



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2MBB  
BMRB ID : 19394  
Title : Solution Structure of the human Polymerase iota UBM1-Ubiquitin Complex  
Authors : Wang, S.; Zhou, P.  
Deposited on : 2013-07-29

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The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

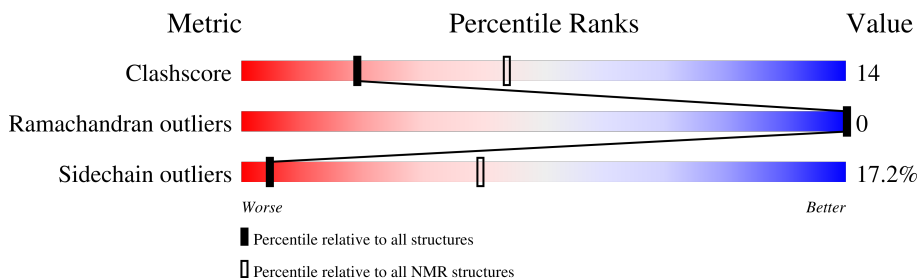
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 86%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	106	
2	B	78	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:66-A:90, B:201-B:272 (97)	0.21	6

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

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

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

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

### 3 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 1835 atoms, of which 934 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	38	607	191	307	49	59	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P06654
A	2	GLN	-	expression tag	UNP P06654
A	57	GLY	-	linker	UNP P06654
A	58	SER	-	linker	UNP P06654
A	99	LEU	-	expression tag	UNP Q9UNA4
A	100	GLU	-	expression tag	UNP Q9UNA4
A	101	HIS	-	expression tag	UNP Q9UNA4
A	102	HIS	-	expression tag	UNP Q9UNA4
A	103	HIS	-	expression tag	UNP Q9UNA4
A	104	HIS	-	expression tag	UNP Q9UNA4
A	105	HIS	-	expression tag	UNP Q9UNA4
A	106	HIS	-	expression tag	UNP Q9UNA4

- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	76	1228	378	627	105	117	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	199	SER	-	expression tag	UNP P0CG47
B	200	HIS	-	expression tag	UNP P0CG47



SER	HLS	W201	K206	T207	L208	T212	I213	V217	E218	T222	V225	V226	K227	K233	Q241	R242	L243	I244	F245	K248	Q249	L250	E251	R254	T255	L256	Y259	R260	I261	Q262	K263	E264	S265	T266	L267	H268	L269	V270	L271	R272	L273	R274	G275	G276
-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	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	2017
Number of shifts mapped to atoms	1333
Number of unparsed shifts	0
Number of shifts with mapping errors	684
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	197	198	198	8±1
2	B	574	597	596	18±3
All	All	15420	15900	15880	445

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 14.

5 of 87 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:217:VAL:HG11	2:B:226:VAL:HG22	0.94	1.39	16	20
1:A:78:LEU:HD13	1:A:82:ILE:HG21	0.93	1.38	20	18
1:A:82:ILE:HG23	2:B:270:VAL:HG11	0.78	1.56	19	18
1:A:78:LEU:HD23	1:A:82:ILE:HG21	0.77	1.56	9	2
2:B:226:VAL:HG21	2:B:256:LEU:HD21	0.72	1.61	18	19

### 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	25/106 (24%)	25±0 (99±2%)	0±0 (1±2%)	0±0 (0±0%)	100	100
2	B	71/78 (91%)	69±1 (97±1%)	2±1 (3±1%)	0±0 (0±0%)	100	100
All	All	1920/3680 (52%)	1869 (97%)	51 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 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	23/92 (25%)	20±1 (89±6%)	3±1 (11±6%)	9	53
2	B	66/70 (94%)	53±2 (81±3%)	13±2 (19±3%)	4	35
All	All	1780/3240 (55%)	1473 (83%)	307 (17%)	5	39

5 of 36 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	206	LYS	20
2	B	208	LEU	20
2	B	212	THR	20
2	B	225	ASN	20
2	B	255	THR	20

