wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2MEJ
BMRB ID	:	19522
Title	:	Solution Structure of the Complex Between BCL-xL and the p53 Core Domain determined with PRE restraints
Authors	:	Viacava Follis, A.; Grace, C.R.; Kriwacki, R.W.
Deposited on	:	2013-09-25

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:

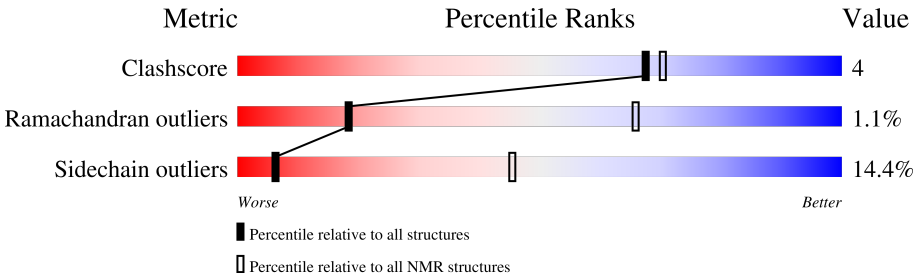
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 20%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	212	52% 16% 32%
2	B	217	76% 14% 10%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:5-A:31, A:86-A:201, B:96-B:290 (338)	0.29	15

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 5 clusters and 8 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3336 atoms, of which 633 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	144	1426	746	258	197	220	5	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q07817
A	2	HIS	-	expression tag	UNP Q07817
A	3	SER	-	expression tag	UNP Q07817

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	195	1909	945	375	285	288	16	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	B	1	1	1

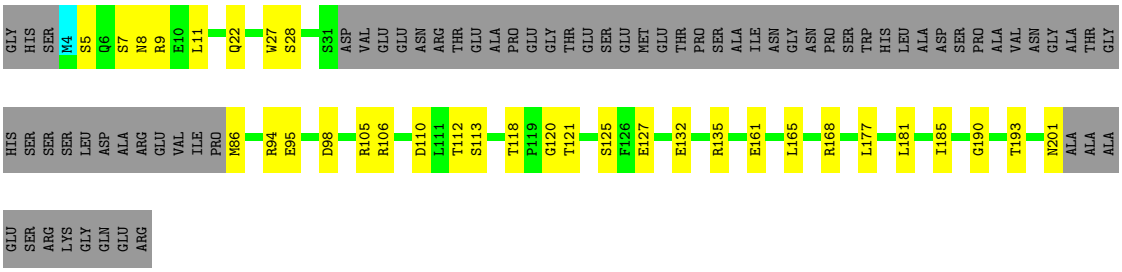
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

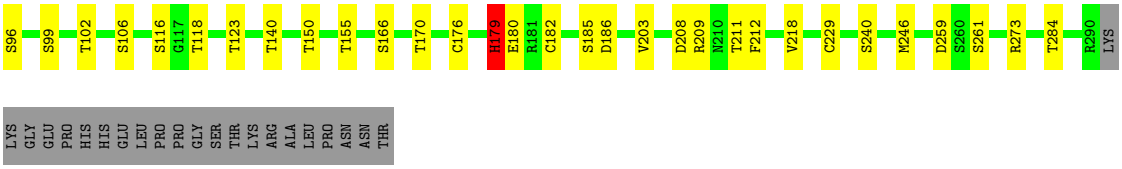
• Molecule 1: Bcl-2-like protein 1

Chain A:



• Molecule 2: Cellular tumor antigen p53

Chain B:

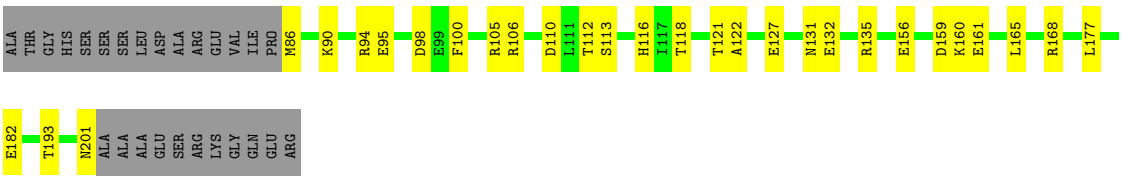


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

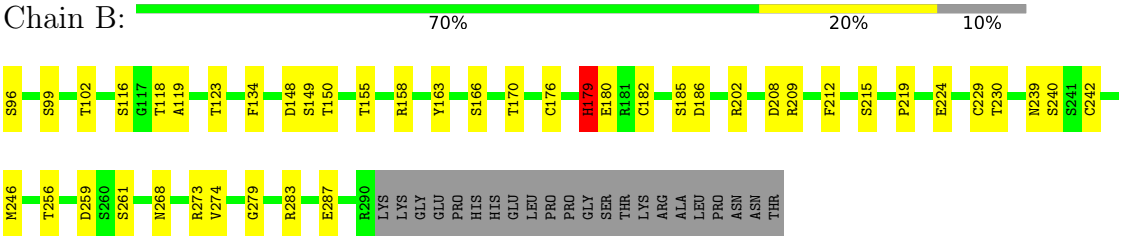
The representative model is number 15. Colouring as in section 4.1 above.

• Molecule 1: Bcl-2-like protein 1

Chain A:



• Molecule 2: Cellular tumor antigen p53



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular 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
HADDOCK	structure solution	
Amber	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	1254
Number of shifts mapped to atoms	762
Number of unparsed shifts	0
Number of shifts with mapping errors	492
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	20%

6 Model quality

6.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.27±0.00	0±0/1188 (0.0± 0.0%)	0.39±0.02	0±0/1607 (0.0± 0.0%)
2	B	0.28±0.00	0±0/1569 (0.0± 0.0%)	0.40±0.00	0±0/2127 (0.0± 0.0%)
All	All	0.27	0/55140 (0.0%)	0.39	2/74680 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	86	MET	N-CA-CB	8.33	125.60	110.60	16	1
1	A	86	MET	N-CA-C	-5.42	96.36	111.00	16	1

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	1160	257	1097	9±2
2	B	1534	375	1496	13±3
3	B	1	0	0	1±1
All	All	53900	12640	51848	414

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 4.

5 of 94 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:176:CYS:SG	3:B:401:ZN:ZN	1.44	1.03	20	19
2:B:176:CYS:HG	3:B:401:ZN:ZN	0.94	0.72	8	8
2:B:240:SER:HA	2:B:246:MET:SD	0.77	2.20	14	20
2:B:155:THR:HG22	2:B:259:ASP:HA	0.73	1.58	20	6
1:A:132:GLU:HA	1:A:135:ARG:HD2	0.71	1.62	1	18

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	140/212 (66%)	122±2 (87±1%)	16±3 (11±2%)	2±1 (2±1%)	14	59
2	B	193/217 (89%)	181±2 (94±1%)	11±2 (5±1%)	1±1 (1±0%)	26	73
All	All	6660/8580 (78%)	6057 (91%)	533 (8%)	70 (1%)	18	66

5 of 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	179	HIS	18
1	A	120	GLY	13
1	A	122	ALA	10
2	B	262	GLY	8
1	A	22	GLN	5

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	122/176 (69%)	101±2 (83±2%)	21±2 (17±2%)	5 40
2	B	175/194 (90%)	153±2 (87±1%)	22±2 (13±1%)	8 50
All	All	5940/7400 (80%)	5086 (86%)	854 (14%)	6 45

