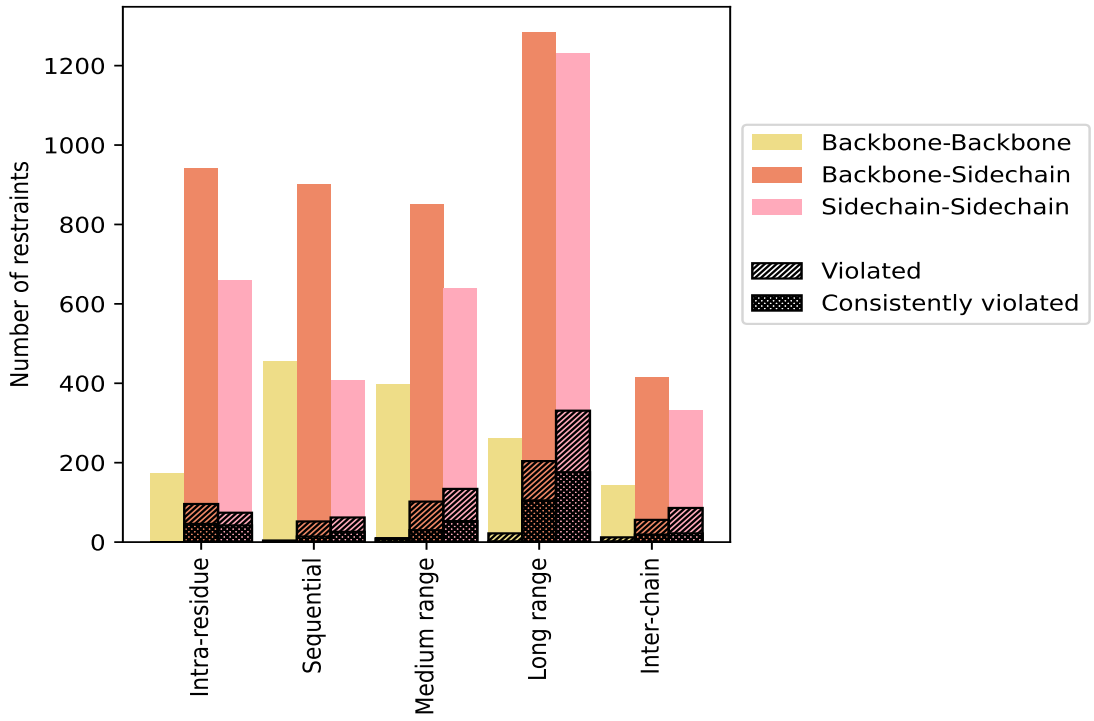
9.1 Summary of distance violations (i)

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)	1774	19.5	170	9.6	1.9	88	5.0	1.0
Backbone-Backbone	174	1.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	940	10.3	96	10.2	1.1	46	4.9	0.5
Sidechain-Sidechain	660	7.3	74	11.2	0.8	42	6.4	0.5
Sequential (|i-j|=1)	1764	19.4	118	6.7	1.3	40	2.3	0.4
Backbone-Backbone	456	5.0	4	0.9	0.0	0	0.0	0.0
Backbone-Sidechain	900	9.9	52	5.8	0.6	14	1.6	0.2
Sidechain-Sidechain	408	4.5	62	15.2	0.7	26	6.4	0.3
Medium range (|i-j|>1 & |i-j|<5)	1888	20.8	246	13.0	2.7	91	4.8	1.0
Backbone-Backbone	398	4.4	10	2.5	0.1	8	2.0	0.1
Backbone-Sidechain	850	9.3	102	12.0	1.1	30	3.5	0.3
Sidechain-Sidechain	640	7.0	134	20.9	1.5	53	8.3	0.6
Long range (|i-j|≥5)	2772	30.5	557	20.1	6.1	283	10.2	3.1
Backbone-Backbone	260	2.9	22	8.5	0.2	2	0.8	0.0
Backbone-Sidechain	1282	14.1	204	15.9	2.2	105	8.2	1.2
Sidechain-Sidechain	1230	13.5	331	26.9	3.6	176	14.3	1.9
Inter-chain	892	9.8	154	17.3	1.7	43	4.8	0.5
Backbone-Backbone	144	1.6	12	8.3	0.1	2	1.4	0.0
Backbone-Sidechain	416	4.6	56	13.5	0.6	19	4.6	0.2
Sidechain-Sidechain	332	3.7	86	25.9	0.9	22	6.6	0.2
Hydrogen bond	2	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	9092	100.0	1245	13.7	13.7	545	6.0	6.0
Backbone-Backbone	1432	15.8	48	3.4	0.5	12	0.8	0.1
Backbone-Sidechain	4390	48.3	510	11.6	5.6	214	4.9	2.4
Sidechain-Sidechain	3270	36.0	687	21.0	7.6	319	9.8	3.5