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 83% 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	2017
Number of shifts mapped to atoms	1333
Number of unparsed shifts	0
Number of shifts with mapping errors	684
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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 684) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HA	4.155	0.020	1
1	A	1	MET	HB2	2.083	0.020	2
1	A	1	MET	HB3	2.209	0.020	2
1	A	1	MET	HG2	2.17	0.020	2
1	A	1	MET	HG3	2.407	0.020	2
1	A	1	MET	HE1	2.11	0.020	1
1	A	1	MET	HE2	2.11	0.020	1
1	A	1	MET	HE3	2.11	0.020	1
1	A	1	MET	CA	54.073	0.400	1
1	A	1	MET	CB	32.187	0.400	1
1	A	1	MET	CG	30.268	0.400	1
1	A	1	MET	CE	15.833	0.400	1
1	A	2	GLN	H	8.338	0.020	1
1	A	2	GLN	HA	4.954	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	GLN	HB2	1.955	0.020	2
1	A	2	GLN	HB3	2.018	0.020	2
1	A	2	GLN	HG2	2.341	0.020	2
1	A	2	GLN	HG3	2.114	0.020	2
1	A	2	GLN	HE21	6.887	0.020	2
1	A	2	GLN	HE22	7.827	0.020	2
1	A	2	GLN	CA	55.411	0.400	1
1	A	2	GLN	CB	29.995	0.400	1
1	A	2	GLN	CG	34.639	0.400	1
1	A	2	GLN	N	123.406	0.400	1
1	A	2	GLN	NE2	112.352	0.400	1
1	A	3	TYR	H	9.082	0.020	1
1	A	3	TYR	HA	5.35	0.020	1
1	A	3	TYR	HB2	2.708	0.020	2
1	A	3	TYR	HB3	3.383	0.020	2
1	A	3	TYR	HD1	7.13	0.020	1
1	A	3	TYR	HD2	7.13	0.020	1
1	A	3	TYR	HE1	6.908	0.020	1
1	A	3	TYR	HE2	6.908	0.020	1
1	A	3	TYR	CA	56.595	0.400	1
1	A	3	TYR	CB	42.987	0.400	1
1	A	3	TYR	CD1	133.033	0.400	1
1	A	3	TYR	CE1	117.444	0.400	1
1	A	3	TYR	N	124.395	0.400	1
1	A	4	LYS	H	9.088	0.020	1
1	A	4	LYS	HA	5.209	0.020	1
1	A	4	LYS	HB2	1.876	0.020	2
1	A	4	LYS	HB3	2.013	0.020	2
1	A	4	LYS	HG2	1.327	0.020	2
1	A	4	LYS	HG3	1.448	0.020	2
1	A	4	LYS	HD2	1.605	0.020	1
1	A	4	LYS	HD3	1.605	0.020	1
1	A	4	LYS	HE2	2.775	0.020	1
1	A	4	LYS	HE3	2.775	0.020	1
1	A	4	LYS	CA	54.057	0.400	1
1	A	4	LYS	CB	35.465	0.400	1
1	A	4	LYS	CG	25.103	0.400	1
1	A	4	LYS	CD	28.441	0.400	1
1	A	4	LYS	CE	41.265	0.400	1
1	A	4	LYS	N	122.232	0.400	1
1	A	5	LEU	H	8.608	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LEU	HA	4.934	0.020	1
1	A	5	LEU	HB2	0.736	0.020	2
1	A	5	LEU	HB3	-1.157	0.020	2
1	A	5	LEU	HG	0.849	0.020	1
1	A	5	LEU	HD11	0.526	0.020	2
1	A	5	LEU	HD12	0.526	0.020	2
1	A	5	LEU	HD13	0.526	0.020	2
1	A	5	LEU	HD21	0.561	0.020	2
1	A	5	LEU	HD22	0.561	0.020	2
1	A	5	LEU	HD23	0.561	0.020	2
1	A	5	LEU	CA	52.143	0.400	1
1	A	5	LEU	CB	42.147	0.400	1
1	A	5	LEU	CG	26.677	0.400	1
1	A	5	LEU	CD1	24.28	0.400	1
1	A	5	LEU	CD2	25.395	0.400	1
1	A	5	LEU	N	126.362	0.400	1
1	A	6	ILE	H	9.073	0.020	1
1	A	6	ILE	HA	4.308	0.020	1
1	A	6	ILE	HB	1.942	0.020	1
1	A	6	ILE	HG12	1.069	0.020	2
1	A	6	ILE	HG13	1.394	0.020	2
1	A	6	ILE	HG21	0.772	0.020	1
1	A	6	ILE	HG22	0.772	0.020	1
1	A	6	ILE	HG23	0.772	0.020	1
1	A	6	ILE	HD11	0.742	0.020	1
1	A	6	ILE	HD12	0.742	0.020	1
1	A	6	ILE	HD13	0.742	0.020	1
1	A	6	ILE	CA	59.636	0.400	1
1	A	6	ILE	CB	37.669	0.400	1
1	A	6	ILE	CG1	26.797	0.400	1
1	A	6	ILE	CG2	16.602	0.400	1
1	A	6	ILE	CD1	12.225	0.400	1
1	A	6	ILE	N	126.117	0.400	1
1	A	7	LEU	H	8.702	0.020	1
1	A	7	LEU	HA	4.462	0.020	1
1	A	7	LEU	HB2	1.421	0.020	2
1	A	7	LEU	HB3	1.332	0.020	2
1	A	7	LEU	HG	1.269	0.020	1
1	A	7	LEU	HD11	0.736	0.020	2
1	A	7	LEU	HD12	0.736	0.020	2
1	A	7	LEU	HD13	0.736	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	LEU	HD21	0.746	0.020	2
1	A	7	LEU	HD22	0.746	0.020	2
1	A	7	LEU	HD23	0.746	0.020	2
1	A	7	LEU	CA	53.842	0.400	1
1	A	7	LEU	CB	41.737	0.400	1
1	A	7	LEU	CG	27.043	0.400	1
1	A	7	LEU	CD1	25.139	0.400	1
1	A	7	LEU	CD2	25.384	0.400	1
1	A	7	LEU	N	125.509	0.400	1
1	A	8	ASN	H	8.831	0.020	1
1	A	8	ASN	HA	5.223	0.020	1
1	A	8	ASN	HB2	2.495	0.020	2
1	A	8	ASN	HB3	2.944	0.020	2
1	A	8	ASN	HD21	7.11	0.020	2
1	A	8	ASN	HD22	6.761	0.020	2
1	A	8	ASN	CA	50.535	0.400	1
1	A	8	ASN	CB	37.815	0.400	1
1	A	8	ASN	N	125.475	0.400	1
1	A	8	ASN	ND2	111.3	0.400	1
1	A	9	GLY	H	7.92	0.020	1
1	A	9	GLY	HA2	4.422	0.020	2
1	A	9	GLY	HA3	4.021	0.020	2
1	A	9	GLY	CA	44.266	0.400	1
1	A	9	GLY	N	109.755	0.400	1
1	A	10	LYS	H	9.283	0.020	1
1	A	10	LYS	HA	4.026	0.020	1
1	A	10	LYS	HB2	1.792	0.020	1
1	A	10	LYS	HB3	1.792	0.020	1
1	A	10	LYS	HG2	1.421	0.020	1
1	A	10	LYS	HG3	1.421	0.020	1
1	A	10	LYS	HD2	1.671	0.020	1
1	A	10	LYS	HD3	1.671	0.020	1
1	A	10	LYS	HE2	2.923	0.020	1
1	A	10	LYS	HE3	2.923	0.020	1
1	A	10	LYS	CA	58.515	0.400	1
1	A	10	LYS	CB	31.958	0.400	1
1	A	10	LYS	CG	24.774	0.400	1
1	A	10	LYS	CD	28.434	0.400	1
1	A	10	LYS	CE	41.279	0.400	1
1	A	10	LYS	N	121.086	0.400	1
1	A	11	THR	H	8.803	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	THR	HA	4.353	0.020	1
1	A	11	THR	HB	4.207	0.020	1
1	A	11	THR	HG21	1.125	0.020	1
1	A	11	THR	HG22	1.125	0.020	1
1	A	11	THR	HG23	1.125	0.020	1
1	A	11	THR	CA	61.46	0.400	1
1	A	11	THR	CB	69.112	0.400	1
1	A	11	THR	CG2	21.314	0.400	1
1	A	11	THR	N	108.583	0.400	1
1	A	12	LEU	H	7.306	0.020	1
1	A	12	LEU	HA	4.432	0.020	1
1	A	12	LEU	HB2	1.405	0.020	2
1	A	12	LEU	HB3	1.53	0.020	2
1	A	12	LEU	HG	1.394	0.020	1
1	A	12	LEU	HD11	0.863	0.020	2
1	A	12	LEU	HD12	0.863	0.020	2
1	A	12	LEU	HD13	0.863	0.020	2
1	A	12	LEU	HD21	0.78	0.020	2
1	A	12	LEU	HD22	0.78	0.020	2
1	A	12	LEU	HD23	0.78	0.020	2
1	A	12	LEU	CA	54.61	0.400	1
1	A	12	LEU	CB	42.938	0.400	1
1	A	12	LEU	CG	27.012	0.400	1
1	A	12	LEU	CD1	23.754	0.400	1
1	A	12	LEU	CD2	24.863	0.400	1
1	A	12	LEU	N	124.89	0.400	1
1	A	13	LYS	H	8.095	0.020	1
1	A	13	LYS	HA	5.114	0.020	1
1	A	13	LYS	HB2	1.877	0.020	2
1	A	13	LYS	HB3	1.705	0.020	2
1	A	13	LYS	HG2	1.435	0.020	1
1	A	13	LYS	HG3	1.435	0.020	1
1	A	13	LYS	HD2	1.72	0.020	1
1	A	13	LYS	HD3	1.72	0.020	1
1	A	13	LYS	HE2	2.902	0.020	2
1	A	13	LYS	HE3	2.986	0.020	2
1	A	13	LYS	CA	53.297	0.400	1
1	A	13	LYS	CB	34.391	0.400	1
1	A	13	LYS	CG	24.585	0.400	1
1	A	13	LYS	CD	28.678	0.400	1
1	A	13	LYS	CE	42.079	0.400	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	LYS	N	123.767	0.400	1
1	A	14	GLY	H	8.386	0.020	1
1	A	14	GLY	HA2	4.136	0.020	2
1	A	14	GLY	HA3	4.247	0.020	2
1	A	14	GLY	CA	44.568	0.400	1
1	A	14	GLY	N	109.323	0.400	1
1	A	15	GLU	H	8.376	0.020	1
1	A	15	GLU	HA	5.591	0.020	1
1	A	15	GLU	HB2	1.893	0.020	2
1	A	15	GLU	HB3	1.993	0.020	2
1	A	15	GLU	HG2	2.126	0.020	1
1	A	15	GLU	HG3	2.126	0.020	1
1	A	15	GLU	CA	54.057	0.400	1
1	A	15	GLU	CB	33.327	0.400	1
1	A	15	GLU	CG	35.58	0.400	1
1	A	15	GLU	N	118.548	0.400	1
1	A	16	THR	H	8.759	0.020	1
1	A	16	THR	HA	4.719	0.020	1
1	A	16	THR	HB	3.888	0.020	1
1	A	16	THR	HG21	0.414	0.020	1
1	A	16	THR	HG22	0.414	0.020	1
1	A	16	THR	HG23	0.414	0.020	1
1	A	16	THR	CA	59.943	0.400	1
1	A	16	THR	CB	68.911	0.400	1
1	A	16	THR	CG2	18.828	0.400	1
1	A	16	THR	N	115.84	0.400	1
1	A	17	THR	H	8.059	0.020	1
1	A	17	THR	HA	5.793	0.020	1
1	A	17	THR	HB	4.276	0.020	1
1	A	17	THR	HG21	1.17	0.020	1
1	A	17	THR	HG22	1.17	0.020	1
1	A	17	THR	HG23	1.17	0.020	1
1	A	17	THR	CA	59.295	0.400	1
1	A	17	THR	CB	72.719	0.400	1
1	A	17	THR	CG2	21.011	0.400	1
1	A	17	THR	N	111.797	0.400	1
1	A	18	THR	H	8.954	0.020	1
1	A	18	THR	HA	4.647	0.020	1
1	A	18	THR	HB	3.822	0.020	1
1	A	18	THR	HG21	0.458	0.020	1
1	A	18	THR	HG22	0.458	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	THR	HG23	0.458	0.020	1
1	A	18	THR	CA	61.725	0.400	1