5 of 84 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	28	SER	20
1	A	105	ARG	20
1	A	118	THR	20
2	B	155	THR	20
2	B	179	HIS	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 20% for the well-defined parts and 20% 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	1254
Number of shifts mapped to atoms	762
Number of unparsed shifts	0
Number of shifts with mapping errors	492
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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 492) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	HIS	H	7.419	0.020	1
1	A	2	HIS	CA	56.562	0.3	1
1	A	2	HIS	CB	38.023	0.3	1
1	A	2	HIS	N	117.497	0.3	1
1	A	11	LEU	HD11	0.173	0.020	1
1	A	11	LEU	HD12	0.173	0.020	1
1	A	11	LEU	HD13	0.173	0.020	1
1	A	11	LEU	HD21	-0.156	0.020	1
1	A	11	LEU	HD22	-0.156	0.020	1
1	A	11	LEU	HD23	-0.156	0.020	1
1	A	12	VAL	HG11	1.041	0.020	1
1	A	12	VAL	HG12	1.041	0.020	1
1	A	12	VAL	HG13	1.041	0.020	1
1	A	12	VAL	HG21	1.162	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	VAL	HG22	1.162	0.020	1
1	A	12	VAL	HG23	1.162	0.020	1
1	A	13	VAL	HG11	0.875	0.020	1
1	A	13	VAL	HG12	0.875	0.020	1
1	A	13	VAL	HG13	0.875	0.020	1
1	A	13	VAL	HG21	0.854	0.020	1
1	A	13	VAL	HG22	0.854	0.020	1
1	A	13	VAL	HG23	0.854	0.020	1
1	A	16	LEU	HD11	0.868	0.020	1
1	A	16	LEU	HD12	0.868	0.020	1
1	A	16	LEU	HD13	0.868	0.020	1
1	A	16	LEU	HD21	0.845	0.020	1
1	A	16	LEU	HD22	0.845	0.020	1
1	A	16	LEU	HD23	0.845	0.020	1
1	A	20	LEU	HD11	0.756	0.020	1
1	A	20	LEU	HD12	0.756	0.020	1
1	A	20	LEU	HD13	0.756	0.020	1
1	A	20	LEU	HD21	0.706	0.020	1
1	A	20	LEU	HD22	0.706	0.020	1
1	A	20	LEU	HD23	0.706	0.020	1
1	A	32	ASP	H	8.223	0.020	1
1	A	32	ASP	C	175.938	0.3	1
1	A	32	ASP	CA	53.446	0.3	1
1	A	32	ASP	CB	39.701	0.3	1
1	A	32	ASP	N	122.131	0.3	1
1	A	33	VAL	H	7.813	0.020	1
1	A	33	VAL	HG11	0.833	0.020	1
1	A	33	VAL	HG12	0.833	0.020	1
1	A	33	VAL	HG13	0.833	0.020	1
1	A	33	VAL	HG21	0.844	0.020	1
1	A	33	VAL	HG22	0.844	0.020	1
1	A	33	VAL	HG23	0.844	0.020	1
1	A	33	VAL	C	176.001	0.3	1
1	A	33	VAL	CA	61.574	0.3	1
1	A	33	VAL	CB	31.31	0.3	1
1	A	33	VAL	CG1	19.971	0.3	1
1	A	33	VAL	CG2	20.651	0.3	1
1	A	33	VAL	N	118.703	0.3	1
1	A	34	GLU	H	8.295	0.020	1
1	A	34	GLU	C	176.34	0.3	1
1	A	34	GLU	CA	55.523	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	34	GLU	CB	28.993	0.3	1
1	A	34	GLU	N	123.764	0.3	1
1	A	35	GLU	H	8.017	0.020	1
1	A	35	GLU	C	175.838	0.3	1
1	A	35	GLU	CA	56.163	0.3	1
1	A	35	GLU	CB	28.913	0.3	1
1	A	35	GLU	N	121.359	0.3	1
1	A	36	ASN	H	8.355	0.020	1
1	A	36	ASN	C	174.719	0.3	1
1	A	36	ASN	CA	52.704	0.3	1
1	A	36	ASN	CB	37.68	0.3	1
1	A	36	ASN	N	119.106	0.3	1
1	A	37	ARG	H	8.202	0.020	1
1	A	37	ARG	C	176.158	0.3	1
1	A	37	ARG	CA	55.261	0.3	1
1	A	37	ARG	CB	29.29	0.3	1
1	A	37	ARG	N	121.744	0.3	1
1	A	38	THR	H	8.165	0.020	1
1	A	38	THR	C	174.12	0.3	1
1	A	38	THR	CA	61.254	0.3	1
1	A	38	THR	CB	68.686	0.3	1
1	A	38	THR	N	115.798	0.3	1
1	A	39	GLU	H	8.286	0.020	1
1	A	39	GLU	C	175.359	0.3	1
1	A	39	GLU	CA	55.341	0.3	1
1	A	39	GLU	CB	29.05	0.3	1
1	A	39	GLU	N	123.018	0.3	1
1	A	40	ALA	H	8.266	0.020	1
1	A	40	ALA	CA	49.587	0.3	1
1	A	40	ALA	CB	16.824	0.3	1
1	A	40	ALA	N	126.206	0.3	1
1	A	42	GLU	H	8.449	0.020	1
1	A	42	GLU	C	176.857	0.3	1
1	A	42	GLU	CA	56.322	0.3	1
1	A	42	GLU	CB	29.233	0.3	1
1	A	42	GLU	N	121.227	0.3	1
1	A	43	GLY	H	8.404	0.020	1
1	A	43	GLY	C	174.18	0.3	1
1	A	43	GLY	CA	44.496	0.3	1
1	A	43	GLY	N	110.018	0.3	1
1	A	44	THR	H	7.96	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	44	THR	C	174.599	0.3	1
1	A	44	THR	CA	61.174	0.3	1
1	A	44	THR	CB	68.766	0.3	1
1	A	44	THR	N	113.043	0.3	1
1	A	45	GLU	H	8.52	0.020	1
1	A	45	GLU	C	177.119	0.3	1
1	A	45	GLU	CA	56.915	0.3	1
1	A	45	GLU	CB	28.571	0.3	1
1	A	45	GLU	N	122.967	0.3	1
1	A	46	SER	H	8.044	0.020	1
1	A	46	SER	C	176.105	0.3	1
1	A	46	SER	CA	58.24	0.3	1
1	A	46	SER	CB	62.236	0.3	1
1	A	46	SER	N	115.037	0.3	1
1	A	47	GLU	H	8.455	0.020	1
1	A	47	GLU	C	177.319	0.3	1
1	A	47	GLU	CA	56.882	0.3	1
1	A	47	GLU	CB	27.155	0.3	1
1	A	47	GLU	N	122.848	0.3	1
1	A	48	MET	H	8.112	0.020	1
1	A	48	MET	C	176.28	0.3	1
1	A	48	MET	CA	55.204	0.3	1
1	A	48	MET	CB	28.993	0.3	1
1	A	48	MET	N	119.852	0.3	1
1	A	49	GLU	H	8.313	0.020	1
1	A	49	GLU	C	175.978	0.3	1
1	A	49	GLU	CA	55.843	0.3	1
1	A	49	GLU	CB	28.97	0.3	1
1	A	49	GLU	N	121.577	0.3	1
1	A	50	THR	H	8.15	0.020	1
1	A	50	THR	CA	58.959	0.3	1
1	A	50	THR	CB	68.606	0.3	1
1	A	50	THR	N	117.663	0.3	1
1	A	52	SER	H	8.273	0.020	1
1	A	52	SER	C	174.2	0.3	1
1	A	52	SER	CA	57.818	0.3	1
1	A	52	SER	CB	62.613	0.3	1
1	A	52	SER	N	115.578	0.3	1
1	A	53	ALA	H	8.198	0.020	1
1	A	53	ALA	C	177.676	0.3	1
1	A	53	ALA	CA	51.665	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	ALA	CB	17.783	0.3	1
1	A	53	ALA	N	125.481	0.3	1
1	A	54	ILE	H	7.934	0.020	1
1	A	54	ILE	HD11	0.808	0.020	1
1	A	54	ILE	HD12	0.808	0.020	1
1	A	54	ILE	HD13	0.808	0.020	1
1	A	54	ILE	C	174.277	0.3	1
1	A	54	ILE	CA	61.494	0.3	1
1	A	54	ILE	CB	37.304	0.3	1
1	A	54	ILE	CD1	12.363	0.3	1
1	A	54	ILE	N	118.586	0.3	1
1	A	55	ASN	H	8.34	0.020	1
1	A	55	ASN	C	175.159	0.3	1
1	A	55	ASN	CA	52.646	0.3	1
1	A	55	ASN	CB	37.783	0.3	1
1	A	55	ASN	N	121.388	0.3	1
1	A	56	GLY	H	8.135	0.020	1
1	A	56	GLY	C	173.083	0.3	1
1	A	56	GLY	CA	44.393	0.3	1
1	A	56	GLY	N	108.575	0.3	1
1	A	57	ASN	H	8.023	0.020	1
1	A	57	ASN	CA	58.115	0.3	1
1	A	57	ASN	CB	37.828	0.3	1
1	A	57	ASN	N	118.964	0.3	1
1	A	59	SER	H	8.196	0.020	1
1	A	59	SER	C	174.182	0.3	1
1	A	59	SER	CA	58.217	0.3	1