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

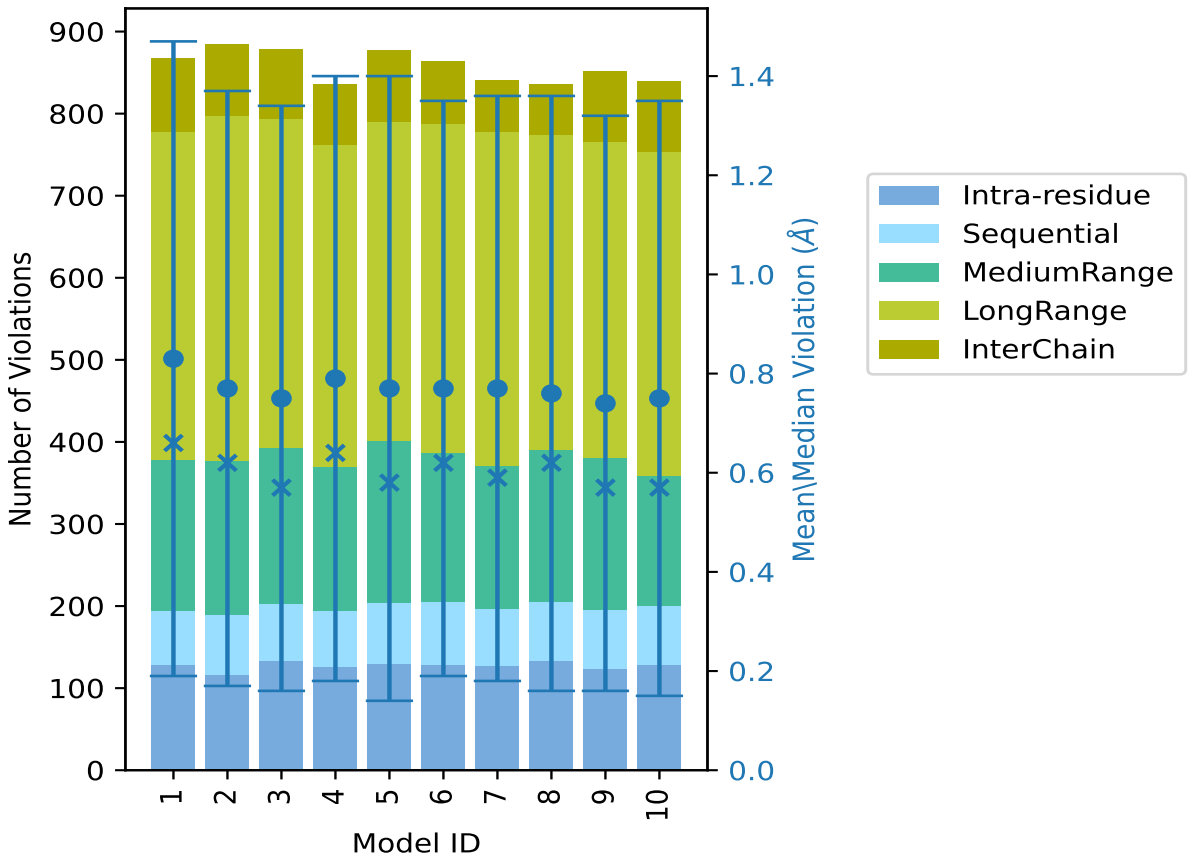
9.2 Distance violation statistics for each model

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	128	67	183	400	90	868	0.83	3.45	0.64	0.66
2	116	74	187	420	87	884	0.77	3.08	0.6	0.62
3	133	70	190	401	85	879	0.75	3.53	0.59	0.57
4	126	68	176	392	74	836	0.79	3.37	0.61	0.64
5	130	74	198	388	87	877	0.77	3.58	0.63	0.58
6	129	76	182	401	76	864	0.77	3.25	0.58	0.62
7	127	70	174	407	63	841	0.77	3.53	0.59	0.59
8	134	71	186	383	62	836	0.76	3.69	0.6	0.62
9	124	72	184	386	86	852	0.74	3.11	0.58	0.57
10	129	71	159	395	86	840	0.75	3.27	0.6	0.57