1	A	18	THR	CB	69.521	0.400	1
1	A	18	THR	CG2	18.557	0.400	1
1	A	18	THR	N	114.492	0.400	1
1	A	19	GLU	H	7.92	0.020	1
1	A	19	GLU	HA	5.155	0.020	1
1	A	19	GLU	HB2	1.919	0.020	1
1	A	19	GLU	HB3	1.919	0.020	1
1	A	19	GLU	HG2	2.031	0.020	2
1	A	19	GLU	HG3	2.263	0.020	2
1	A	19	GLU	CA	53.843	0.400	1
1	A	19	GLU	CB	29.809	0.400	1
1	A	19	GLU	CG	35.232	0.400	1
1	A	19	GLU	N	125.896	0.400	1
1	A	20	ALA	H	9.32	0.020	1
1	A	20	ALA	HA	4.919	0.020	1
1	A	20	ALA	HB1	1.325	0.020	1
1	A	20	ALA	HB2	1.325	0.020	1
1	A	20	ALA	HB3	1.325	0.020	1
1	A	20	ALA	CA	50.26	0.400	1
1	A	20	ALA	CB	23.199	0.400	1
1	A	20	ALA	N	127.308	0.400	1
1	A	21	VAL	H	8.474	0.020	1
1	A	21	VAL	HA	4.082	0.020	1
1	A	21	VAL	HB	2.183	0.020	1
1	A	21	VAL	HG11	0.989	0.020	2
1	A	21	VAL	HG12	0.989	0.020	2
1	A	21	VAL	HG13	0.989	0.020	2
1	A	21	VAL	HG21	0.981	0.020	2
1	A	21	VAL	HG22	0.981	0.020	2
1	A	21	VAL	HG23	0.981	0.020	2
1	A	21	VAL	CA	62.975	0.400	1
1	A	21	VAL	CB	31.421	0.400	1
1	A	21	VAL	CG1	20.424	0.400	1
1	A	21	VAL	CG2	19.662	0.400	1
1	A	21	VAL	N	115.712	0.400	1
1	A	22	ASP	H	7.296	0.020	1
1	A	22	ASP	HA	4.74	0.020	1
1	A	22	ASP	HB2	2.944	0.020	2
1	A	22	ASP	HB3	3.026	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	ASP	CA	51.939	0.400	1
1	A	22	ASP	CB	41.543	0.400	1
1	A	22	ASP	N	115.055	0.400	1
1	A	23	ALA	H	8.276	0.020	1
1	A	23	ALA	HA	3.301	0.020	1
1	A	23	ALA	HB1	1.161	0.020	1
1	A	23	ALA	HB2	1.161	0.020	1
1	A	23	ALA	HB3	1.161	0.020	1
1	A	23	ALA	CA	54.038	0.400	1
1	A	23	ALA	CB	16.945	0.400	1
1	A	23	ALA	N	121.34	0.400	1
1	A	24	ALA	H	8.034	0.020	1
1	A	24	ALA	HA	3.943	0.020	1
1	A	24	ALA	HB1	1.27	0.020	1
1	A	24	ALA	HB2	1.27	0.020	1
1	A	24	ALA	HB3	1.27	0.020	1
1	A	24	ALA	CA	54.14	0.400	1
1	A	24	ALA	CB	17.275	0.400	1
1	A	24	ALA	N	120.414	0.400	1
1	A	25	THR	H	8.269	0.020	1
1	A	25	THR	HA	3.683	0.020	1
1	A	25	THR	HB	3.998	0.020	1
1	A	25	THR	HG21	1.207	0.020	1
1	A	25	THR	HG22	1.207	0.020	1
1	A	25	THR	HG23	1.207	0.020	1
1	A	25	THR	CA	66.348	0.400	1
1	A	25	THR	CB	67.268	0.400	1
1	A	25	THR	CG2	20.488	0.400	1
1	A	25	THR	N	116.322	0.400	1
1	A	26	ALA	H	7.135	0.020	1
1	A	26	ALA	HA	3.057	0.020	1
1	A	26	ALA	HB1	0.488	0.020	1
1	A	26	ALA	HB2	0.488	0.020	1
1	A	26	ALA	HB3	0.488	0.020	1
1	A	26	ALA	CA	54.338	0.400	1
1	A	26	ALA	CB	16.929	0.400	1
1	A	26	ALA	N	123.563	0.400	1
1	A	27	GLU	H	8.299	0.020	1
1	A	27	GLU	HA	2.608	0.020	1
1	A	27	GLU	HB2	1.829	0.020	2
1	A	27	GLU	HB3	1.931	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	GLU	HG2	1.603	0.020	1
1	A	27	GLU	HG3	1.603	0.020	1
1	A	27	GLU	CA	59.053	0.400	1
1	A	27	GLU	CB	28.681	0.400	1
1	A	27	GLU	CG	35.265	0.400	1
1	A	27	GLU	N	116.527	0.400	1
1	A	28	LYS	H	6.924	0.020	1
1	A	28	LYS	HA	3.705	0.020	1
1	A	28	LYS	HB2	1.813	0.020	1
1	A	28	LYS	HB3	1.813	0.020	1
1	A	28	LYS	HG2	1.305	0.020	2
1	A	28	LYS	HG3	1.527	0.020	2
1	A	28	LYS	HD2	1.592	0.020	1
1	A	28	LYS	HD3	1.592	0.020	1
1	A	28	LYS	HE2	2.874	0.020	1
1	A	28	LYS	HE3	2.874	0.020	1
1	A	28	LYS	CA	59.095	0.400	1
1	A	28	LYS	CB	31.691	0.400	1
1	A	28	LYS	CG	24.598	0.400	1
1	A	28	LYS	CD	28.719	0.400	1
1	A	28	LYS	CE	41.425	0.400	1
1	A	28	LYS	N	116.49	0.400	1
1	A	29	VAL	H	7.306	0.020	1
1	A	29	VAL	HA	3.619	0.020	1
1	A	29	VAL	HB	1.73	0.020	1
1	A	29	VAL	HG11	0.768	0.020	2
1	A	29	VAL	HG12	0.768	0.020	2
1	A	29	VAL	HG13	0.768	0.020	2
1	A	29	VAL	HG21	0.877	0.020	2
1	A	29	VAL	HG22	0.877	0.020	2
1	A	29	VAL	HG23	0.877	0.020	2
1	A	29	VAL	CA	65.349	0.400	1
1	A	29	VAL	CB	31.179	0.400	1
1	A	29	VAL	CG1	19.923	0.400	1
1	A	29	VAL	CG2	21.099	0.400	1
1	A	29	VAL	N	120.468	0.400	1
1	A	30	PHE	H	8.498	0.020	1
1	A	30	PHE	HA	4.755	0.020	1
1	A	30	PHE	HB2	2.812	0.020	2
1	A	30	PHE	HB3	3.3	0.020	2
1	A	30	PHE	HD1	6.899	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	PHE	HD2	6.899	0.020	1
1	A	30	PHE	HE1	7.078	0.020	1
1	A	30	PHE	HE2	7.078	0.020	1
1	A	30	PHE	HZ	7.168	0.020	1
1	A	30	PHE	CA	55.977	0.400	1
1	A	30	PHE	CB	36.854	0.400	1
1	A	30	PHE	CD1	129.211	0.400	1
1	A	30	PHE	CE1	130.036	0.400	1
1	A	30	PHE	CZ	129.763	0.400	1
1	A	30	PHE	N	120.532	0.400	1
1	A	31	LYS	H	9.058	0.020	1
1	A	31	LYS	HA	4.148	0.020	1
1	A	31	LYS	HB2	1.606	0.020	2
1	A	31	LYS	HB3	1.54	0.020	2
1	A	31	LYS	HG2	0.445	0.020	2
1	A	31	LYS	HG3	0.779	0.020	2
1	A	31	LYS	HD2	1.028	0.020	2
1	A	31	LYS	HD3	1.086	0.020	2
1	A	31	LYS	HE2	1.639	0.020	2
1	A	31	LYS	HE3	1.861	0.020	2
1	A	31	LYS	CA	59.299	0.400	1
1	A	31	LYS	CB	31.118	0.400	1
1	A	31	LYS	CG	25.363	0.400	1
1	A	31	LYS	CD	28.182	0.400	1
1	A	31	LYS	CE	40.67	0.400	1
1	A	31	LYS	N	122.701	0.400	1
1	A	32	GLN	H	7.423	0.020	1
1	A	32	GLN	HA	4.024	0.020	1
1	A	32	GLN	HB2	2.184	0.020	2
1	A	32	GLN	HB3	2.231	0.020	2
1	A	32	GLN	HG2	2.397	0.020	2
1	A	32	GLN	HG3	2.427	0.020	2
1	A	32	GLN	HE21	6.863	0.020	2
1	A	32	GLN	HE22	7.918	0.020	2
1	A	32	GLN	CA	57.95	0.400	1
1	A	32	GLN	CB	27.592	0.400	1
1	A	32	GLN	CG	32.832	0.400	1
1	A	32	GLN	N	119.507	0.400	1
1	A	32	GLN	NE2	115.204	0.400	1
1	A	33	TYR	H	8.232	0.020	1
1	A	33	TYR	HA	4.255	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	33	TYR	HB2	3.287	0.020	1
1	A	33	TYR	HB3	3.287	0.020	1
1	A	33	TYR	HD1	6.968	0.020	1
1	A	33	TYR	HD2	6.968	0.020	1
1	A	33	TYR	HE1	6.714	0.020	1
1	A	33	TYR	HE2	6.714	0.020	1
1	A	33	TYR	CA	61.241	0.400	1
1	A	33	TYR	CB	38.192	0.400	1
1	A	33	TYR	CD1	132.213	0.400	1
1	A	33	TYR	CE1	117.726	0.400	1
1	A	33	TYR	N	120.872	0.400	1
1	A	34	ALA	H	9.16	0.020	1
1	A	34	ALA	HA	3.774	0.020	1
1	A	34	ALA	HB1	1.821	0.020	1
1	A	34	ALA	HB2	1.821	0.020	1
1	A	34	ALA	HB3	1.821	0.020	1
1	A	34	ALA	CA	55.731	0.400	1
1	A	34	ALA	CB	17.381	0.400	1
1	A	34	ALA	N	122.479	0.400	1
1	A	35	ASN	H	8.229	0.020	1
1	A	35	ASN	HA	4.42	0.020	1
1	A	35	ASN	HB2	2.9	0.020	2
1	A	35	ASN	HB3	2.943	0.020	2
1	A	35	ASN	HD21	7.601	0.020	2
1	A	35	ASN	HD22	6.955	0.020	2
1	A	35	ASN	CA	56.368	0.400	1
1	A	35	ASN	CB	38.301	0.400	1
1	A	35	ASN	N	117.521	0.400	1
1	A	35	ASN	ND2	112.17	0.400	1
1	A	36	ASP	H	8.917	0.020	1
1	A	36	ASP	HA	4.345	0.020	1
1	A	36	ASP	HB2	2.713	0.020	2
1	A	36	ASP	HB3	2.542	0.020	2
1	A	36	ASP	CA	56.333	0.400	1
1	A	36	ASP	CB	39.413	0.400	1
1	A	36	ASP	N	121.311	0.400	1
1	A	37	ASN	H	7.357	0.020	1
1	A	37	ASN	HA	4.575	0.020	1
1	A	37	ASN	HB2	2.077	0.020	2
1	A	37	ASN	HB3	2.667	0.020	2
1	A	37	ASN	HD21	6.253	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	37	ASN	HD22	6.619	0.020	2
1	A	37	ASN	CA	53.194	0.400	1
1	A	37	ASN	CB	39.449	0.400	1
1	A	37	ASN	N	115.211	0.400	1
1	A	37	ASN	ND2	114.79	0.400	1
1	A	38	GLY	H	7.772	0.020	1
1	A	38	GLY	HA2	3.897	0.020	1
1	A	38	GLY	HA3	3.897	0.020	1
1	A	38	GLY	CA	46.224	0.400	1
1	A	38	GLY	N	108.012	0.400	1
1	A	39	VAL	H	8.099	0.020	1
1	A	39	VAL	HA	4.124	0.020	1
1	A	39	VAL	HB	1.711	0.020	1
1	A	39	VAL	HG11	0.615	0.020	2
1	A	39	VAL	HG12	0.615	0.020	2
1	A	39	VAL	HG13	0.615	0.020	2
1	A	39	VAL	HG21	0.784	0.020	2
1	A	39	VAL	HG22	0.784	0.020	2
1	A	39	VAL	HG23	0.784	0.020	2
1	A	39	VAL	CA	61.42	0.400	1
1	A	39	VAL	CB	32.712	0.400	1
1	A	39	VAL	CG1	21.005	0.400	1
1	A	39	VAL	CG2	21.289	0.400	1
1	A	39	VAL	N	120.706	0.400	1
1	A	40	ASP	H	8.468	0.020	1
1	A	40	ASP	HA	4.863	0.020	1
1	A	40	ASP	HB2	2.574	0.020	2
1	A	40	ASP	HB3	2.702	0.020	2
1	A	40	ASP	CA	51.913	0.400	1
1	A	40	ASP	CB	42.636	0.400	1