1	A	59	SER	CB	62.133	0.3	1
1	A	59	SER	N	114.72	0.3	1
1	A	60	TRP	H	7.739	0.020	1
1	A	60	TRP	HE1	10.044	0.020	1
1	A	60	TRP	C	177.557	0.3	1
1	A	60	TRP	CA	56.482	0.3	1
1	A	60	TRP	CB	28.274	0.3	1
1	A	60	TRP	N	121.715	0.3	1
1	A	60	TRP	NE1	129.191	0.3	1
1	A	61	HIS	H	7.861	0.020	1
1	A	61	HIS	C	177.557	0.3	1
1	A	61	HIS	CA	56.379	0.3	1
1	A	61	HIS	CB	30.032	0.3	1
1	A	61	HIS	N	126.423	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	62	LEU	H	7.807	0.020	1
1	A	62	LEU	HD11	0.774	0.020	1
1	A	62	LEU	HD12	0.774	0.020	1
1	A	62	LEU	HD13	0.774	0.020	1
1	A	62	LEU	C	176.717	0.3	1
1	A	62	LEU	CA	53.982	0.3	1
1	A	62	LEU	CB	40.477	0.3	1
1	A	62	LEU	CD1	23.127	0.3	1
1	A	62	LEU	N	122.945	0.3	1
1	A	63	ALA	H	8.086	0.020	1
1	A	63	ALA	C	179.954	0.3	1
1	A	63	ALA	CA	51.448	0.3	1
1	A	63	ALA	CB	17.383	0.3	1
1	A	63	ALA	N	123.85	0.3	1
1	A	64	ASP	H	8.1	0.020	1
1	A	64	ASP	C	175.601	0.3	1
1	A	64	ASP	CA	53.366	0.3	1
1	A	64	ASP	CB	39.941	0.3	1
1	A	64	ASP	N	118.641	0.3	1
1	A	65	SER	H	7.99	0.020	1
1	A	65	SER	CA	55.443	0.3	1
1	A	65	SER	CB	62.396	0.3	1
1	A	65	SER	N	116.272	0.3	1
1	A	67	ALA	H	8.169	0.020	1
1	A	67	ALA	C	175.914	0.3	1
1	A	67	ALA	CA	51.528	0.3	1
1	A	67	ALA	CB	17.566	0.3	1
1	A	67	ALA	N	123.345	0.3	1
1	A	68	VAL	H	7.909	0.020	1
1	A	68	VAL	HG11	0.857	0.020	1
1	A	68	VAL	HG12	0.857	0.020	1
1	A	68	VAL	HG13	0.857	0.020	1
1	A	68	VAL	CA	61.037	0.3	1
1	A	68	VAL	CB	31.31	0.3	1
1	A	68	VAL	CG1	20.825	0.3	1
1	A	68	VAL	N	118.753	0.3	1
1	A	69	ASN	H	8.369	0.020	1
1	A	69	ASN	C	175.399	0.3	1
1	A	69	ASN	CA	52.726	0.3	1
1	A	69	ASN	CB	37.783	0.3	1
1	A	69	ASN	N	121.462	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	70	GLY	H	8.248	0.020	1
1	A	70	GLY	C	177.057	0.3	1
1	A	70	GLY	CA	44.553	0.3	1
1	A	70	GLY	N	109.223	0.3	1
1	A	71	ALA	H	8.065	0.020	1
1	A	71	ALA	C	175.459	0.3	1
1	A	71	ALA	CA	51.767	0.3	1
1	A	71	ALA	CB	17.543	0.3	1
1	A	71	ALA	N	123.297	0.3	1
1	A	72	THR	H	8.024	0.020	1
1	A	72	THR	C	174.999	0.3	1
1	A	72	THR	CA	61.094	0.3	1
1	A	72	THR	CB	68.766	0.3	1
1	A	72	THR	N	112.143	0.3	1
1	A	73	GLY	H	8.227	0.020	1
1	A	73	GLY	C	177.297	0.3	1
1	A	73	GLY	CA	44.473	0.3	1
1	A	73	GLY	N	110.366	0.3	1
1	A	74	HIS	H	7.853	0.020	1
1	A	74	HIS	C	177.414	0.3	1
1	A	74	HIS	CA	58.006	0.3	1
1	A	74	HIS	CB	27.155	0.3	1
1	A	74	HIS	N	117.513	0.3	1
1	A	75	SER	H	8.169	0.020	1
1	A	75	SER	C	175.832	0.3	1
1	A	75	SER	CA	60.514	0.3	1
1	A	75	SER	CB	62.156	0.3	1
1	A	75	SER	N	116.418	0.3	1
1	A	76	SER	H	8.253	0.020	1
1	A	76	SER	C	176.36	0.3	1
1	A	76	SER	CA	60.398	0.3	1
1	A	76	SER	CB	61.676	0.3	1
1	A	76	SER	N	117.428	0.3	1
1	A	77	SER	H	8.24	0.020	1
1	A	77	SER	C	174.42	0.3	1
1	A	77	SER	CA	58.16	0.3	1
1	A	77	SER	CB	62.156	0.3	1
1	A	77	SER	N	116.656	0.3	1
1	A	78	LEU	H	8.125	0.020	1
1	A	78	LEU	HD11	0.785	0.020	1
1	A	78	LEU	HD12	0.785	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	78	LEU	HD13	0.785	0.020	1
1	A	78	LEU	C	176.96	0.3	1
1	A	78	LEU	CA	54.484	0.3	1
1	A	78	LEU	CB	40.877	0.3	1
1	A	78	LEU	CD1	22.937	0.3	1
1	A	78	LEU	N	123.323	0.3	1
1	A	79	ASP	H	8.08	0.020	1
1	A	79	ASP	C	175.698	0.3	1
1	A	79	ASP	CA	53.685	0.3	1
1	A	79	ASP	CB	40.26	0.3	1
1	A	79	ASP	N	120.229	0.3	1
1	A	80	ALA	H	8.021	0.020	1
1	A	80	ALA	C	174.24	0.3	1
1	A	80	ALA	CA	51.745	0.3	1
1	A	80	ALA	CB	17.783	0.3	1
1	A	80	ALA	N	124.162	0.3	1
1	A	81	ARG	H	7.988	0.020	1
1	A	81	ARG	C	175.961	0.3	1
1	A	81	ARG	CA	60.398	0.3	1
1	A	81	ARG	CB	31.39	0.3	1
1	A	81	ARG	N	119.064	0.3	1
1	A	82	GLU	H	8.269	0.020	1
1	A	82	GLU	C	175.858	0.3	1
1	A	82	GLU	CA	55.843	0.3	1
1	A	82	GLU	CB	28.993	0.3	1
1	A	82	GLU	N	121.381	0.3	1
1	A	83	VAL	H	8.664	0.020	1
1	A	83	VAL	HG11	0.831	0.020	1
1	A	83	VAL	HG12	0.831	0.020	1
1	A	83	VAL	HG13	0.831	0.020	1
1	A	83	VAL	HG21	0.889	0.020	1
1	A	83	VAL	HG22	0.889	0.020	1
1	A	83	VAL	HG23	0.889	0.020	1
1	A	83	VAL	C	176.34	0.3	1
1	A	83	VAL	CA	61.197	0.3	1
1	A	83	VAL	CB	29.392	0.3	1
1	A	83	VAL	CG1	20.844	0.3	1
1	A	83	VAL	CG2	20.263	0.3	1
1	A	83	VAL	N	122.576	0.3	1
1	A	84	ILE	H	8.282	0.020	1
1	A	84	ILE	HD11	0.785	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	84	ILE	HD12	0.785	0.020	1
1	A	84	ILE	HD13	0.785	0.020	1
1	A	84	ILE	CA	57.738	0.3	1
1	A	84	ILE	CB	37.121	0.3	1
1	A	84	ILE	CD1	12.48	0.3	1
1	A	84	ILE	N	125.51	0.3	1
1	A	89	VAL	HG11	0.274	0.020	1
1	A	89	VAL	HG12	0.274	0.020	1
1	A	89	VAL	HG13	0.274	0.020	1
1	A	89	VAL	HG21	0.471	0.020	1
1	A	89	VAL	HG22	0.471	0.020	1
1	A	89	VAL	HG23	0.471	0.020	1
1	A	93	LEU	HD11	-0.423	0.020	1
1	A	93	LEU	HD12	-0.423	0.020	1
1	A	93	LEU	HD13	-0.423	0.020	1
1	A	93	LEU	HD21	0.099	0.020	1
1	A	93	LEU	HD22	0.099	0.020	1
1	A	93	LEU	HD23	0.099	0.020	1
1	A	102	LEU	HD11	0.83	0.020	1
1	A	102	LEU	HD12	0.83	0.020	1
1	A	102	LEU	HD13	0.83	0.020	1
1	A	102	LEU	HD21	0.539	0.020	1
1	A	102	LEU	HD22	0.539	0.020	1
1	A	102	LEU	HD23	0.539	0.020	1
1	A	111	LEU	HD11	0.582	0.020	1
1	A	111	LEU	HD12	0.582	0.020	1
1	A	111	LEU	HD13	0.582	0.020	1
1	A	111	LEU	HD21	0.533	0.020	1
1	A	111	LEU	HD22	0.533	0.020	1
1	A	111	LEU	HD23	0.533	0.020	1
1	A	115	LEU	HD11	0.505	0.020	1
1	A	115	LEU	HD12	0.505	0.020	1
1	A	115	LEU	HD13	0.505	0.020	1
1	A	115	LEU	HD21	0.855	0.020	1
1	A	115	LEU	HD22	0.855	0.020	1
1	A	115	LEU	HD23	0.855	0.020	1
1	A	117	ILE	HD11	0.863	0.020	1
1	A	117	ILE	HD12	0.863	0.020	1
1	A	117	ILE	HD13	0.863	0.020	1
1	A	129	VAL	HG11	0.938	0.020	1
1	A	129	VAL	HG12	0.938	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	129	VAL	HG13	0.938	0.020	1