[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, 7845(IR:1604, SQ:1646, MR:1642, LR:2215, IC:738) 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]	%
18	16	26	59	30	149	1	10.0
12	14	22	28	22	98	2	20.0
4	9	12	28	16	69	3	30.0

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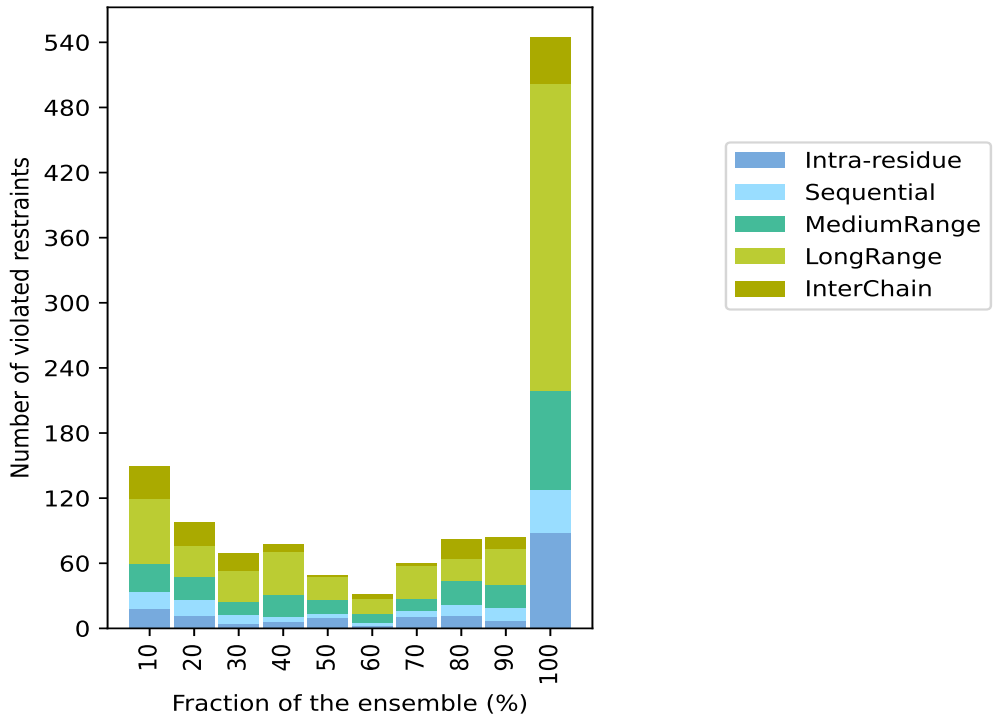
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
6	5	20	40	7	78	4	40.0
10	4	12	22	1	49	5	50.0
3	2	9	13	4	31	6	60.0
11	5	11	31	2	60	7	70.0
11	11	22	20	18	82	8	80.0
7	12	21	33	11	84	9	90.0
88	40	91	283	43	545	10	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble

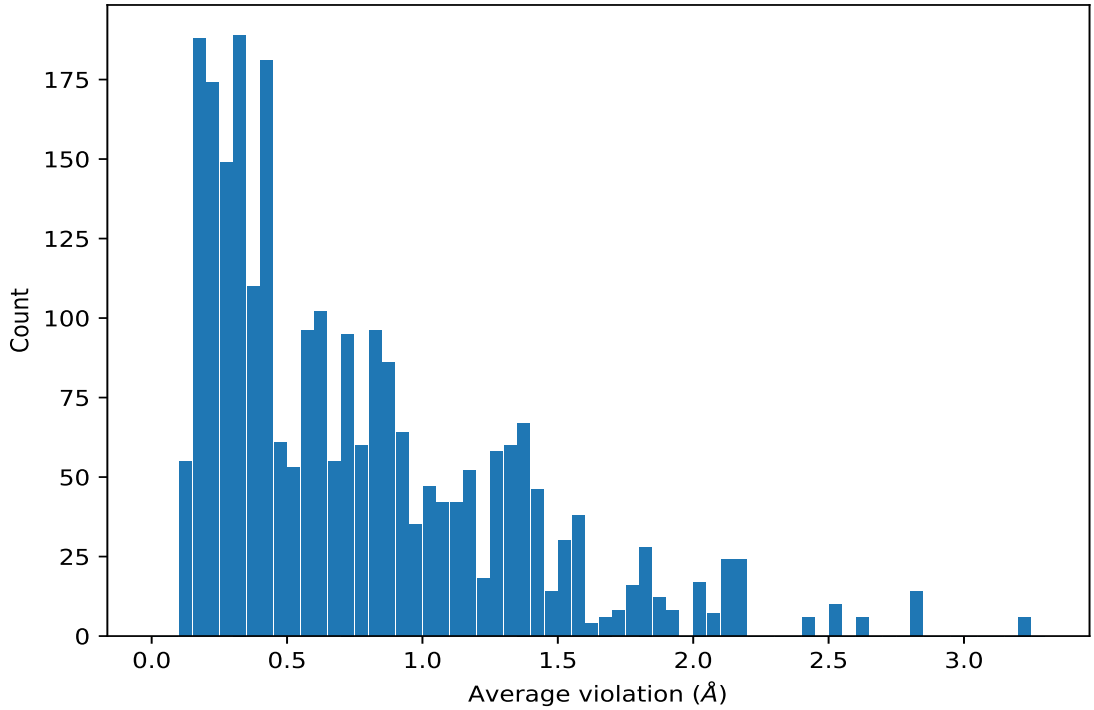


9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

in the ensemble



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,5301)	1:106:A:ALA:HB2	1:112:A:TYR:HB3	10	3.24	0.25	3.26
(1,5301)	1:106:A:ALA:HB1	1:112:A:TYR:HB3	10	3.24	0.25	3.26
(1,5301)	1:106:A:ALA:HB3	1:112:A:TYR:HB3	10	3.24	0.25	3.26
(1,5302)	1:106:B:ALA:HB2	1:112:B:TYR:HB3	10	3.24	0.25	3.26
(1,5302)	1:106:B:ALA:HB1	1:112:B:TYR:HB3	10	3.24	0.25	3.26
(1,5302)	1:106:B:ALA:HB3	1:112:B:TYR:HB3	10	3.24	0.25	3.26
(3,295)	1:94:A:THR:HG21	1:86:A:LEU:H	10	2.83	0.13	2.84
(3,295)	1:94:A:THR:HG22	1:86:A:LEU:H	10	2.83	0.13	2.84
(3,295)	1:94:A:THR:HG23	1:86:A:LEU:H	10	2.83	0.13	2.84
(3,296)	1:94:B:THR:HG21	1:86:B:LEU:H	10	2.83	0.13	2.84
(3,296)	1:94:B:THR:HG22	1:86:B:LEU:H	10	2.83	0.13	2.84
(3,296)	1:94:B:THR:HG23	1:86:B:LEU:H	10	2.83	0.13	2.84
(3,2062)	1:85:B:GLN:HG2	1:124:B:LYS:HD3	10	2.82	0.22	2.88
(3,2062)	1:85:B:GLN:HG3	1:124:B:LYS:HD3	10	2.82	0.22	2.88
(3,2062)	1:85:B:GLN:HG3	1:124:B:LYS:HG2	10	2.82	0.22	2.88