1	A	40	ASP	N	127.304	0.400	1
1	A	41	GLY	H	7.912	0.020	1
1	A	41	GLY	HA2	3.731	0.020	2
1	A	41	GLY	HA3	4.216	0.020	2
1	A	41	GLY	CA	44.866	0.400	1
1	A	41	GLY	N	107.327	0.400	1
1	A	42	GLU	H	8.024	0.020	1
1	A	42	GLU	HA	4.674	0.020	1
1	A	42	GLU	HB2	2.028	0.020	2
1	A	42	GLU	HB3	1.95	0.020	2
1	A	42	GLU	HG2	2.245	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	42	GLU	HG3	2.338	0.020	2
1	A	42	GLU	CA	54.95	0.400	1
1	A	42	GLU	CB	30.956	0.400	1
1	A	42	GLU	CG	35.811	0.400	1
1	A	42	GLU	N	120.524	0.400	1
1	A	43	TRP	H	9.294	0.020	1
1	A	43	TRP	HA	5.354	0.020	1
1	A	43	TRP	HB2	3.141	0.020	2
1	A	43	TRP	HB3	3.351	0.020	2
1	A	43	TRP	HD1	7.554	0.020	1
1	A	43	TRP	HE3	7.601	0.020	1
1	A	43	TRP	HZ2	7.322	0.020	1
1	A	43	TRP	HZ3	6.595	0.020	1
1	A	43	TRP	HH2	6.727	0.020	1
1	A	43	TRP	CA	57.201	0.400	1
1	A	43	TRP	CB	30.057	0.400	1
1	A	43	TRP	CD1	126.469	0.400	1
1	A	43	TRP	CE3	118.812	0.400	1
1	A	43	TRP	CZ2	113.889	0.400	1
1	A	43	TRP	CZ3	120.179	0.400	1
1	A	43	TRP	CH2	122.367	0.400	1
1	A	43	TRP	N	128.082	0.400	1
1	A	44	THR	H	9.247	0.020	1
1	A	44	THR	HA	4.803	0.020	1
1	A	44	THR	HB	4.215	0.020	1
1	A	44	THR	HG21	1.167	0.020	1
1	A	44	THR	HG22	1.167	0.020	1
1	A	44	THR	HG23	1.167	0.020	1
1	A	44	THR	CA	59.89	0.400	1
1	A	44	THR	CB	71.686	0.400	1
1	A	44	THR	CG2	21.312	0.400	1
1	A	44	THR	N	114.405	0.400	1
1	A	45	TYR	H	8.559	0.020	1
1	A	45	TYR	HA	4.946	0.020	1
1	A	45	TYR	HB2	2.48	0.020	2
1	A	45	TYR	HB3	2.854	0.020	2
1	A	45	TYR	HD1	7.791	0.020	1
1	A	45	TYR	HD2	7.791	0.020	1
1	A	45	TYR	HE1	6.335	0.020	1
1	A	45	TYR	HE2	6.335	0.020	1
1	A	45	TYR	CA	56.317	0.400	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	TYR	CB	41.007	0.400	1
1	A	45	TYR	CD1	131.666	0.400	1
1	A	45	TYR	CE1	116.897	0.400	1
1	A	45	TYR	N	120.527	0.400	1
1	A	46	ASP	H	7.604	0.020	1
1	A	46	ASP	HA	4.564	0.020	1
1	A	46	ASP	HB2	2.244	0.020	2
1	A	46	ASP	HB3	2.582	0.020	2
1	A	46	ASP	CA	51.153	0.400	1
1	A	46	ASP	CB	42.435	0.400	1
1	A	46	ASP	N	128.305	0.400	1
1	A	47	ASP	H	8.55	0.020	1
1	A	47	ASP	HA	4.115	0.020	1
1	A	47	ASP	HB2	2.502	0.020	2
1	A	47	ASP	HB3	2.806	0.020	2
1	A	47	ASP	CA	55.741	0.400	1
1	A	47	ASP	CB	41.549	0.400	1
1	A	47	ASP	N	124.821	0.400	1
1	A	48	ALA	H	8.319	0.020	1
1	A	48	ALA	HA	4.105	0.020	1
1	A	48	ALA	HB1	1.482	0.020	1
1	A	48	ALA	HB2	1.482	0.020	1
1	A	48	ALA	HB3	1.482	0.020	1
1	A	48	ALA	CA	54.624	0.400	1
1	A	48	ALA	CB	17.741	0.400	1
1	A	48	ALA	N	119.765	0.400	1
1	A	49	THR	H	6.989	0.020	1
1	A	49	THR	HA	4.38	0.020	1
1	A	49	THR	HB	4.384	0.020	1
1	A	49	THR	HG21	1.061	0.020	1
1	A	49	THR	HG22	1.061	0.020	1
1	A	49	THR	HG23	1.061	0.020	1
1	A	49	THR	CA	59.812	0.400	1
1	A	49	THR	CB	69.519	0.400	1
1	A	49	THR	CG2	20.533	0.400	1
1	A	49	THR	N	103.111	0.400	1
1	A	50	LYS	H	7.84	0.020	1
1	A	50	LYS	HA	4.167	0.020	1
1	A	50	LYS	HB2	2.08	0.020	2
1	A	50	LYS	HB3	2.022	0.020	2
1	A	50	LYS	HG2	1.22	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	50	LYS	HG3	1.397	0.020	2
1	A	50	LYS	HD2	1.418	0.020	2
1	A	50	LYS	HD3	1.677	0.020	2
1	A	50	LYS	HE2	2.934	0.020	2
1	A	50	LYS	HE3	3.084	0.020	2
1	A	50	LYS	CA	56.039	0.400	1
1	A	50	LYS	CB	28.705	0.400	1
1	A	50	LYS	CG	24.059	0.400	1
1	A	50	LYS	CD	27.791	0.400	1
1	A	50	LYS	N	123.033	0.400	1
1	A	51	THR	H	7.356	0.020	1
1	A	51	THR	HA	5.477	0.020	1
1	A	51	THR	HB	3.742	0.020	1
1	A	51	THR	HG21	0.97	0.020	1
1	A	51	THR	HG22	0.97	0.020	1
1	A	51	THR	HG23	0.97	0.020	1
1	A	51	THR	CA	61.62	0.400	1
1	A	51	THR	CB	71.382	0.400	1
1	A	51	THR	CG2	20.235	0.400	1
1	A	51	THR	N	111.03	0.400	1
1	A	52	PHE	H	10.378	0.020	1
1	A	52	PHE	HA	5.66	0.020	1
1	A	52	PHE	HB2	3.221	0.020	2
1	A	52	PHE	HB3	3.288	0.020	2
1	A	52	PHE	HD1	7.781	0.020	1
1	A	52	PHE	HD2	7.781	0.020	1
1	A	52	PHE	HE1	7.207	0.020	1
1	A	52	PHE	HE2	7.207	0.020	1
1	A	52	PHE	HZ	6.984	0.020	1
1	A	52	PHE	CA	56.579	0.400	1
1	A	52	PHE	CB	42.155	0.400	1
1	A	52	PHE	CD1	131.677	0.400	1
1	A	52	PHE	CE1	130.845	0.400	1
1	A	52	PHE	CZ	130.572	0.400	1
1	A	52	PHE	N	130.82	0.400	1
1	A	53	THR	H	9.087	0.020	1
1	A	53	THR	HA	5.194	0.020	1
1	A	53	THR	HB	3.803	0.020	1
1	A	53	THR	HG21	0.933	0.020	1
1	A	53	THR	HG22	0.933	0.020	1
1	A	53	THR	HG23	0.933	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	THR	CA	60.937	0.400	1
1	A	53	THR	CB	70.455	0.400	1
1	A	53	THR	CG2	19.978	0.400	1
1	A	53	THR	N	116.885	0.400	1
1	A	54	VAL	H	8.177	0.020	1
1	A	54	VAL	HA	4.463	0.020	1
1	A	54	VAL	HB	-0.324	0.020	1
1	A	54	VAL	HG11	0.365	0.020	2
1	A	54	VAL	HG12	0.365	0.020	2
1	A	54	VAL	HG13	0.365	0.020	2
1	A	54	VAL	HG21	-0.364	0.020	2
1	A	54	VAL	HG22	-0.364	0.020	2
1	A	54	VAL	HG23	-0.364	0.020	2
1	A	54	VAL	CA	57.398	0.400	1
1	A	54	VAL	CB	31.788	0.400	1
1	A	54	VAL	CG1	19.166	0.400	1
1	A	54	VAL	CG2	20.192	0.400	1
1	A	54	VAL	N	123.065	0.400	1
1	A	55	THR	H	8.322	0.020	1
1	A	55	THR	HA	4.691	0.020	1
1	A	55	THR	HB	3.826	0.020	1
1	A	55	THR	HG21	1.143	0.020	1
1	A	55	THR	HG22	1.143	0.020	1
1	A	55	THR	HG23	1.143	0.020	1
1	A	55	THR	CA	60.411	0.400	1
1	A	55	THR	CB	69.948	0.400	1
1	A	55	THR	CG2	20.761	0.400	1
1	A	55	THR	N	123.192	0.400	1
1	A	56	GLU	H	8.086	0.020	1
1	A	56	GLU	HA	4.517	0.020	1
1	A	56	GLU	HB2	1.984	0.020	2
1	A	56	GLU	HB3	2.146	0.020	2
1	A	56	GLU	HG2	2.388	0.020	1
1	A	56	GLU	HG3	2.388	0.020	1
1	A	56	GLU	CA	55.735	0.400	1
1	A	56	GLU	CB	31.402	0.400	1
1	A	56	GLU	CG	36.079	0.400	1
1	A	56	GLU	N	128.667	0.400	1
1	A	57	GLY	H	8.762	0.020	1
1	A	57	GLY	HA2	4.051	0.020	2
1	A	57	GLY	HA3	3.928	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	GLY	CA	44.569	0.400	1
1	A	57	GLY	N	112.349	0.400	1
1	A	58	SER	H	8.306	0.020	1
1	A	58	SER	HA	4.43	0.020	1
1	A	58	SER	HB2	3.811	0.020	1
1	A	58	SER	HB3	3.811	0.020	1
1	A	58	SER	CA	57.476	0.400	1
1	A	58	SER	CB	63.353	0.400	1
1	A	58	SER	N	115.095	0.400	1
1	A	59	ASN	HA	4.661	0.020	1
1	A	59	ASN	HB2	2.663	0.020	2
1	A	59	ASN	HB3	2.74	0.020	2
1	A	59	ASN	HD21	6.87	0.020	2
1	A	59	ASN	HD22	7.554	0.020	2
1	A	59	ASN	CA	52.684	0.400	1
1	A	59	ASN	CB	38.28	0.400	1
1	A	59	ASN	ND2	112.729	0.400	1
1	A	60	GLU	H	8.254	0.020	1
1	A	60	GLU	HA	4.157	0.020	1
1	A	60	GLU	HB2	1.76	0.020	2
1	A	60	GLU	HB3	1.846	0.020	2
1	A	60	GLU	HG2	2.017	0.020	1
1	A	60	GLU	CA	56.05	0.400	1
1	A	60	GLU	CB	30.054	0.400	1
1	A	60	GLU	CG	35.557	0.400	1
1	A	60	GLU	N	120.738	0.400	1
1	A	61	PHE	H	8.227	0.020	1
1	A	61	PHE	HA	4.836	0.020	1
1	A	61	PHE	HB2	2.913	0.020	2
1	A	61	PHE	HB3	3.079	0.020	2
1	A	61	PHE	HD1	7.247	0.020	1
1	A	61	PHE	HD2	7.247	0.020	1
1	A	61	PHE	HE1	7.436	0.020	1
1	A	61	PHE	HE2	7.436	0.020	1
1	A	61	PHE	HZ	7.228	0.020	1
1	A	61	PHE	CA	54.935	0.400	1
1	A	61	PHE	CB	38.54	0.400	1
1	A	61	PHE	CD1	131.392	0.400	1
1	A	61	PHE	CE1	129.478	0.400	1
1	A	61	PHE	CZ	129.204	0.400	1
1	A	61	PHE	N	121.332	0.400	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	GLU	H	8.339	0.020	1
1	A	100	GLU	HB2	1.842	0.020	1
1	A	100	GLU	HB3	1.842	0.020	1
1	A	100	GLU	HG2	2.112	0.020	1
1	A	100	GLU	HG3	2.112	0.020	1
1	A	100	GLU	CB	29.695	0.400	1
1	A	100	GLU	CG	35.547	0.400	1
1	A	100	GLU	N	121.442	0.400	1
1	B	200	HIS	HA	4.701	0.020	1
1	B	200	HIS	HB2	3.027	0.020	1
1	B	200	HIS	HB3	3.027	0.020	1
1	B	200	HIS	HD2	6.896	0.020	1
1	B	200	HIS	CA	55.778	0.400	1
1	B	200	HIS	CB	30.309	0.400	1

### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	175	$0.56 \pm 0.13$	Should be applied
$^{13}\text{C}_\beta$	160	$0.63 \pm 0.13$	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	166	$0.61 \pm 0.45$	None needed (imprecise)

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 1173 atoms were assigned a chemical shift out of a possible 1362. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	381/481 (79%)	194/195 (99%)	97/194 (50%)	90/92 (98%)
Sidechain	758/835 (91%)	519/539 (96%)	228/267 (85%)	11/29 (38%)
Aromatic	34/46 (74%)	21/23 (91%)	13/22 (59%)	0/1 (0%)
Overall	1173/1362 (86%)	734/757 (97%)	338/483 (70%)	101/122 (83%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

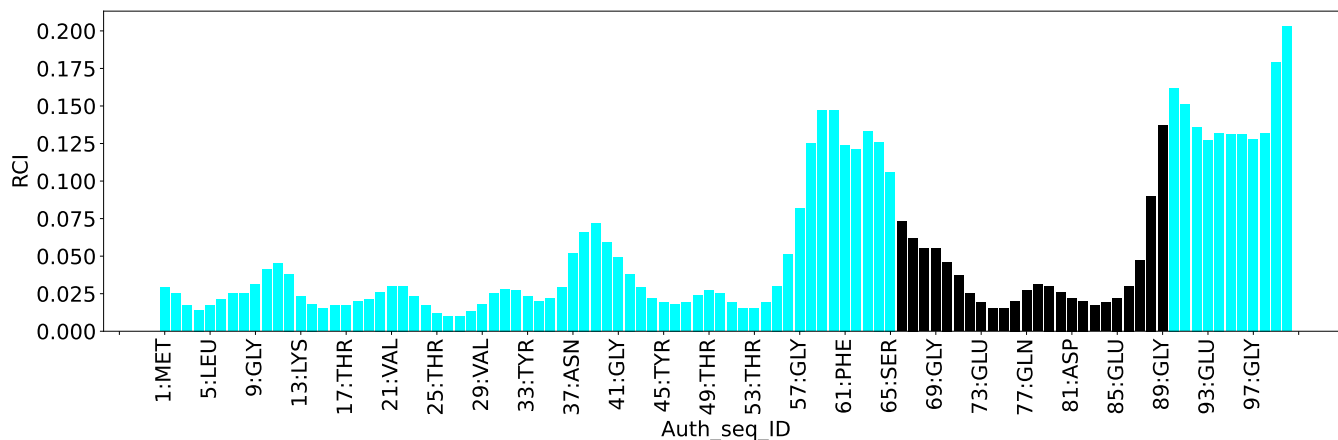
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	5	LEU	HB3	-1.16	-0.26 – 3.31	-7.5
1	A	54	VAL	HB	-0.32	0.43 – 3.54	-7.4
1	A	31	LYS	HE2	1.64	1.95 – 3.88	-6.6
1	A	31	LYS	HE3	1.86	1.92 – 3.89	-5.3