1	A	129	VAL	HG21	0.962	0.020	1
1	A	129	VAL	HG22	0.962	0.020	1
1	A	129	VAL	HG23	0.962	0.020	1
1	A	130	VAL	HG11	0.07	0.020	1
1	A	130	VAL	HG12	0.07	0.020	1
1	A	130	VAL	HG13	0.07	0.020	1
1	A	130	VAL	HG21	-0.083	0.020	1
1	A	130	VAL	HG22	-0.083	0.020	1
1	A	130	VAL	HG23	-0.083	0.020	1
1	A	133	LEU	HD11	0.448	0.020	1
1	A	133	LEU	HD12	0.448	0.020	1
1	A	133	LEU	HD13	0.448	0.020	1
1	A	133	LEU	HD21	0.35	0.020	1
1	A	133	LEU	HD22	0.35	0.020	1
1	A	133	LEU	HD23	0.35	0.020	1
1	A	138	VAL	HG11	0.282	0.020	1
1	A	138	VAL	HG12	0.282	0.020	1
1	A	138	VAL	HG13	0.282	0.020	1
1	A	138	VAL	HG21	-0.747	0.020	1
1	A	138	VAL	HG22	-0.747	0.020	1
1	A	138	VAL	HG23	-0.747	0.020	1
1	A	143	ILE	HD11	0.234	0.020	1
1	A	143	ILE	HD12	0.234	0.020	1
1	A	143	ILE	HD13	0.234	0.020	1
1	A	144	VAL	HG11	1.046	0.020	1
1	A	144	VAL	HG12	1.046	0.020	1
1	A	144	VAL	HG13	1.046	0.020	1
1	A	144	VAL	HG21	0.788	0.020	1
1	A	144	VAL	HG22	0.788	0.020	1
1	A	144	VAL	HG23	0.788	0.020	1
1	A	153	LEU	HD11	0.822	0.020	1
1	A	153	LEU	HD12	0.822	0.020	1
1	A	153	LEU	HD13	0.822	0.020	1
1	A	153	LEU	HD21	0.789	0.020	1
1	A	153	LEU	HD22	0.789	0.020	1
1	A	153	LEU	HD23	0.789	0.020	1
1	A	155	VAL	HG11	0.945	0.020	1
1	A	155	VAL	HG12	0.945	0.020	1
1	A	155	VAL	HG13	0.945	0.020	1
1	A	155	VAL	HG21	0.976	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	155	VAL	HG22	0.976	0.020	1
1	A	155	VAL	HG23	0.976	0.020	1
1	A	158	VAL	HG11	0.124	0.020	1
1	A	158	VAL	HG12	0.124	0.020	1
1	A	158	VAL	HG13	0.124	0.020	1
1	A	158	VAL	HG21	0.349	0.020	1
1	A	158	VAL	HG22	0.349	0.020	1
1	A	158	VAL	HG23	0.349	0.020	1
1	A	164	VAL	HG11	0.82	0.020	1
1	A	164	VAL	HG12	0.82	0.020	1
1	A	164	VAL	HG13	0.82	0.020	1
1	A	164	VAL	HG21	0.843	0.020	1
1	A	164	VAL	HG22	0.843	0.020	1
1	A	164	VAL	HG23	0.843	0.020	1
1	A	165	LEU	HD11	0.607	0.020	1
1	A	165	LEU	HD12	0.607	0.020	1
1	A	165	LEU	HD13	0.607	0.020	1
1	A	165	LEU	HD21	0.658	0.020	1
1	A	165	LEU	HD22	0.658	0.020	1
1	A	165	LEU	HD23	0.658	0.020	1
1	A	166	VAL	HG11	0.233	0.020	1
1	A	166	VAL	HG12	0.233	0.020	1
1	A	166	VAL	HG13	0.233	0.020	1
1	A	166	VAL	HG21	0.43	0.020	1
1	A	166	VAL	HG22	0.43	0.020	1
1	A	166	VAL	HG23	0.43	0.020	1
1	A	169	ILE	HD11	0.45	0.020	1
1	A	169	ILE	HD12	0.45	0.020	1
1	A	169	ILE	HD13	0.45	0.020	1
1	A	177	LEU	HD11	1.09	0.020	1
1	A	177	LEU	HD12	1.09	0.020	1
1	A	177	LEU	HD13	1.09	0.020	1
1	A	177	LEU	HD21	1.077	0.020	1
1	A	177	LEU	HD22	1.077	0.020	1
1	A	177	LEU	HD23	1.077	0.020	1
1	A	181	LEU	HD11	-0.304	0.020	1
1	A	181	LEU	HD12	-0.304	0.020	1
1	A	181	LEU	HD13	-0.304	0.020	1
1	A	181	LEU	HD21	0.193	0.020	1
1	A	181	LEU	HD22	0.193	0.020	1
1	A	181	LEU	HD23	0.193	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	185	ILE	HD11	0.504	0.020	1
1	A	185	ILE	HD12	0.504	0.020	1
1	A	185	ILE	HD13	0.504	0.020	1
1	A	195	VAL	HG11	0.842	0.020	1
1	A	195	VAL	HG12	0.842	0.020	1
1	A	195	VAL	HG13	0.842	0.020	1
1	A	195	VAL	HG21	1.055	0.020	1
1	A	195	VAL	HG22	1.055	0.020	1
1	A	195	VAL	HG23	1.055	0.020	1
1	A	197	LEU	HD11	0.813	0.020	1
1	A	197	LEU	HD12	0.813	0.020	1
1	A	197	LEU	HD13	0.813	0.020	1
1	A	197	LEU	HD21	0.848	0.020	1
1	A	197	LEU	HD22	0.848	0.020	1
1	A	197	LEU	HD23	0.848	0.020	1
1	A	202	ALA	H	8.096	0.020	1
1	A	202	ALA	C	178.056	0.3	1
1	A	202	ALA	CA	52.384	0.3	1
1	A	202	ALA	CB	17.543	0.3	1
1	A	202	ALA	N	123.312	0.3	1
1	A	203	ALA	H	8.048	0.020	1
1	A	203	ALA	C	178.056	0.3	1
1	A	203	ALA	CA	52.224	0.3	1
1	A	203	ALA	CB	17.303	0.3	1
1	A	203	ALA	N	121.596	0.3	1
1	A	204	ALA	H	7.948	0.020	1
1	A	204	ALA	C	178.516	0.3	1
1	A	204	ALA	CA	52.384	0.3	1
1	A	204	ALA	CB	17.303	0.3	1
1	A	204	ALA	N	122.138	0.3	1
1	A	205	GLU	H	8.204	0.020	1
1	A	205	GLU	C	177.137	0.3	1
1	A	205	GLU	CA	56.699	0.3	1
1	A	205	GLU	CB	28.411	0.3	1
1	A	205	GLU	N	118.578	0.3	1
1	A	206	SER	H	8.045	0.020	1
1	A	206	SER	C	174.719	0.3	1
1	A	206	SER	CA	58.377	0.3	1
1	A	206	SER	CB	62.373	0.3	1
1	A	206	SER	N	115.312	0.3	1
1	A	207	ARG	H	7.999	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	207	ARG	C	175.978	0.3	1
1	A	207	ARG	CA	55.74	0.3	1
1	A	207	ARG	CB	28.571	0.3	1
1	A	207	ARG	N	121.799	0.3	1
1	A	208	LYS	H	8.164	0.020	1
1	A	208	LYS	C	177.157	0.3	1
1	A	208	LYS	CA	56.22	0.3	1
1	A	208	LYS	CB	31.128	0.3	1
1	A	208	LYS	N	121.165	0.3	1
1	A	209	GLY	H	8.342	0.020	1
1	A	209	GLY	C	173.9	0.3	1
1	A	209	GLY	CA	44.553	0.3	1
1	A	209	GLY	N	109.505	0.3	1
1	A	210	GLN	H	8.06	0.020	1
1	A	210	GLN	C	176.877	0.3	1
1	A	210	GLN	CA	55.101	0.3	1
1	A	210	GLN	CB	28.011	0.3	1
1	A	210	GLN	N	119.207	0.3	1
1	A	211	GLU	H	8.517	0.020	1
1	A	211	GLU	C	175.741	0.3	1
1	A	211	GLU	CA	56.3	0.3	1
1	A	211	GLU	CB	28.913	0.3	1
1	A	211	GLU	N	121.15	0.3	1
1	A	212	ARG	H	8.397	0.020	1
1	A	212	ARG	CA	55.9	0.3	1
1	A	212	ARG	CB	29.05	0.3	1
1	A	212	ARG	N	122.133	0.3	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
$^{13}C_{\alpha}$	203	0.10 ± 0.37	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	188	1.75 ± 0.11	Should be checked
$^{13}C'$	192	-0.18 ± 0.22	None needed (< 0.5 ppm)
^{15}N	203	1.06 ± 0.23	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 20%, i.e. 918 atoms were assigned a chemical shift out of a possible 4589. 0 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	561/1681 (33%)	141/683 (21%)	279/676 (41%)	141/322 (44%)
Sidechain	347/2497 (14%)	162/1617 (10%)	185/761 (24%)	0/119 (0%)
Aromatic	10/411 (2%)	5/203 (2%)	0/193 (0%)	5/15 (33%)
Overall	918/4589 (20%)	308/2503 (12%)	464/1630 (28%)	146/456 (32%)