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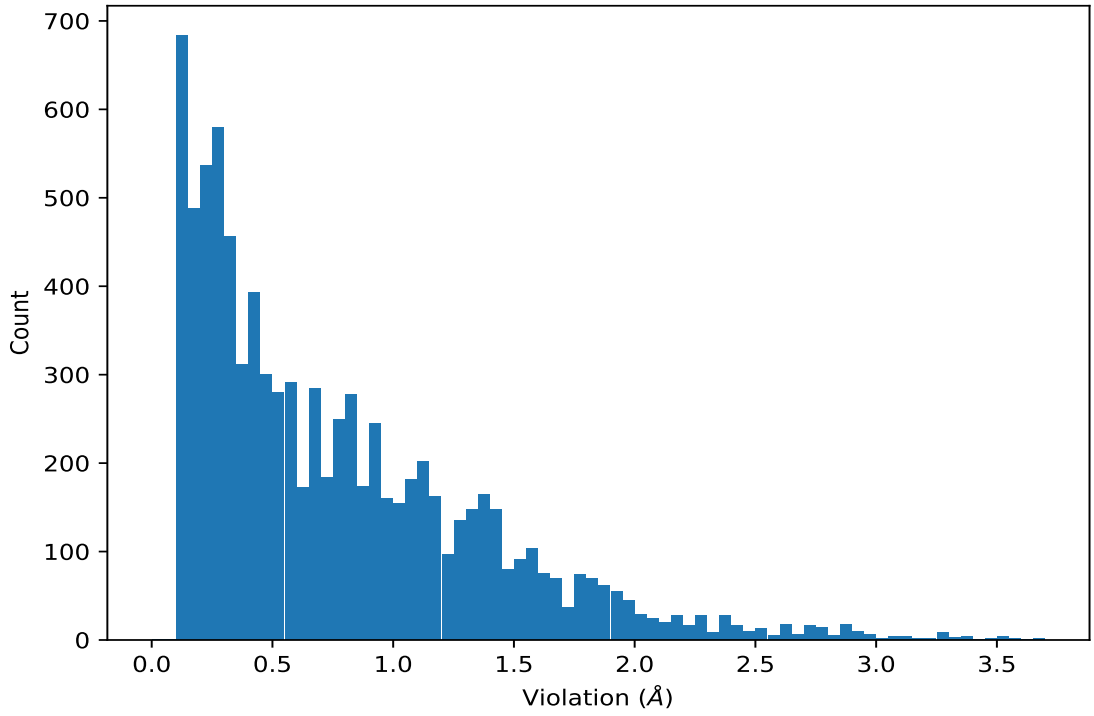
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,2062)	1:85:B:GLN:HG2	1:124:B:LYS:HG2	10	2.82	0.22	2.88
(3,2061)	1:85:A:GLN:HG2	1:124:A:LYS:HD3	10	2.81	0.21	2.88
(3,2061)	1:85:A:GLN:HG3	1:124:A:LYS:HD3	10	2.81	0.21	2.88
(3,2061)	1:85:A:GLN:HG3	1:124:A:LYS:HG2	10	2.81	0.21	2.88
(3,2061)	1:85:A:GLN:HG2	1:124:A:LYS:HG2	10	2.81	0.21	2.88
(3,933)	1:45:A:ILE:HG23	1:129:A:LYS:HB2	10	2.64	0.15	2.62
(3,933)	1:45:A:ILE:HG21	1:129:A:LYS:HB2	10	2.64	0.15	2.62
(3,933)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	10	2.64	0.15	2.62
(3,934)	1:45:B:ILE:HG23	1:129:B:LYS:HB2	10	2.64	0.15	2.62
(3,934)	1:45:B:ILE:HG21	1:129:B:LYS:HB2	10	2.64	0.15	2.62
(3,934)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	10	2.64	0.15	2.62
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	10	2.54	0.29	2.58
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	10	2.54	0.29	2.58

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

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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)
(1,4564)	1:87:B:THR:HG21	1:98:B:LYS:HE3	8	3.69
(1,4563)	1:87:A:THR:HG21	1:98:A:LYS:HE3	8	3.69
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE2	5	3.58
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE2	5	3.58
(1,5302)	1:106:B:ALA:HB3	1:112:B:TYR:HB3	3	3.53
(1,5302)	1:106:B:ALA:HB3	1:112:B:TYR:HB3	7	3.53
(1,5301)	1:106:A:ALA:HB3	1:112:A:TYR:HB3	3	3.53
(1,5301)	1:106:A:ALA:HB3	1:112:A:TYR:HB3	7	3.52
(1,5302)	1:106:B:ALA:HB2	1:112:B:TYR:HB3	1	3.45
(1,5301)	1:106:A:ALA:HB2	1:112:A:TYR:HB3	1	3.45