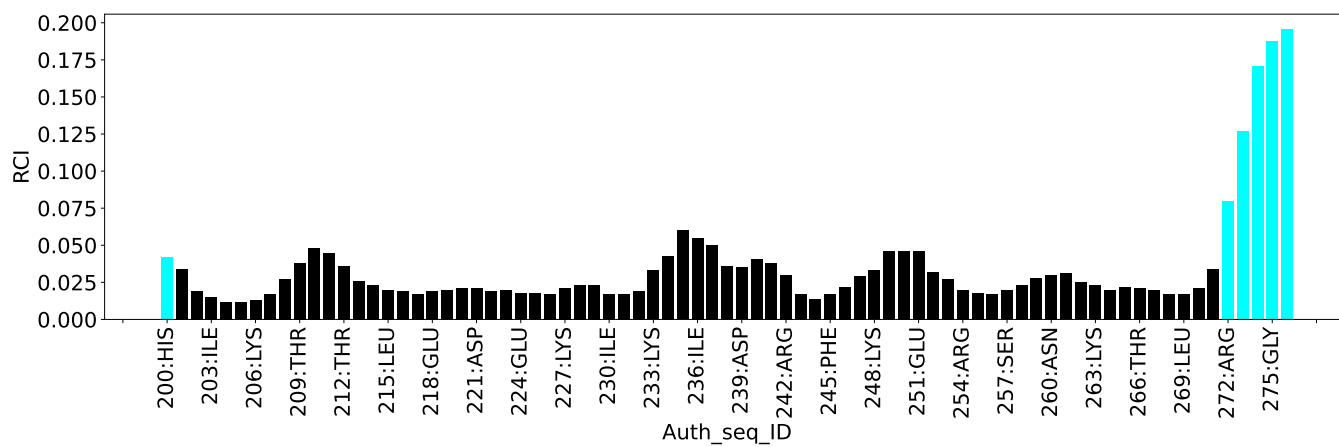
### 7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3742
Intra-residue ( $ i-j =0$ )	514
Sequential ( $ i-j =1$ )	793
Medium range ( $ i-j >1$ and $ i-j <5$ )	844
Long range ( $ i-j \geq 5$ )	1274
Inter-chain	232
Hydrogen bond restraints	85
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	20.3
Number of long range restraints per residue <sup>1</sup>	7.1

<sup>1</sup>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)	2.1	0.19
0.2-0.5 (Medium)	0.3	0.45
>0.5 (Large)	2.4	2.06

### 8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations



## 9 Distance violation analysis [\(i\)](#)

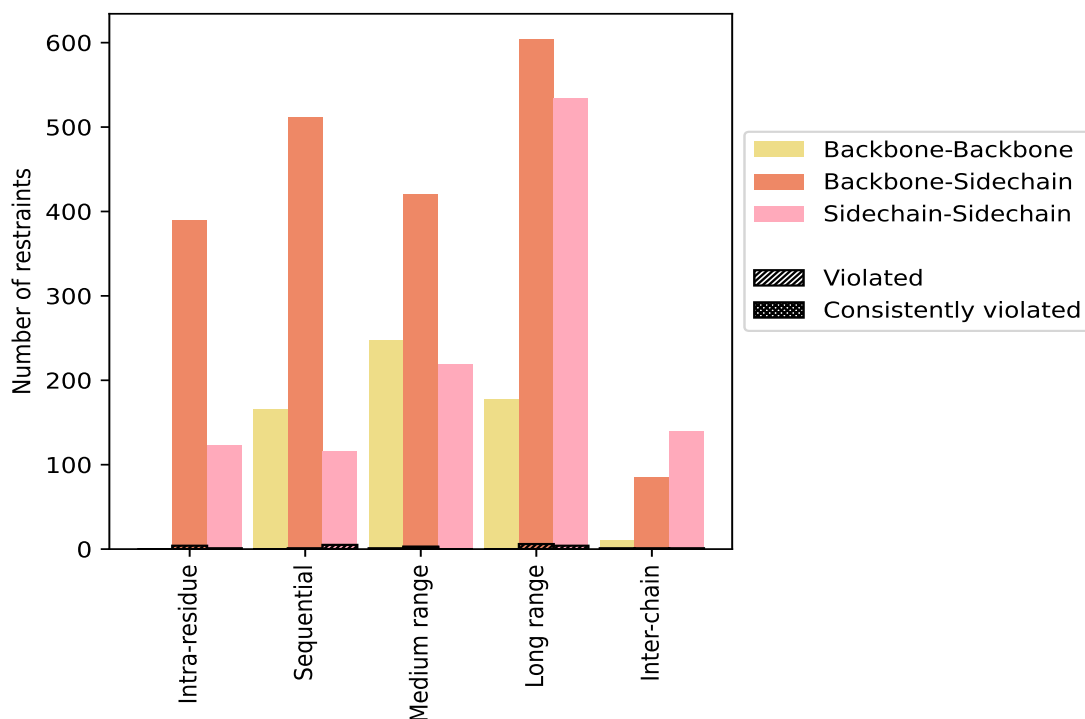
### 9.1 Summary of distance violations [\(i\)](#)

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.