7.1.4 Statistically unusual chemical shifts

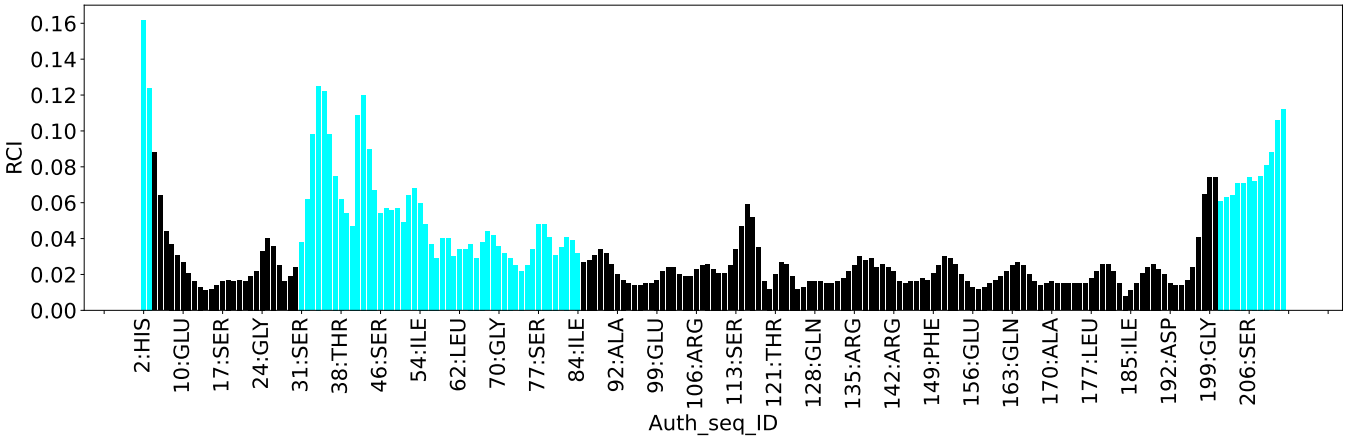
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	138	VAL	HG21	-0.75	-0.58 – 2.19	-5.6
1	A	138	VAL	HG22	-0.75	-0.58 – 2.19	-5.6
1	A	138	VAL	HG23	-0.75	-0.58 – 2.19	-5.6