10 Dihedral-angle violation analysis

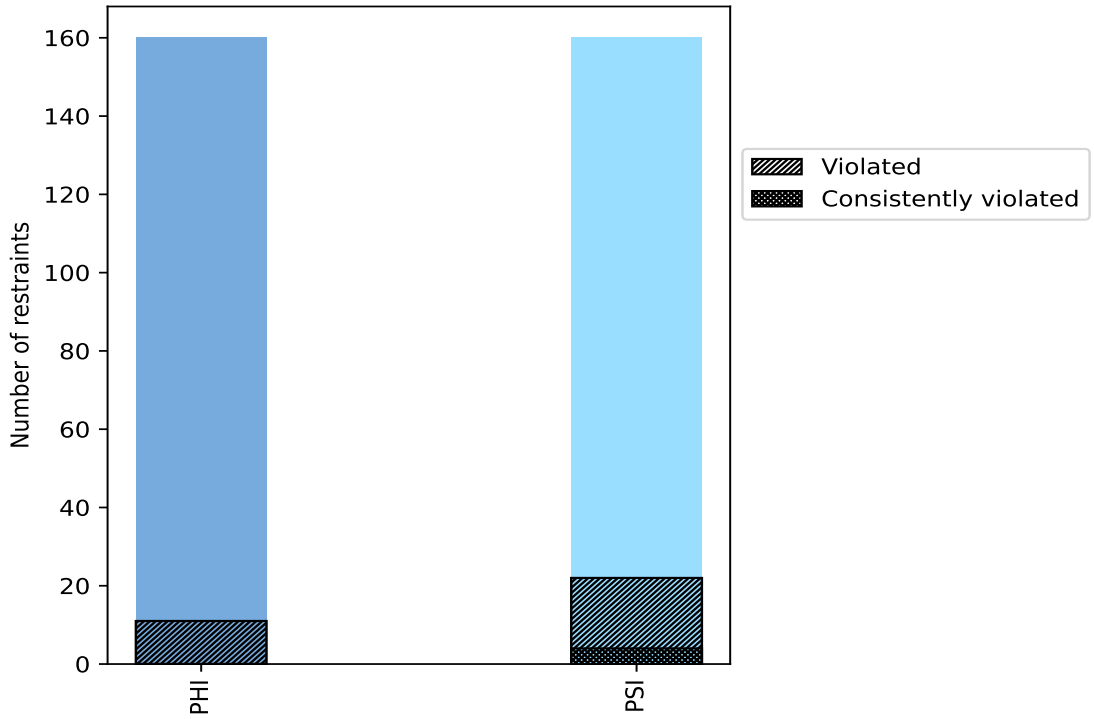
10.1 Summary of dihedral-angle violations

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	160	50.0	11	6.9	3.4	0	0.0	0.0
PSI	160	50.0	22	13.8	6.9	4	2.5	1.2
Total	320	100.0	33	10.3	10.3	4	1.2	1.2

[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



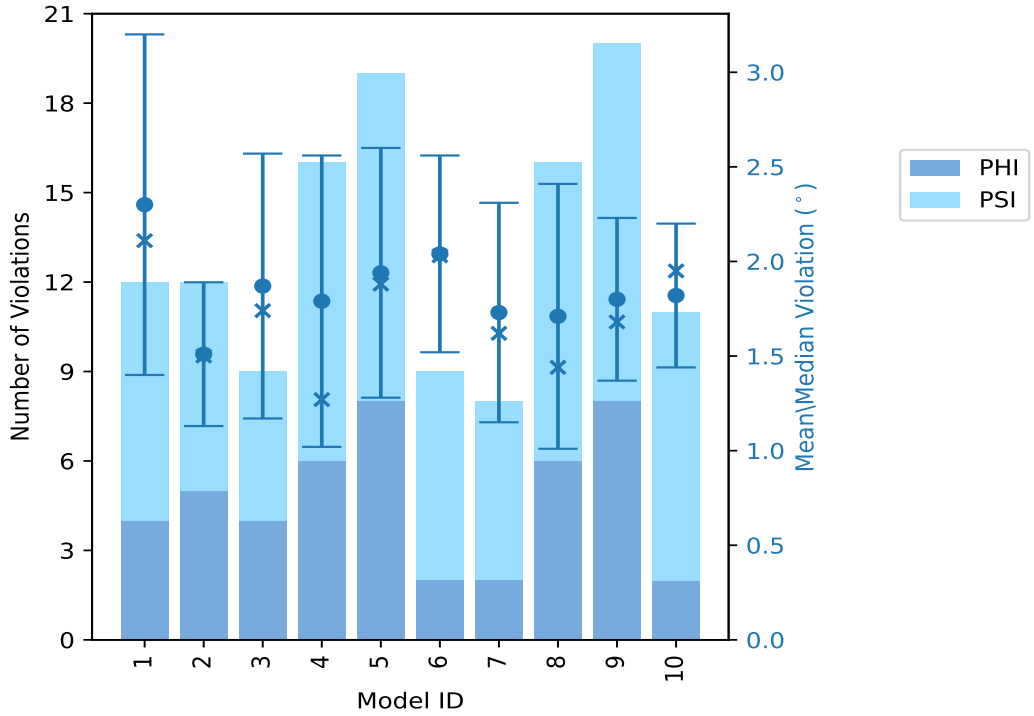
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	4	8	12	2.3	3.54	0.9	2.11
2	5	7	12	1.51	2.22	0.38	1.5
3	4	5	9	1.87	3.02	0.7	1.74
4	6	10	16	1.79	2.95	0.77	1.27
5	8	11	19	1.94	3.48	0.66	1.88
6	2	7	9	2.04	2.63	0.52	2.03
7	2	6	8	1.73	2.72	0.58	1.62
8	6	10	16	1.71	3.13	0.7	1.44
9	8	12	20	1.8	2.56	0.43	1.68
10	2	9	11	1.82	2.26	0.38	1.95