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>514</b>	<b>13.7</b>	<b>5</b>	<b>1.0</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	390	10.4	4	1.0	0.1	0	0.0	0.0
Sidechain-Sidechain	123	3.3	1	0.8	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>793</b>	<b>21.2</b>	<b>6</b>	<b>0.8</b>	<b>0.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	165	4.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	512	13.7	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	116	3.1	5	4.3	0.1	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>844</b>	<b>22.6</b>	<b>3</b>	<b>0.4</b>	<b>0.1</b>	<b>2</b>	<b>0.2</b>	<b>0.1</b>
Backbone-Backbone	205	5.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	420	11.2	3	0.7	0.1	2	0.5	0.1
Sidechain-Sidechain	219	5.9	0	0.0	0.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>1274</b>	<b>34.0</b>	<b>9</b>	<b>0.7</b>	<b>0.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	140	3.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	600	16.0	5	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	534	14.3	4	0.7	0.1	0	0.0	0.0
<b>Inter-chain</b>	<b>232</b>	<b>6.2</b>	<b>3</b>	<b>1.3</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	8	0.2	1	12.5	0.0	0	0.0	0.0
Backbone-Sidechain	85	2.3	1	1.2	0.0	0	0.0	0.0
Sidechain-Sidechain	139	3.7	1	0.7	0.0	0	0.0	0.0
Hydrogen bond	85	2.3	2	2.4	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Total</b>	<b>3742</b>	<b>100.0</b>	<b>28</b>	<b>0.7</b>	<b>0.7</b>	<b>2</b>	<b>0.1</b>	<b>0.1</b>
Backbone-Backbone	600	16.0	2	0.3	0.1	0	0.0	0.0
Backbone-Sidechain	2011	53.7	15	0.7	0.4	2	0.1	0.1
Sidechain-Sidechain	1131	30.2	11	1.0	0.3	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	0	2	2	0	4	1.0	1.91	0.72	0.96
2	0	0	2	2	0	4	0.93	1.96	0.81	0.82
3	0	0	2	3	0	5	0.88	1.92	0.69	0.92
4	0	1	2	2	0	5	0.88	2.06	0.79	0.37
5	0	1	2	0	1	4	1.04	1.95	0.71	1.04
6	0	0	2	1	0	3	1.15	1.99	0.78	1.35
7	0	0	2	2	1	5	0.97	1.89	0.71	1.26
8	0	0	2	0	2	4	0.9	1.93	0.75	0.78
9	0	0	2	1	0	3	1.19	1.94	0.76	1.48
10	0	0	2	4	1	7	0.62	1.91	0.64	0.38
11	0	0	2	0	0	2	1.65	1.88	0.22	1.65

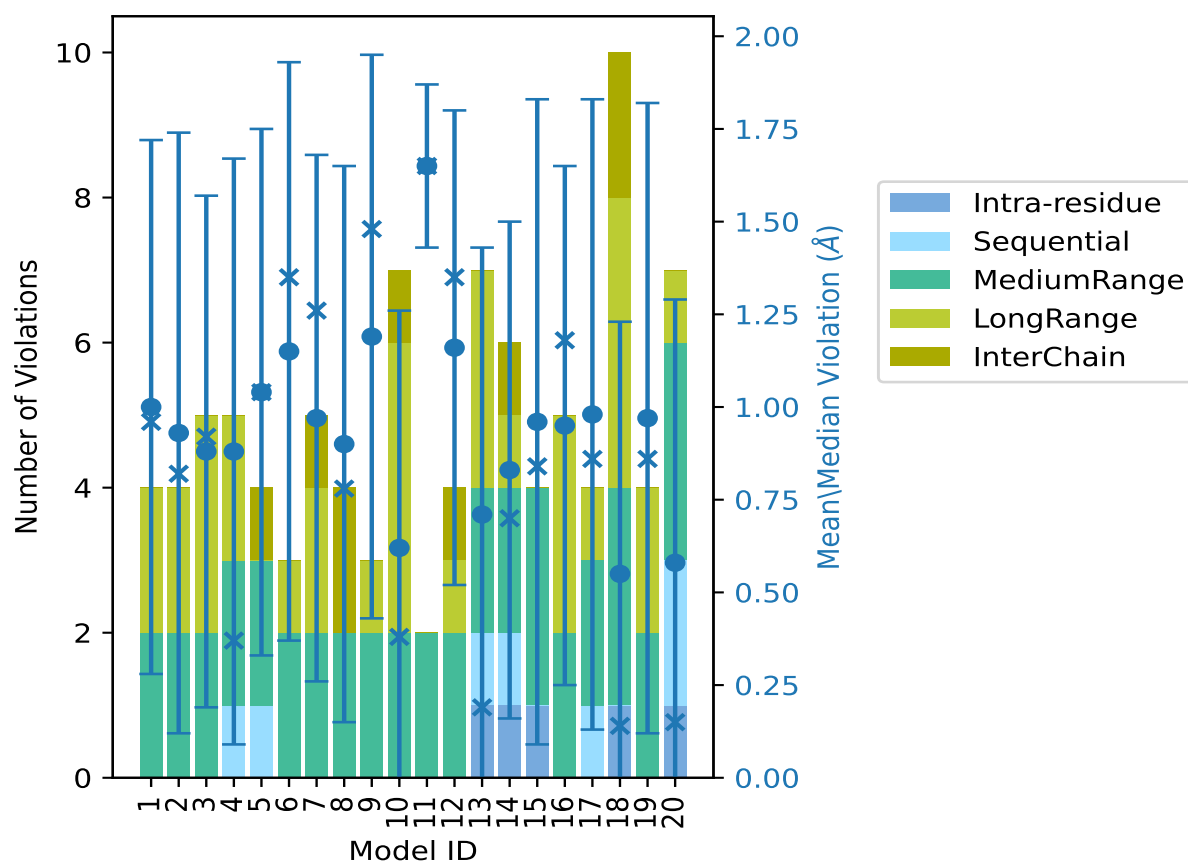
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
12	0	0	2	1	1	4	1.16	1.83	0.64	1.35
13	1	1	2	3	0	7	0.71	2.01	0.72	0.19
14	1	1	2	1	1	6	0.83	1.89	0.67	0.7
15	1	0	3	0	0	4	0.96	2.05	0.87	0.84
16	0	0	2	3	0	5	0.95	1.87	0.7	1.18
17	0	1	2	1	0	4	0.98	2.06	0.85	0.86
18	1	0	3	4	2	10	0.55	1.98	0.68	0.14
19	0	0	2	2	0	4	0.97	2.05	0.85	0.86
20	1	2	3	1	0	7	0.58	1.92	0.71	0.15

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [\(i\)](#)



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

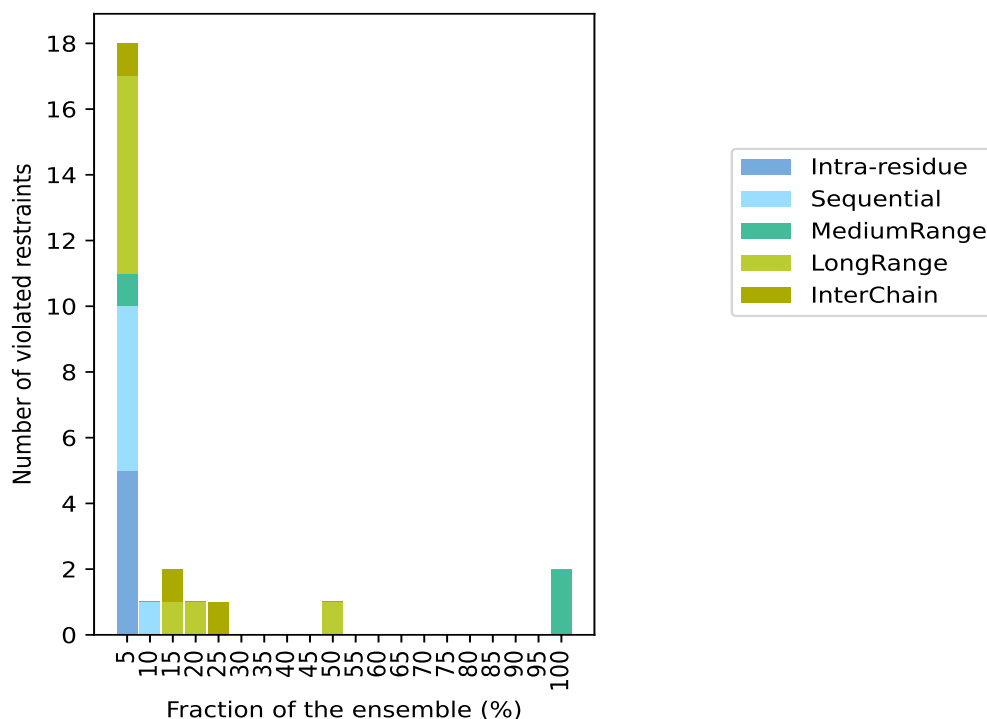
### 9.3 Distance violation statistics for the ensemble