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
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
2:HIS
10:GLU
17:SER
24:GLY
31:SER
38:THR
46:SER
54:ILE
62:LEU
70:GLY
77:SER
84:ILE
92:ALA
99:GLU
106:ARG
113:SER
121:THR
128:GLN
135:ARG
142:ARG
149:PHE
156:GLU
163:GLN
170:ALA
177:LEU
185:ILE
192:ASP
199:GLY
206:SER
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	241
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	0
Medium range (|i-j|>1 and |i-j|<5)	0
Long range (|i-j|≥5)	0
Inter-chain	235
Hydrogen bond restraints	0
Disulfide bond restraints	6
Total dihedral-angle restraints	0
Number of unmapped restraints	1
Number of restraints per residue	0.6
Number of long range restraints per residue[1]	0.0

[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)	0.9	0.2
0.2-0.5 (Medium)	3.2	0.5
>0.5 (Large)	6.8	4.72

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

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

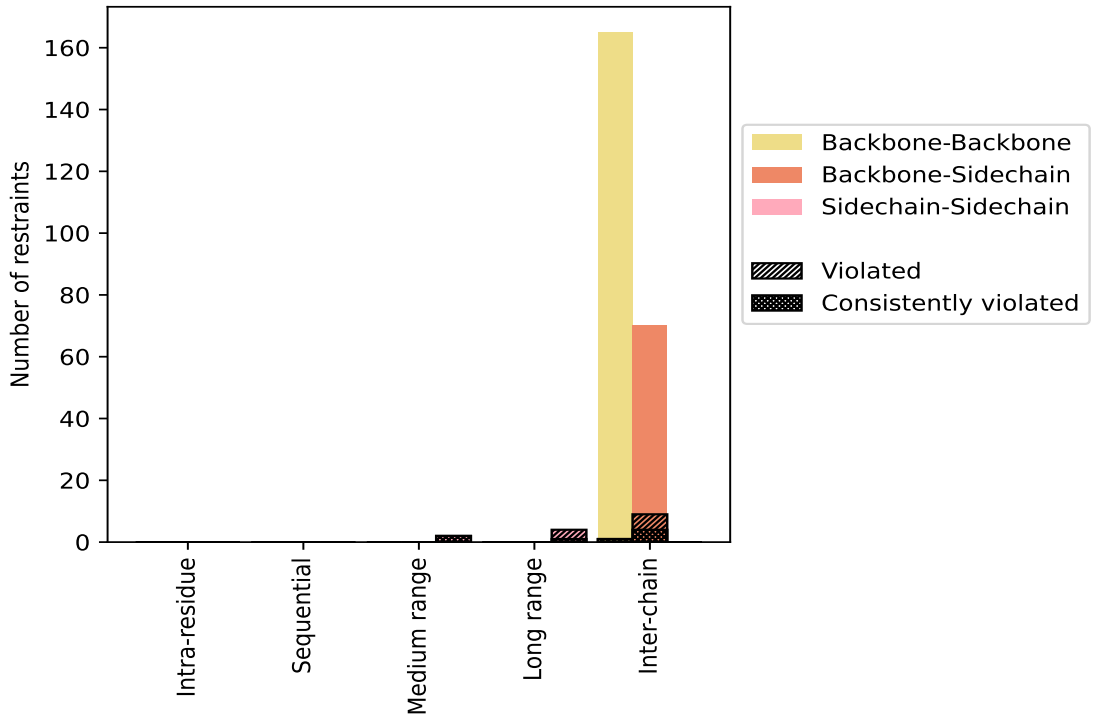
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	235	97.5	10	4.3	4.1	5	2.1	2.1
Backbone-Backbone	165	68.5	1	0.6	0.4	1	0.6	0.4
Backbone-Sidechain	70	29.0	9	12.9	3.7	4	5.7	1.7
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	6	2.5	6	100.0	2.5	3	50.0	1.2
Total	241	100.0	16	6.6	6.6	8	3.3	3.3
Backbone-Backbone	165	68.5	1	0.6	0.4	1	0.6	0.4
Backbone-Sidechain	70	29.0	9	12.9	3.7	4	5.7	1.7
Sidechain-Sidechain	6	2.5	6	100.0	2.5	3	50.0	1.2

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	2	2	6	10	1.4	3.75	1.21	0.76
2	0	0	2	2	7	11	1.51	4.24	1.44	0.74
3	0	0	2	2	7	11	1.43	3.81	1.37	0.66
4	0	0	2	2	7	11	1.46	3.81	1.35	0.88
5	0	0	2	2	7	11	1.36	3.83	1.24	0.78
6	0	0	2	2	8	12	1.42	4.13	1.44	0.7
7	0	0	2	2	8	12	1.27	3.64	1.22	0.7
8	0	0	2	2	6	10	1.58	4.72	1.54	0.69
9	0	0	2	3	7	12	1.24	3.88	1.29	0.48
10	0	0	2	2	6	10	1.49	3.75	1.29	0.73
11	0	0	2	2	6	10	1.49	3.73	1.34	0.9

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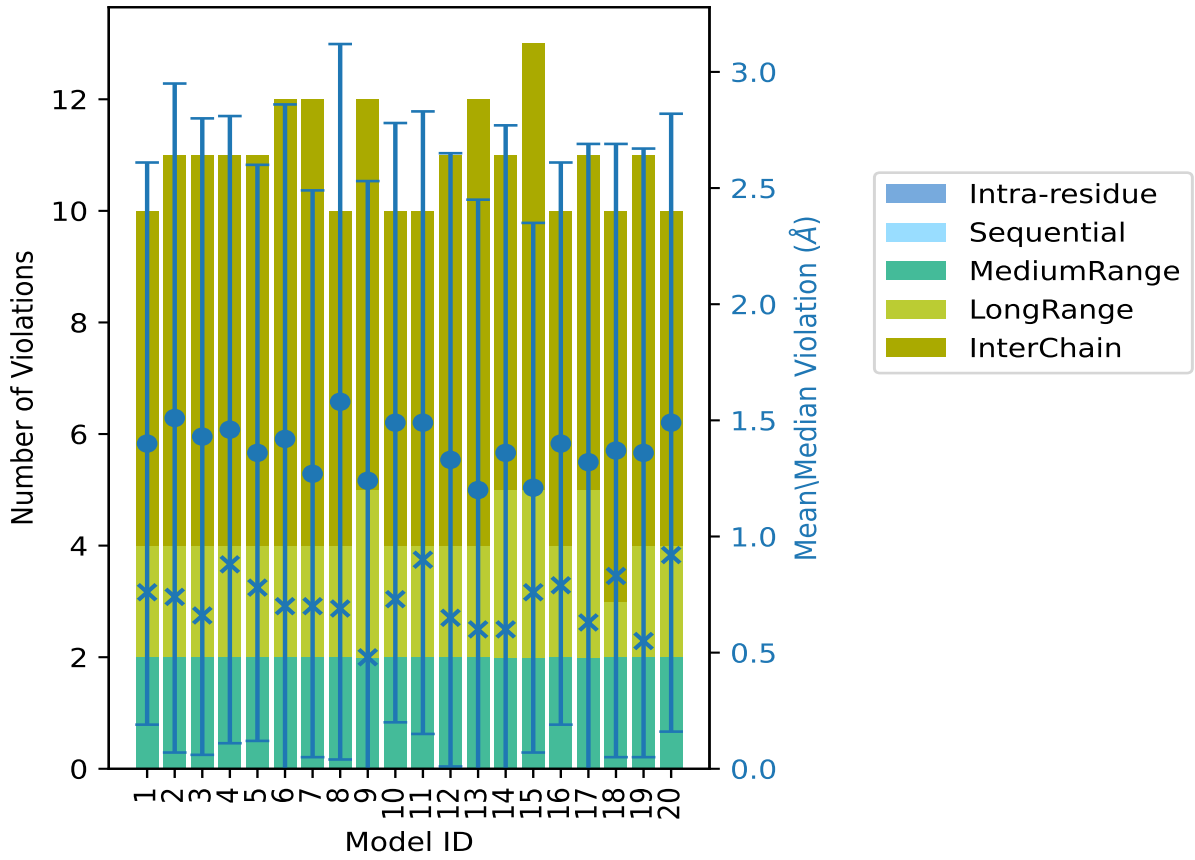
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	2	2	7	11	1.33	3.85	1.32	0.65
13	0	0	2	2	8	12	1.2	3.84	1.25	0.6
14	0	0	2	3	6	11	1.36	3.79	1.41	0.6
15	0	0	2	3	8	13	1.21	3.83	1.14	0.76
16	0	0	2	2	6	10	1.4	3.76	1.21	0.79
17	0	0	2	3	6	11	1.32	3.84	1.37	0.63
18	0	0	2	1	7	10	1.37	4.07	1.32	0.83
19	0	0	2	2	7	11	1.36	4.01	1.31	0.55
20	0	0	2	2	6	10	1.49	3.85	1.33	0.92