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

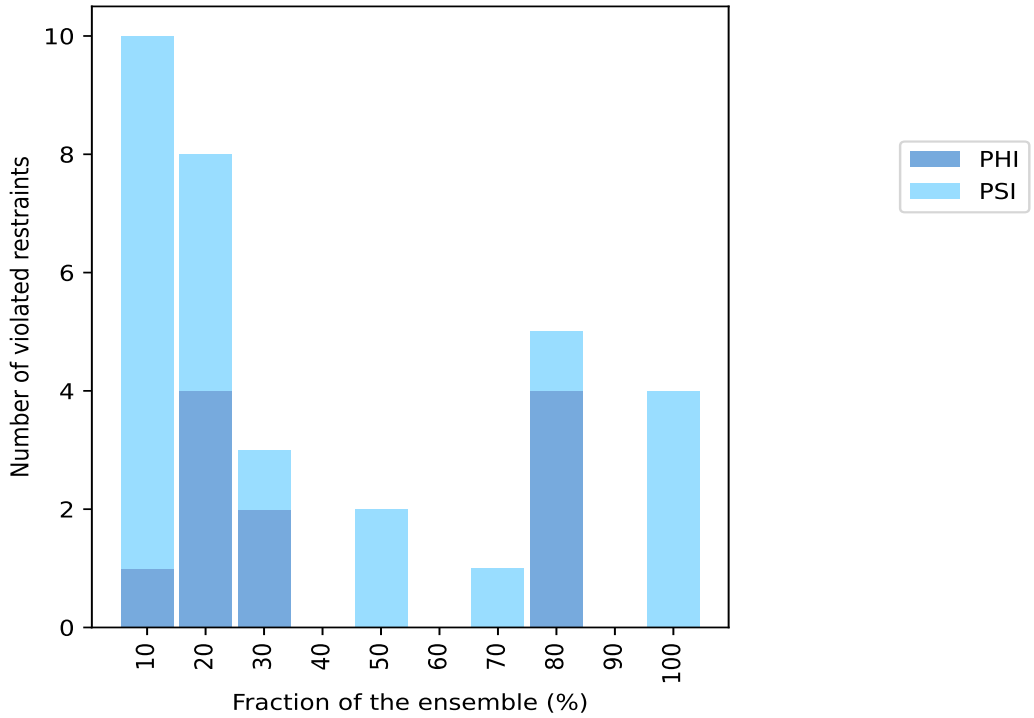
10.3 Dihedral-angle violation statistics for the ensemble

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

[1] Number of models with violations

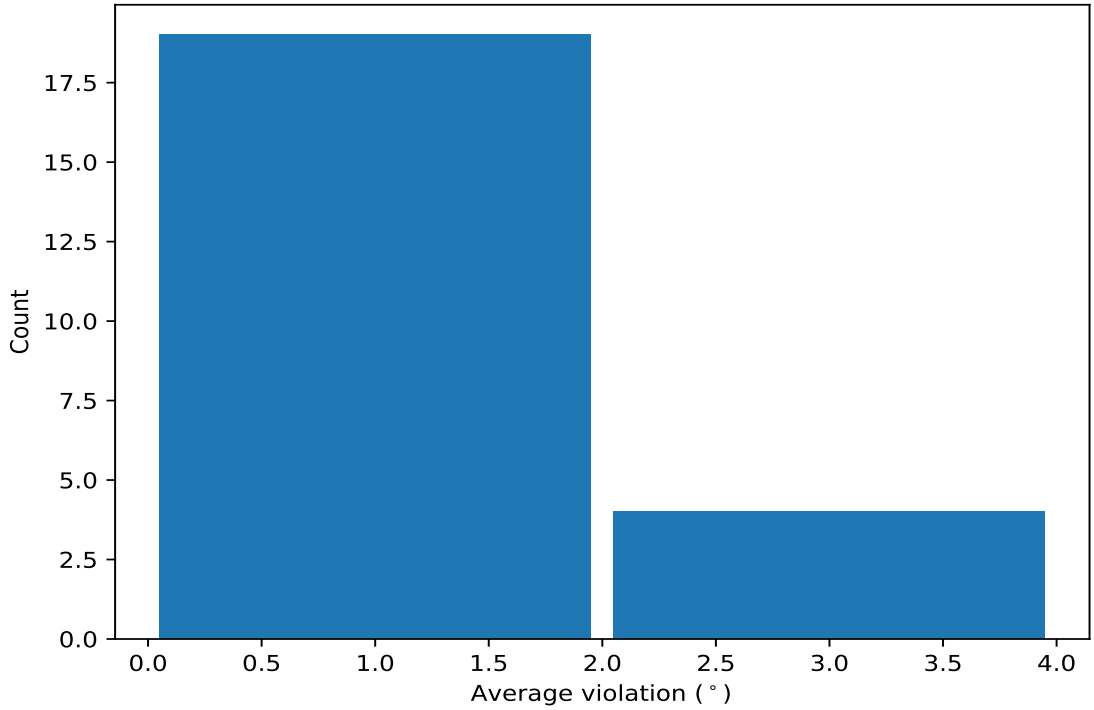
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