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, 3631(IR:509, SQ:787, MR:841, LR:1265, IC:229) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
5	5	1	6	1	18	1	5.0
0	1	0	0	0	1	2	10.0
0	0	0	1	1	2	3	15.0
0	0	0	1	0	1	4	20.0
0	0	0	0	1	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	1	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	2	0	0	2	20	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

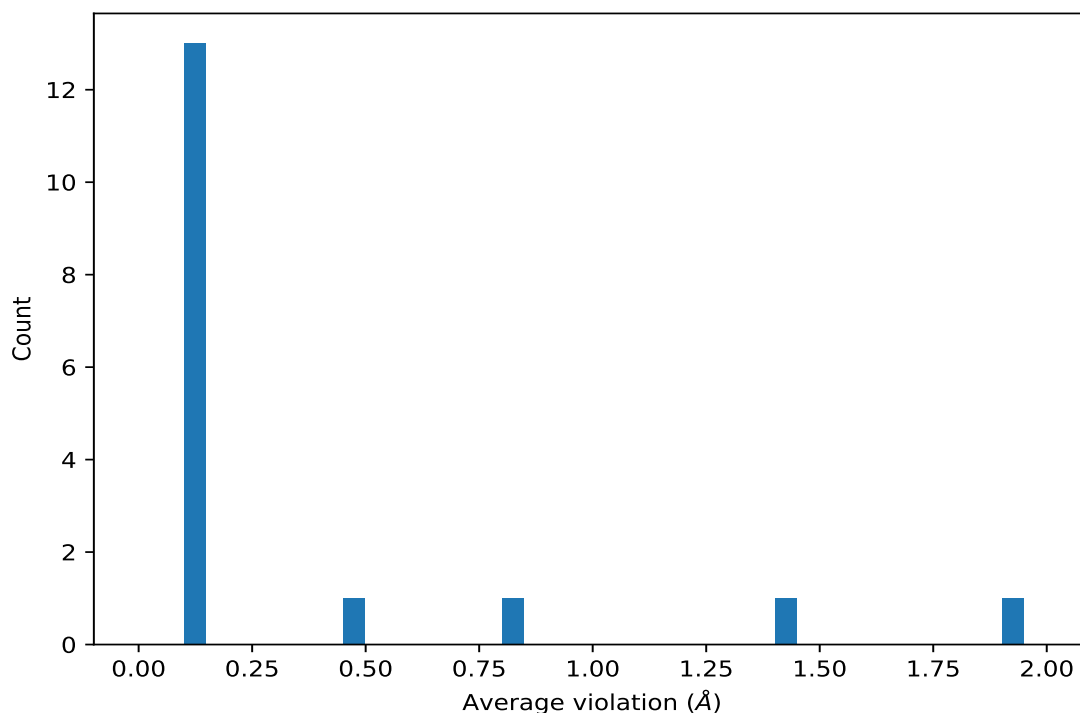
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

The following table provides the mean and the standard deviation of the 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	20	1.95	0.07	1.94
(3,68)	1:A:71:ASP:OD2	1:A:73:GLU:N	20	1.45	0.09	1.46
(3,64)	2:B:211:LYS:NZ	2:B:234:GLU:OE2	10	0.8	0.41	0.88
(3,67)	2:B:236:ILE:O	2:B:241:GLN:HE22	10	0.15	0.02	0.15
(3,88)	1:A:85:GLU:OE1	2:B:242:ARG:NH1	5	0.48	0.3	0.42
(1,746)	2:B:201:MET:HB2	2:B:263:LYS:HG2	4	0.12	0.01	0.12
(1,746)	2:B:201:MET:HB2	2:B:263:LYS:HG3	4	0.12	0.01	0.12
(1,746)	2:B:201:MET:HB3	2:B:263:LYS:HG2	4	0.12	0.01	0.12
(1,746)	2:B:201:MET:HB3	2:B:263:LYS:HG3	4	0.12	0.01	0.12
(1,2830)	1:A:71:ASP:H	2:B:208:LEU:HA	3	0.13	0.01	0.13
(1,739)	2:B:201:MET:HA	2:B:263:LYS:HG2	3	0.12	0.01	0.12
(1,739)	2:B:201:MET:HA	2:B:263:LYS:HG3	3	0.12	0.01	0.12
(1,604)	1:A:94:LYS:HD2	1:A:95:PHE:HD1	2	0.15	0.02	0.15
(1,604)	1:A:94:LYS:HD2	1:A:95:PHE:HD2	2	0.15	0.02	0.15
(1,604)	1:A:94:LYS:HD3	1:A:95:PHE:HD1	2	0.15	0.02	0.15
(1,604)	1:A:94:LYS:HD3	1:A:95:PHE:HD2	2	0.15	0.02	0.15

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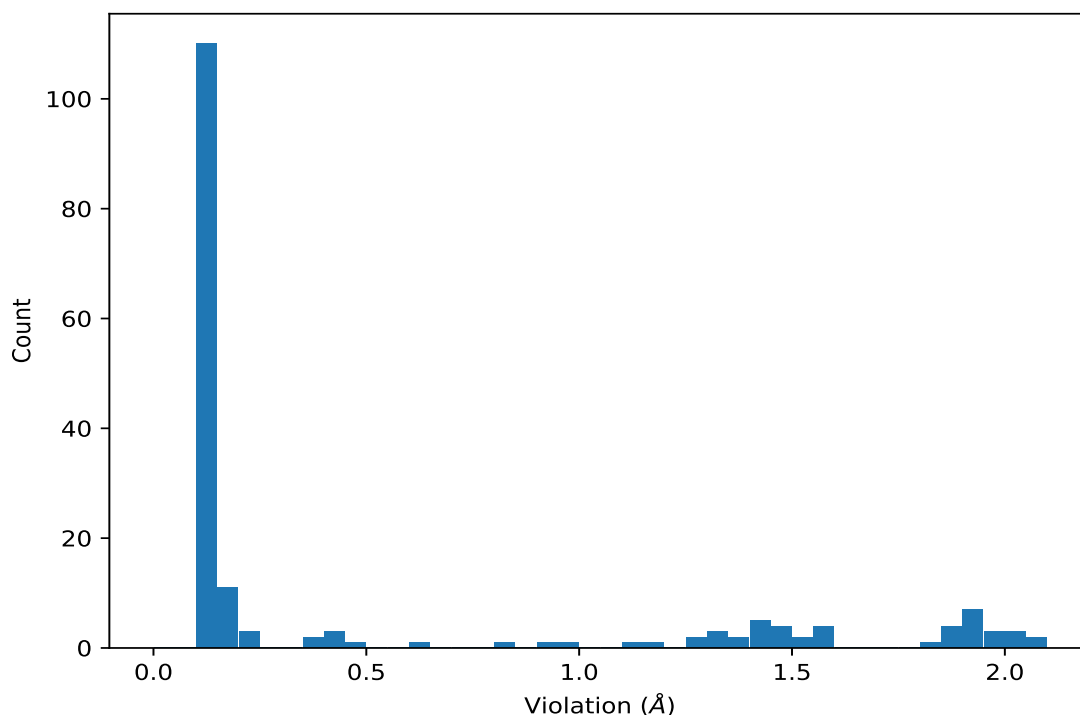
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,58)	2:B:228:ALA:O	2:B:232:ASP:H	2	0.12	0.0	0.12

<sup>1</sup>Number of violated models, <sup>2</sup>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)
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	4	2.06
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	17	2.06
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	15	2.05
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	19	2.05

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<b>Key</b>	<b>Atom-1</b>	<b>Atom-2</b>	<b>Model ID</b>	<b>Violation (Å)</b>
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	13	2.01
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	6	1.99
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	18	1.98
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	2	1.96
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	5	1.95
(3,69)	1:A:71:ASP:OD2	1:A:73:GLU:H	9	1.94



## 10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value