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

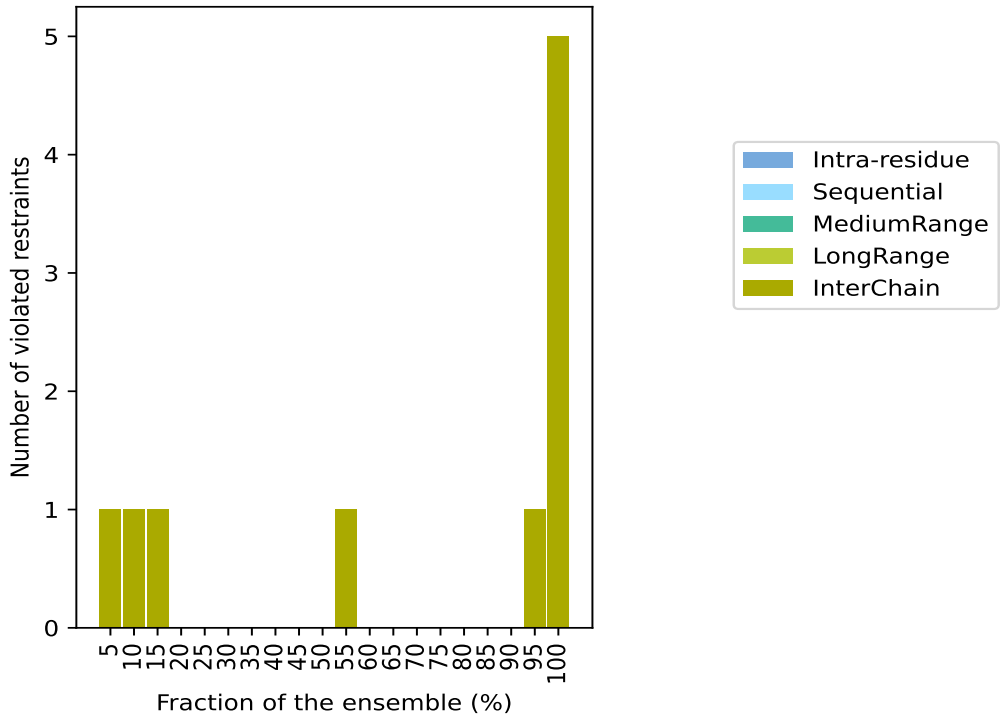
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 225(IR:0, SQ:0, MR:0, LR:0, IC:225) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	1	1	1	5.0
0	0	0	0	1	1	2	10.0
0	0	0	0	1	1	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	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	0	0	0	10	50.0
0	0	0	0	1	1	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	1	1	19	95.0
0	0	0	0	5	5	20	100.0

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

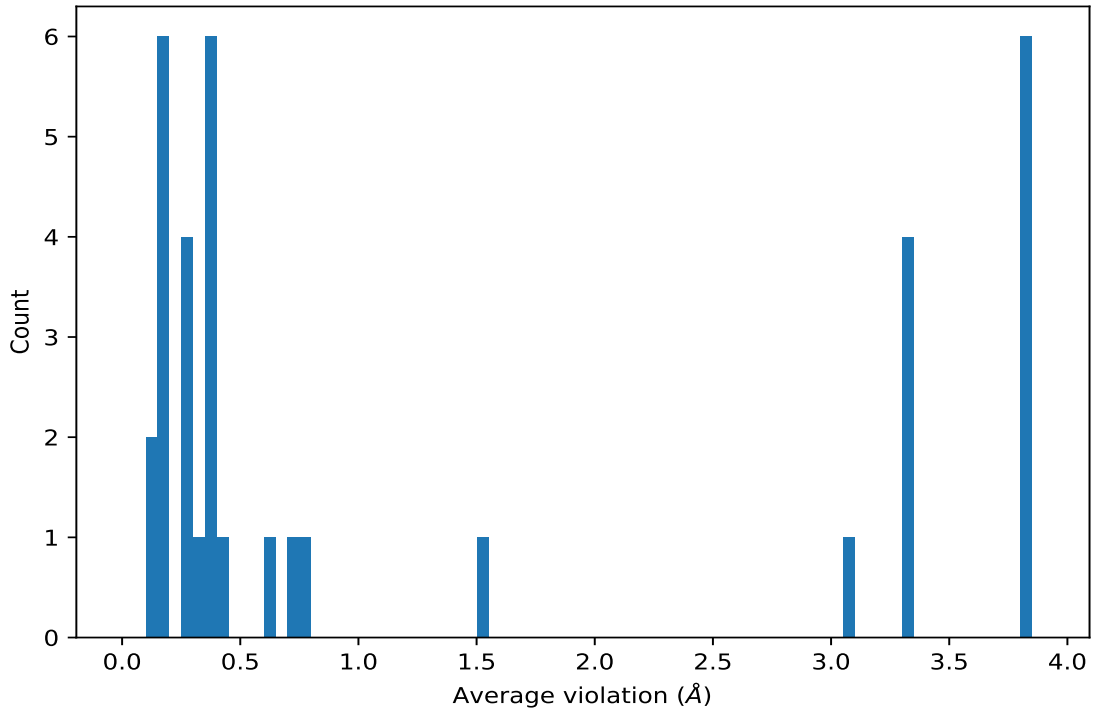
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,88)	1:A:160:LYS:C	2:B:179:HIS:ND1	20	3.83	0.1	3.83
(2,88)	1:A:160:LYS:CA	2:B:179:HIS:ND1	20	3.83	0.1	3.83
(2,88)	1:A:160:LYS:CB	2:B:179:HIS:ND1	20	3.83	0.1	3.83
(2,88)	1:A:160:LYS:CD	2:B:179:HIS:ND1	20	3.83	0.1	3.83
(2,88)	1:A:160:LYS:CE	2:B:179:HIS:ND1	20	3.83	0.1	3.83
(2,88)	1:A:160:LYS:CG	2:B:179:HIS:ND1	20	3.83	0.1	3.83
(1,58)	1:A:125:SER:CA	2:B:248:ARG:N	20	3.32	0.56	3.25
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NE	20	3.32	0.56	3.25
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NH1	20	3.32	0.56	3.25
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NH2	20	3.32	0.56	3.25
(3,13)	2:B:245:GLY:N	1:A:160:LYS:CD	20	3.09	0.22	3.08
(2,84)	1:A:122:ALA:CA	2:B:179:HIS:ND1	20	1.54	0.2	1.58
(3,20)	2:B:179:HIS:ND1	2:B:242:CYS:SG	20	0.75	0.22	0.66
(4,3)	2:B:238:CYS:SG	2:B:242:CYS:SG	20	0.7	0.17	0.75
(3,1)	1:A:116:HIS:C	2:B:179:HIS:ND1	20	0.36	0.12	0.38
(3,1)	1:A:116:HIS:CA	2:B:179:HIS:ND1	20	0.36	0.12	0.38