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

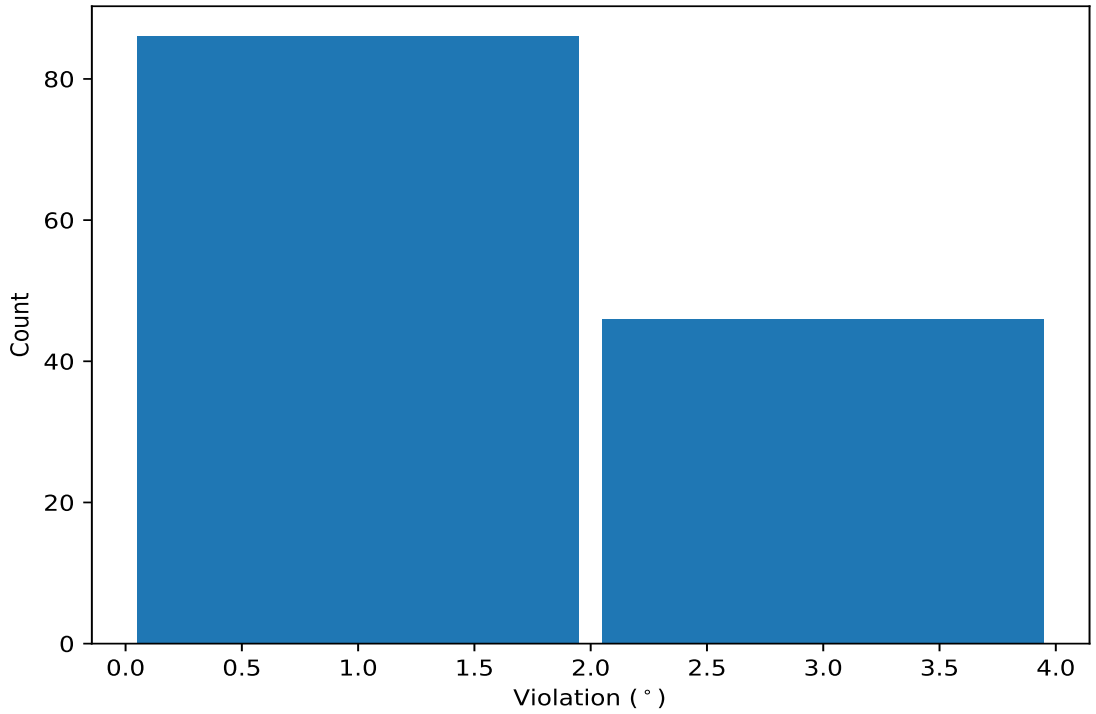
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	10	2.63	0.59	2.65
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	10	2.62	0.56	2.59
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	10	2.17	0.55	2.01
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	10	2.14	0.52	2.04
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	8	1.91	0.73	1.78
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	8	1.85	0.72	1.74
(1,24)	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	1:64:B:VAL:N	8	1.69	0.6	1.4
(1,29)	1:65:B:PHE:C	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	8	1.57	0.37	1.42
(2,29)	1:65:A:PHE:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	8	1.57	0.42	1.41
(2,24)	1:63:A:PRO:N	1:63:A:PRO:CA	1:63:A:PRO:C	1:64:A:VAL:N	7	1.79	0.57	1.65

[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 (°)
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	1	3.54
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	1	3.51
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	5	3.48
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	1	3.43
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	1	3.41
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	5	3.24
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	8	3.13
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	8	3.1
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	3	3.02
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	3	2.95