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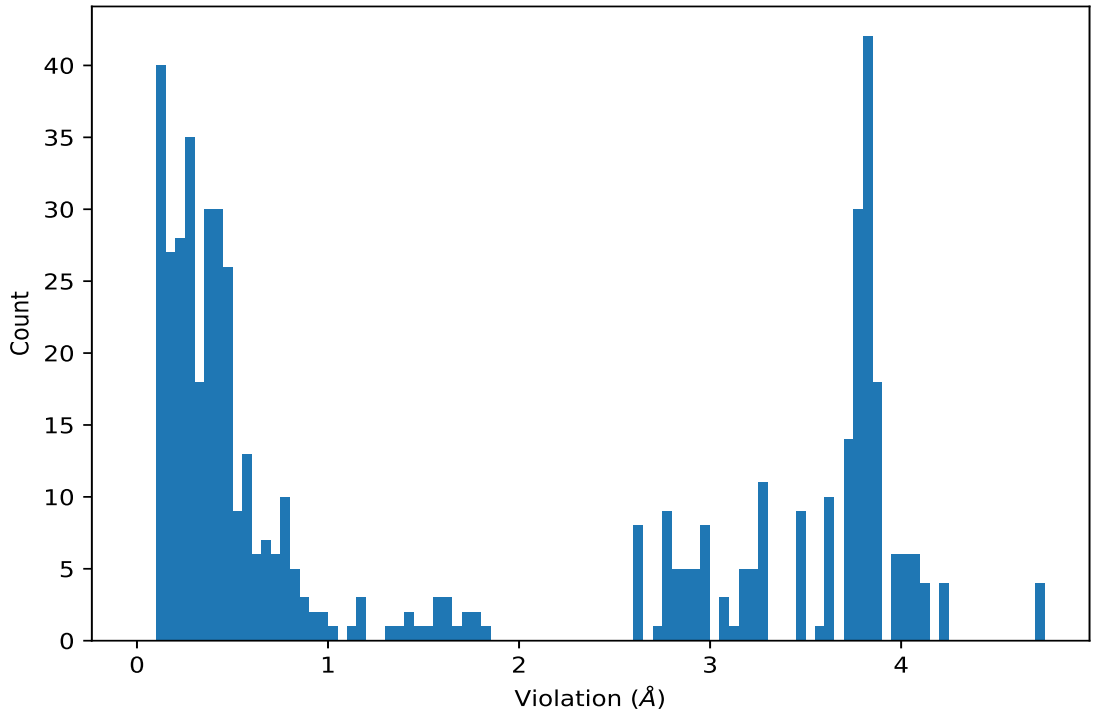
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,1)	1:A:116:HIS:CB	2:B:179:HIS:ND1	20	0.36	0.12	0.38
(3,1)	1:A:116:HIS:CD2	2:B:179:HIS:ND1	20	0.36	0.12	0.38
(3,1)	1:A:116:HIS:CE1	2:B:179:HIS:ND1	20	0.36	0.12	0.38
(3,1)	1:A:116:HIS:CG	2:B:179:HIS:ND1	20	0.36	0.12	0.38
(3,18)	2:B:176:CYS:SG	2:B:179:HIS:ND1	20	0.3	0.04	0.3
(4,1)	2:B:176:CYS:SG	2:B:238:CYS:SG	19	0.64	0.21	0.72
(3,15)	2:B:276:ALA:N	1:A:121:THR:CG2	19	0.42	0.09	0.41

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:A:125:SER:CA	2:B:248:ARG:N	8	4.72
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NE	8	4.72
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NH1	8	4.72
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NH2	8	4.72
(1,58)	1:A:125:SER:CA	2:B:248:ARG:N	2	4.24
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NE	2	4.24
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NH1	2	4.24
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NH2	2	4.24
(1,58)	1:A:125:SER:CA	2:B:248:ARG:N	6	4.13
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NE	6	4.13
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NH1	6	4.13
(1,58)	1:A:125:SER:CA	2:B:248:ARG:NH2	6	4.13
(2,88)	1:A:160:LYS:C	2:B:179:HIS:ND1	18	4.07
(2,88)	1:A:160:LYS:CA	2:B:179:HIS:ND1	18	4.07
(2,88)	1:A:160:LYS:CB	2:B:179:HIS:ND1	18	4.07
(2,88)	1:A:160:LYS:CD	2:B:179:HIS:ND1	18	4.07
(2,88)	1:A:160:LYS:CE	2:B:179:HIS:ND1	18	4.07
(2,88)	1:A:160:LYS:CG	2:B:179:HIS:ND1	18	4.07
(2,88)	1:A:160:LYS:C	2:B:179:HIS:ND1	19	4.01
(2,88)	1:A:160:LYS:CA	2:B:179:HIS:ND1	19	4.01
(2,88)	1:A:160:LYS:CB	2:B:179:HIS:ND1	19	4.01
(2,88)	1:A:160:LYS:CD	2:B:179:HIS:ND1	19	4.01
(2,88)	1:A:160:LYS:CE	2:B:179:HIS:ND1	19	4.01
(2,88)	1:A:160:LYS:CG	2:B:179:HIS:ND1	19	4.01
(2,88)	1:A:160:LYS:C	2:B:179:HIS:ND1	6	3.99
(2,88)	1:A:160:LYS:CA	2:B:179:HIS:ND1	6	3.99
(2,88)	1:A:160:LYS:CB	2:B:179:HIS:ND1	6	3.99
(2,88)	1:A:160:LYS:CD	2:B:179:HIS:ND1	6	3.99
(2,88)	1:A:160:LYS:CE	2:B:179:HIS:ND1	6	3.99
(2,88)	1:A:160:LYS:CG	2:B:179:HIS:ND1	6	3.99
(2,88)	1:A:160:LYS:C	2:B:179:HIS:ND1	9	3.88
(2,88)	1:A:160:LYS:CA	2:B:179:HIS:ND1	9	3.88
(2,88)	1:A:160:LYS:CB	2:B:179:HIS:ND1	9	3.88
(2,88)	1:A:160:LYS:CD	2:B:179:HIS:ND1	9	3.88
(2,88)	1:A:160:LYS:CE	2:B:179:HIS:ND1	9	3.88
(2,88)	1:A:160:LYS:CG	2:B:179:HIS:ND1	9	3.88
(2,88)	1:A:160:LYS:C	2:B:179:HIS:ND1	12	3.85
(2,88)	1:A:160:LYS:CA	2:B:179:HIS:ND1	12	3.85
(2,88)	1:A:160:LYS:CB	2:B:179:HIS:ND1	12	3.85
(2,88)	1:A:160:LYS:CD	2:B:179:HIS:ND1	12	3.85
(2,88)	1:A:160:LYS:CE	2:B:179:HIS:ND1	12	3.85
(2,88)	1:A:160:LYS:CG	2:B:179:HIS:ND1	12	3.85
(2,88)	1:A:160:LYS:C	2:B:179:HIS:ND1	20	3.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,88)	1:A:160:LYS:CA	2:B:179:HIS:ND1	20	3.85
(2,88)	1:A:160:LYS:CB	2:B:179:HIS:ND1	20	3.85
(2,88)	1:A:160:LYS:CD	2:B:179:HIS:ND1	20	3.85
(2,88)	1:A:160:LYS:CE	2:B:179:HIS:ND1	20	3.85
(2,88)	1:A:160:LYS:CG	2:B:179:HIS:ND1	20	3.85
(2,88)	1:A:160:LYS:C	2:B:179:HIS:ND1	8	3.84

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found